# Dinuclear Oxidative Addition Reactions Using an Isostructural Series of $Ni_2$, $Co_2$, and $Fe_2$ Complexes

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**Supporting Information**

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## 1. General Information

**General Considerations.** All manipulations were carried out using standard Schlenk or glovebox techniques under an atmosphere of $N_2$. Solvents were dried and degassed by passing through a column of activated alumina and sparging with Ar gas. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc., degassed, and stored over activated 3 Å molecular sieves prior to use. All other reagents and starting materials were purchased from commercial vendors and used without further purification unless otherwise noted. Liquid reagents were degassed and stored over activated 3 Å molecular sieves prior to use. Elemental analyses were performed by Midwest Microlab (Indianapolis, IN).

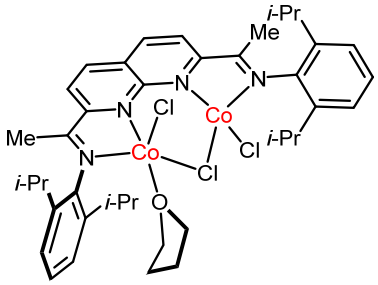
**Physical Methods.** $^1$H NMR spectra were collected at room temperature on Varian INOVA 600 MHz or Bruker DRX 500 MHz spectrometers. $^1$H and $^{13}$C NMR spectra are reported in parts per million relative to tetramethylsilane, using the residual solvent resonances as an internal standard. GC/MS data were collected on a Shimadzu GC-2010/MS-QP2010 spectrometer containing a mini-bore capillary GC column and single quad EI detector. ATR-IR data were collected on a Thermo Nicolet Nexus spectrometer containing a MCT* detector and KBr beam splitter with a range of 350–7400 $cm^{-1}$. UV–vis measurements were acquired on a Perkin Elmer Lambda 950 UV–VIS–NIR spectrophotometer using a 1-cm two-window quartz cuvette. High-resolution mass data were obtained using a 6320 Ion Trap MS system.

**X-Ray Crystallography.** Data were collected using either a Rigaku R-axis curved image plate diffractometer with Cu-Kα radiation (λ = 1.54178 Å), a Nonius Kappa CCD diffractometer with Mo-Kα radiation (λ = 0.71073 Å) at Purdue University, or a Bruker AXS D8 Quest CMOS diffractometer with Mo-Kα radiation (λ = 0.71073 Å) at Youngstown State University. The Rigaku R-axis instrument has a Cu microsource X-ray tube with a laterally graded multilayer (Goebel) mirror. The KappaCCD instrument features a fine focus sealed tube X-ray source with graphite monochromator. The Prospector CCD instrument is equipped with an IμS microsource with a laterally graded multilayer (Goebel) mirror for monochromatization. Single crystals were mounted on Mitegen micromesh or loop mounts using a trace of mineral oil and cooled in-situ to 200(2), 150(2) or 100(2) K for data collection. Data on the Rigaku R-axis were collected using the dTrek option of the CrystalClear software.[1] Data on the KappaCCD instrument were collected using the Nonius Collect software.[2] Both were processed using HKL3000.[3] Data were corrected for absorption and scaled using Scalepack.[3] Data on the Bruker Quest instrument were collected, reflections were indexed and processed, and the files scaled and corrected for absorption using APEX2.[4] The space groups were assigned and the structures were solved by direct methods using XPREP within the SHELXTL suite of programs[5] and refined by full matrix least squares against $F^2$ with all reflections using Shelxl 2013 or 2014[6] using the graphical interface Shelxle.[7] If not specified otherwise H

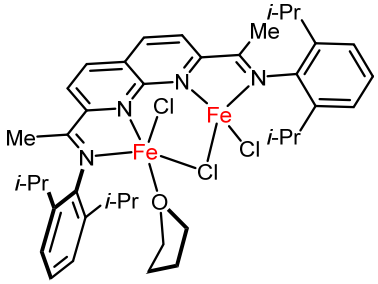
[1] Nonius (1998). Collect Users Manual, Nonius Delft, The Netherlands.
[2] Rigaku Corp. (2014). CrystalClear, The Woodlands, Texas, USA.
[3] Otwinowski Z. & Minor, W. (1997). Methods Enzymol., 276, 307—327.
[4] Apex2 v2013.4-1, v2014.11, v2014.1-1, Saint V8.34A, *SAINT* V8.30C, Bruker AXS Inc.: Madison (WI), USA, 2013/2014.
[5] a) SHELXTL (Version 6.14) (2000-2003) Bruker Advanced X-ray Solutions, Bruker AXS Inc., Madison, Wisconsin: USA. b) Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
[6] a) Sheldrick, G. M. (2015). Acta Cryst. C71, 3-8. b) Sheldrick, G. M. (2013). University of Göttingen, Germany.
[7] SHELXLE Rev656, Rev714 (Hübschle *et al.*, 2011), SHELXLE. Hübschle, C. B., Sheldrick, G. M. and Dittrich, B. (2011). J. Appl. Cryst., 44, 1281--1284.

atoms attached to carbon atoms were positioned geometrically and constrained to ride on their parent atoms, with carbon hydrogen bond distances of 0.95 Å for and aromatic and alkene C-H, 1.00, and 0.98 Å for aliphatic C-H and $CH_3$ moieties, respectively. Methyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density. $U_{iso}(H)$ values were set to a multiple of $U_{eq}(C)$ with 1.5 for $CH_3$, and 1.2 for C-H units, respectively. Experimental details for each crystal are included in Section 7, X-Ray Diffraction Data.

## 2. Synthetic Procedures

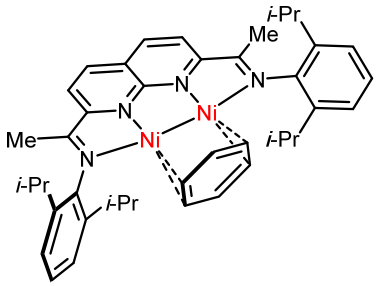



**[$^{i\text{-Pr}}$NDI]$Co_2$(THF)$Cl_3$ (3).** Under an atmosphere of $N_2$, $^{i\text{-Pr}}$NDI (**1**) (159 mg, 0.299 mmol) was dissolved in THF (4 mL) and stirred over Na/Hg amalgam (23.0 mg of Na, 1.00 mmol, 3.34 equiv), yielding a violet then dark orange solution. Separately, $CoCl_2$ (102 mg, 0.785 mmol, 2.62 equiv) was mixed with THF (10 mL) to form a blue suspension. After 1 h, the orange $Na_2$[NDI] (**2**) solution was carefully decanted from the Na/Hg amalgam and added to the $CoCl_2$ suspension, resulting in the immediate formation of a dark brown reaction mixture. After stirring at room temperature for 4 h, the solvent was removed under reduced pressure. The residue was resuspended in pentane then concentrated to dryness. The powder was dissolved in a minimal amount of THF and filtered through a celite pad (approx. 0.5 cm). The filtrate (approx. 4 mL total volume) was placed in a 20-mL vial and carefully layered with pentane (approx. 16 mL) for crystallization. After approx. 48 h, the mother liquor was decanted, and the crystals were washed with pentane (4 x 1 mL). The product was isolated as a darkly colored crystalline solid (178.9 mg, 72% yield). Single crystals obtained by this method were suitable for XRD. $^1$H NMR (300 MHz, $C_6D_6$) δ 2.63, 1.00, –0.91, –7.10, –24.20, –54.27, –104.89. UV–Vis–NIR (THF): $\lambda_{max}$, nm (ε, $M^{-1}$ $cm^{-1}$): 211 (60000), 245 (66000), 328 (17500), 338 (17000). $\mu_{eff}$ = 5.74 $\mu_B$ (Evans method, 300 K, THF containing TMS). Anal. Calc'd. for ($C_{40}H_{52}Cl_3Co_2N_4O$): C 57.95, H 6.32, N 6.76; found: C 57.84, H 6.38, N 6.61%.

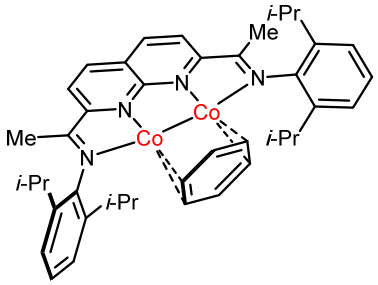



**[$^{i\text{-Pr}}$NDI]$Fe_2$(THF)$Cl_3$ (4).** Under an atmosphere of $N_2$, $^{i\text{-Pr}}$NDI (**1**) (143 mg, 0.269 mmol) was dissolved in THF (3 mL) and stirred over Na/Hg amalgam (23.0 mg of Na, 1.00 mmol, 3.72 equiv), yielding a violet then dark orange solution. Separately, $FeCl_2$ (86.5 mg, 0.682 mmol, 2.53 equiv) was mixed with THF (3 mL) to form a yellow suspension. After 1 h, the orange $Na_2$[NDI] (**2**) solution was carefully decanted from the Na/Hg amalgam and added to the $FeCl_2$ suspension, resulting in the formation of a dark brown reaction mixture. After stirring at room temperature for 2 h, the solvent was removed under reduced pressure. The residue was dissolved in a minimal amount of THF and filtered through a celite pad (approx. 0.5cm). The filtrate (approx. 8 mL total volume) was placed into two 20-mL vials and carefully layered with pentane (approx. 16 mL ea.) for crystallization. After approx. 48 h, the mother liquor was decanted, and the crystals were washed with pentane (4 x 1 mL). The product was isolated as a darkly colored crystalline solid (147.6 mg, 67% yield). Single crystals obtained by this method were suitable for XRD. The product is stable in THF solution but undergoes decomposition in $C_6H_6$. $^1$H NMR (300 MHz,

$C_6D_6$) δ 4.85, 4.24, 1.90, –3.85, –19.18, –29.94, –83.29, –117.41. UV–Vis–NIR (THF): $\lambda_{max}$, nm (ε): 230 (50000), 243 (40000). $\mu_{eff}$ = 7.56 $\mu_B$ (Evans method, 300 K, THF containing TMS). Anal. Calc'd. for ($C_{40}H_{52}Cl_3Fe_2N_4O$): C 58.38, H 6.37, N 6.81; found: C 57.87, H 6.20, N 6.59%.

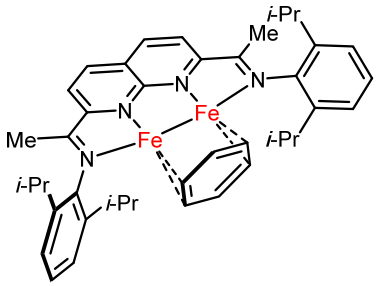



**[$^{i\text{-Pr}}$NDI]$Ni_2(C_6H_6)$ (5)**. Compound **5** was prepared according to the previously reported procedure.[8]

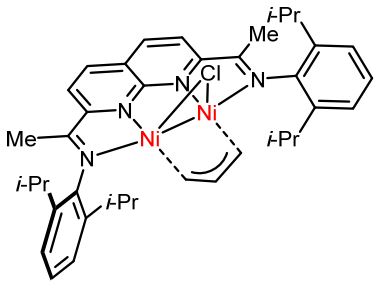



**[$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ (6)**. Under an atmosphere of $N_2$, [$^{i\text{-Pr}}$NDI]$Co_2(THF)Cl_3$ (**3**) (153 mg, 0.184 mmol) was dissolved in THF (5 mL) containing a small amount of $C_6H_6$ (200 µL). $KEt_3BH$ (1.0 M solution in THF, 0.554 mL, 3.0 equiv) was added dropwise with stirring. An immediate color change from brown to green was observed. After stirring for an additional 2 h, the solvent was removed under vacuum and the residue was resuspended in pentane and concentrated under reduced pressure, yielding a darkly colored powder. The crude material was dissolved in a minimal amount of 1:1 $C_6H_6$/pentane (approx. 10 mL), filtered through a pad of celite, and concentrated under reduced pressure. The resulting complex was dissolved in 1:1 pentane/$Et_2O$ (20 mL), filtered through celite, and crystallized by solvent evaporation (diffusion of $Et_2O$/pentane vapor into HMDSO). After 48 h, the mother liquor (approx. 3mL final volume) was carefully decanted, the crystals were washed with cold (–30 °C) pentane (4 x 1 mL), and dried under reduced pressure. The product was isolated as a dark green crystalline solid (46.2 mg, 34% yield). Single crystals suitable for XRD were obtained by slow evaporation of a pentane solution of **1** at room temperature. $^1$H NMR (500 MHz, $C_6D_6$) δ 8.06 (s, 6H, $C_6H_6$), 7.27 (t, *J* = 7.7 Hz, 2H, Ar H), 7.03 (m, 2H, Ar H), 7.01 (d, *J* = 7.7 Hz, 4H, Ar H), 4.73 (dd, *J* = 8.6, 4.7 Hz, 2H, Ar H), 1.15 (d, *J* = 6.7 Hz, 12H, iPr $CH_3$), 0.89 (sept, *J* = 6.7 Hz, 4H, iPr CH), 0.27 (d, *J* = 6.7 Hz, 12H, iPr $CH_3$), –0.94 (s, 6H, $CH_3$). $^{13}$C{$^1$H} NMR (125 MHz, $C_6D_6$) δ 153.1, 152.8, 145.8, 137.7, 131.8, 130.4, 125.3, 123.6, 119.3, 78.3, 26.6, 24.1, 23.6, 14.5. UV–Vis–NIR (THF) $\lambda_{max}$, nm (ε, $M^{-1}$ $cm^{-1}$): 208 (95000), 240 (52000), 310 (28000), 372 (18000), 555 (8000), 715 (8000), 940 (8000). Anal. Calc'd. for ($C_{42}H_{50}Co_2N_4$): C 69.22, H 6.92, N 7.69; found: C 68.35, H 7.01, N 7.74%

[8] Zhou, Y.-Y.; Hartline, D. R.; Steiman, T. J.; Fanwick, P. E.; Uyeda, C. *Inorg. Chem.*, **2014**, *53*, 11770-11777.

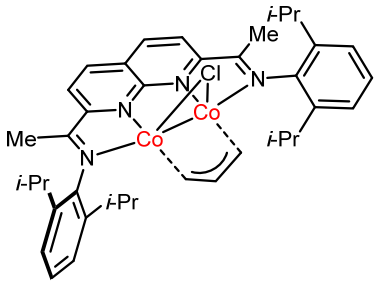



**[$^{i\text{-Pr}}$NDI]$Fe_2(C_6H_6)$ (7)**. Under an atmosphere of $N_2$, [$^{i\text{-Pr}}$NDI]$Fe_2$(THF)$Cl_3$ (**4**) (148 mg, 0.179 mmol) was dissolved in THF (5 mL) containing a small amount of $C_6H_6$ (200 µL). Separately, $KC_8$ (72.8 mg, 0.539 mmol, 3.01 equiv) was weighed into a 20-mL vial. The solution containing the $Fe_2$ complex was added to the solid $KC_8$, and the resulting brown reaction mixture was stirred at room temperature. After 1 h, the solvent was removed under reduced pressure. The residue was dissolved in $C_6H_6$ and filtered through a celite pad (approx. 0.5cm). The filtrate was concentrated to dryness under reduced pressure then redissolved in a 40:60 mixture of $Et_2O$ and pentane (20 mL). The solution was filtered through a glass fiber pad, and the product was allowed to crystallize from the filtrate by slow evaporation (diffusion of $Et_2O$/pentane vapor into HMDSO). After 48 h, the mother liquor (approx. 3mL final volume) was carefully decanted, the crystals were washed with cold (–30 °C) pentane (3 x 200 µL), and dried under reduced pressure. The product was isolated as a dark brown crystalline solid (71.4 mg, 55% yield). Single crystals suitable for XRD were obtained by slow evaporation of a 1:5 $Et_2O$/pentane solution of **1** at –30 °C. The product is stable indefinitely in $C_6H_6$ solution but undergoes decomposition in THF. $^1$H NMR (500 MHz, $C_6D_6$) δ 19.77, 11.13, 9.65, 1.37, 0.98, 0.30, –0.73, –15.70, –86.79. UV–Vis–NIR (THF) $\lambda_{max}$, nm (ε, $M^{-1}$ $cm^{-1}$): 784 (22000), 975 (40000), 1205 (10000). $\mu_{eff}$ = 4.34 $\mu_B$ (Evans method, 300 K, $C_6D_6$). Anal. Calc'd. for ($C_{42}H_{50}Fe_2N_4$): C 69.81, H 6.98, N 7.75; found: C 70.06, H 6.45, N 7.80.

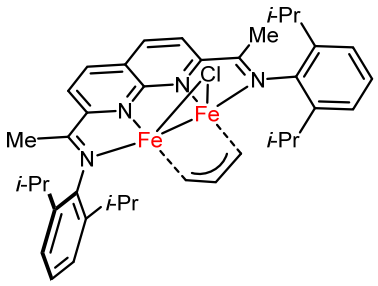



**[$^{i\text{-Pr}}$NDI]$Ni_2$(allyl)Cl (8)**. Under an atmosphere of $N_2$, [$^{i\text{-Pr}}$NDI]$Ni_2(C_6H_6)$ (**5**) (73.0 mg, 0.10 mmol, 1.0 equiv) was dissolved in $C_6H_6$ (2 mL). Allyl chloride (0.88 mg, 0.0115 mmol, 1.15 equiv) was added as a solution in $C_6H_6$ (1.2 mL) with stirring, resulting in an immediate color change from dark brown to green. After the addition was complete, the reaction mixture was concentrated to dryness under reduced pressure. The residue was washed with pentane (2 x 2 mL), redissolved in 5:1 $C_6H_6$/pentane (approx. 2 mL), and filtered through a glass fiber pad. The filtrate was concentrated to dryness, yielding **8** as a green powder (50 mg, 69% yield). Single crystals suitable for XRD were obtained by slow diffusion of pentane vapor into a concentrated solution of **8** in $C_6H_6$. The product is thermally unstable and decomposes over several days at room temperature. $^1$H NMR (500 MHz, $C_6D_6$) δ 8.59 (d, *J* = 8.4 Hz, 2H, Naph H), 7.37 (dd, *J* = 7.7, 1.3 Hz, 2H, Ar H), 7.34 (t, *J* = 7.7 Hz, Ar H), 7.17 (dd, *J* = 7.7, 1.3 Hz, 2H, Ar H), 5.90 (d, *J* = 8.4 Hz, 2H, Naph H), 5.07 (d, *J* = 7.3 Hz, Allyl $CH_2$), 4.19 (sept, *J* = 6.8 Hz, 2H, iPr CH), 3.34 (d, *J* = 13.1 Hz, 2H, Allyl H), 2.13 (sept, *J* = 6.8 Hz, 2H, iPr CH), 1.48 (d, *J* = 6.8 Hz, 6H, iPr $CH_3$), 1.10 (d, *J* = 6.8 Hz, 6H, iPr $CH_3$), 0.95 (d, *J* = 6.8 Hz, 6H, iPr $CH_3$), 0.81 (d, *J* = 6.8 Hz, 6H, iPr $CH_3$), 0.81 (m, 1H, Allyl CH), –0.10 (s, 6H, $CH_3$). $^{13}$C NMR (126 MHz, $C_6D_6$) δ 176.4, 162.0, 153.4, 151.1, 139.0, 137.9, 137.6, 129.4, 128.6, 128.4, 126.8, 126.5, 124.7,

123.6, 83.1, 35.3, 28.7, 27.8, 24.8, 24.1, 23.8, 18.9. UV–Vis–NIR (THF) $\lambda_{max}$, nm (ε, $M^{-1}$ $cm^{-1}$): 283 (34,000), 364 (18,000), 469 (sh), 650 (9600), 858 (2700). Anal. Calcd. for ($C_{39}H_{49}ClN_4Ni_2$): C 64.46, H 6.80, N 7.71; found: C 64.67, H 6.71, N 7.55.




**[$^{i\text{-Pr}}$NDI]$Co_2$(allyl)Cl (9)**. Under an atmosphere of $N_2$, [$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ (**6**) (14.6 mg , 0.0201 mmol, 1.0 equiv) was dissolved in THF (2 mL), and allyl chloride (1.53 mg , 0.201 mmol, 1.0 equiv) was added a solution in diethyl ether (1 mL). Following the addition, the reaction mixture was immediately concentrated to dryness under reduced pressure. The residue was redissolved in pentane (approx. 4 mL) and filtered through a glass fiber pad. The filtrate was concentrated to dryness, yielding **9** as a dark brown powder (9.0 mg, 62% yield). Single crystals suitable for XRD were obtained by slow evaporation of a 1:1 $Et_2O$/pentane solution of **9** at –30 °C. The product is thermally unstable and decomposes over several days at room temperature. $^1$H NMR (800 MHz, $C_6D_6$) δ 75.72 (br s, 2H, Allyl $CH_2$), 22.56 (br s, 2H, Allyl $CH_2$), 13.64 (d, *J* = 6.5Hz, 2H, Naph H), 10.22 (d, *J* = 6.5 Hz, 2H, Naph H), 6.75 (d, *J* = 8.4 Hz, 2H, Ar H), 6.32 (d, *J* = 7.8 Hz, 2H, Ar H), 5.31 (t, *J* = 8.1 Hz, 2H, Ar H), 3.36 (s, 2H, iPr CH), 2.63 (s, 6H, $CH_3$), 1.84 (s, 6H, $CH_3$), 1.01 (s, 6H, $CH_3$), –0.39 (s, 6H, $CH_3$), –0.92 (s, 6H, $CH_3$), –1.14 (s, 2H, iPr CH), –3.44 (br s, 1H, Allyl CH). UV–Vis–NIR (THF) $\lambda_{max}$, nm (ε, $M^{-1}$ $cm^{-1}$): 215 (80000), 243 (31000), 340 (sh), 724 (8440). $\mu_{eff}$ = 1.44 $\mu_B$ (Evans method, 300K, Benzene-$d_6$). Anal. Calcd. for ($C_{39}H_{49}ClN_4Co_2$): C 64.42, H 6.79, N 7.70; found: C 63.50, H 6.70, N 7.18 %.




**[$^{i\text{-Pr}}$NDI]$Fe_2$(allyl)Cl (10)**. Under an atmosphere of $N_2$, [$^{i\text{-Pr}}$NDI]$Fe_2(C_6H_6)$ (**7**) (13.2 mg, 0.0183 mmol, 1.0 equiv) was dissolved in THF (1 mL). Allyl chloride (1.41 mg, 0.0184mmol, 1.01 equiv) was added as a solution in $Et_2O$ (1 mL), resulting in a color change from red-brown to yellow-brown. The reaction mixture was stirred for 5 min then concentrated to dryness under reduced pressure. The residue was redissolved in pentane (approx. 4 mL) and filtered through a glass fiber pad. The filtrate was concentrated to dryness under reduced pressure yielding **10** as a yellow-brown solid (9.0 mg, 68% yield). Single crystals suitable for XRD were obtained by slow evaporation of a pentane solution of **10** at –30°C. $^1$H NMR (300MHz, $C_6D_6$) δ 27.61 (br s, 2H), 9.32 (s, 2H), 4.78 (s, 2H), 1.57 (s, 6H), 0.21 (s, 6H), –0.97 (s, 2H), –1.68 (s, 6H), –2.23 (s, 6H), –3.21 (s, 2H), –3.69 (s, 6H), –4.15 (br s, 2H), –92.27 (br s, 1H). UV–Vis–NIR (THF) $\lambda_{max}$, nm (ε, $M^{-1}$ $cm^{-1}$): 208 (57000), 400 (sh), 978 (7400). $\mu_{eff}$ = 4.87 $\mu_B$ (Evans method, 296 K, $C_6D_6$). Anal. Calcd. for ($C_{39}H_{49}ClN_4Fe_2$): C 64.46, H 6.80, N 7.71; found: C 64.27, H 6.87, N 7.52 %.

## 3. NMR Spectra

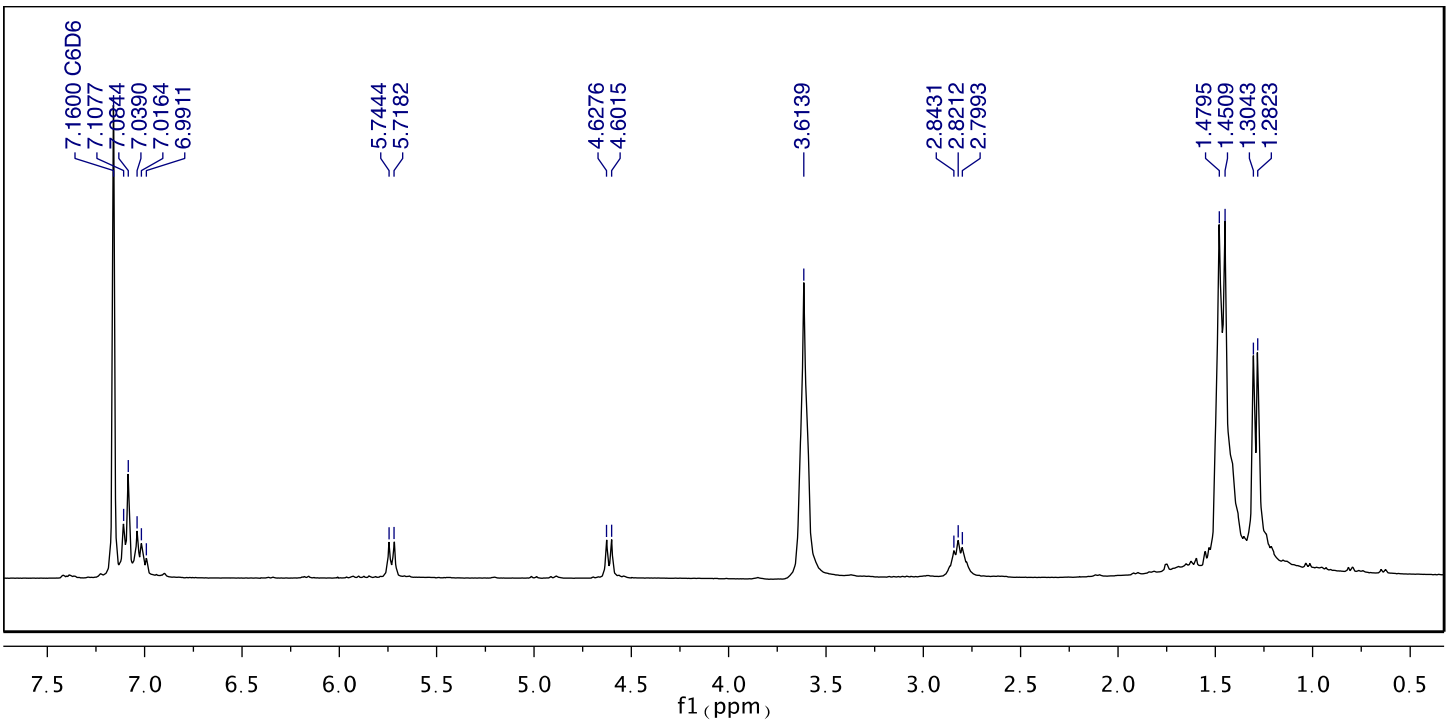



**Figure S1.** $^{1}$H NMR spectrum of $Na_2[^{i\text{-}Pr}NDI]$ (**2**) in $C_6D_6$.

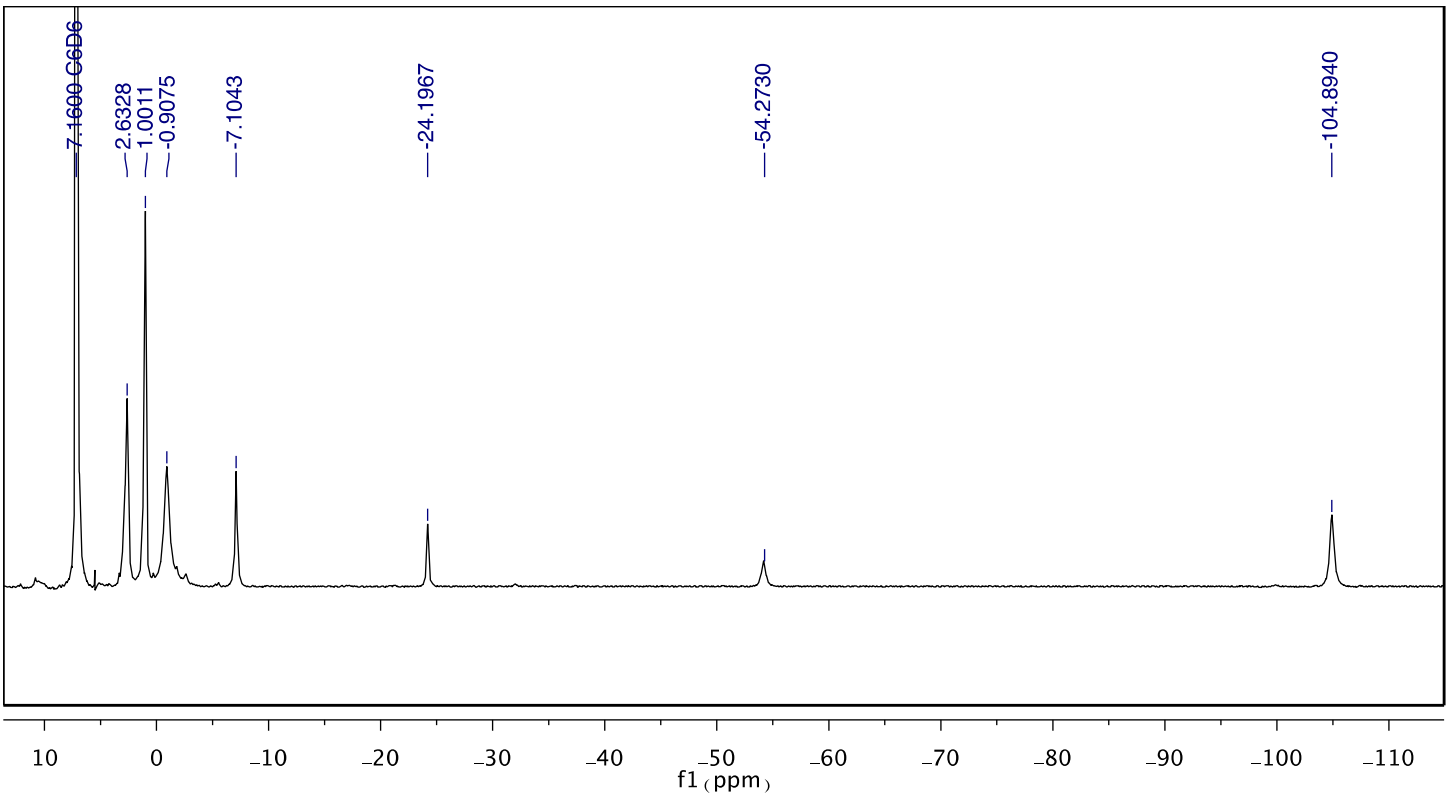



**Figure S2.** $^{1}$H NMR spectrum of $[^{i\text{-}Pr}NDI]Co_2(THF)Cl_3$ (**3**) in $C_6D_6$.

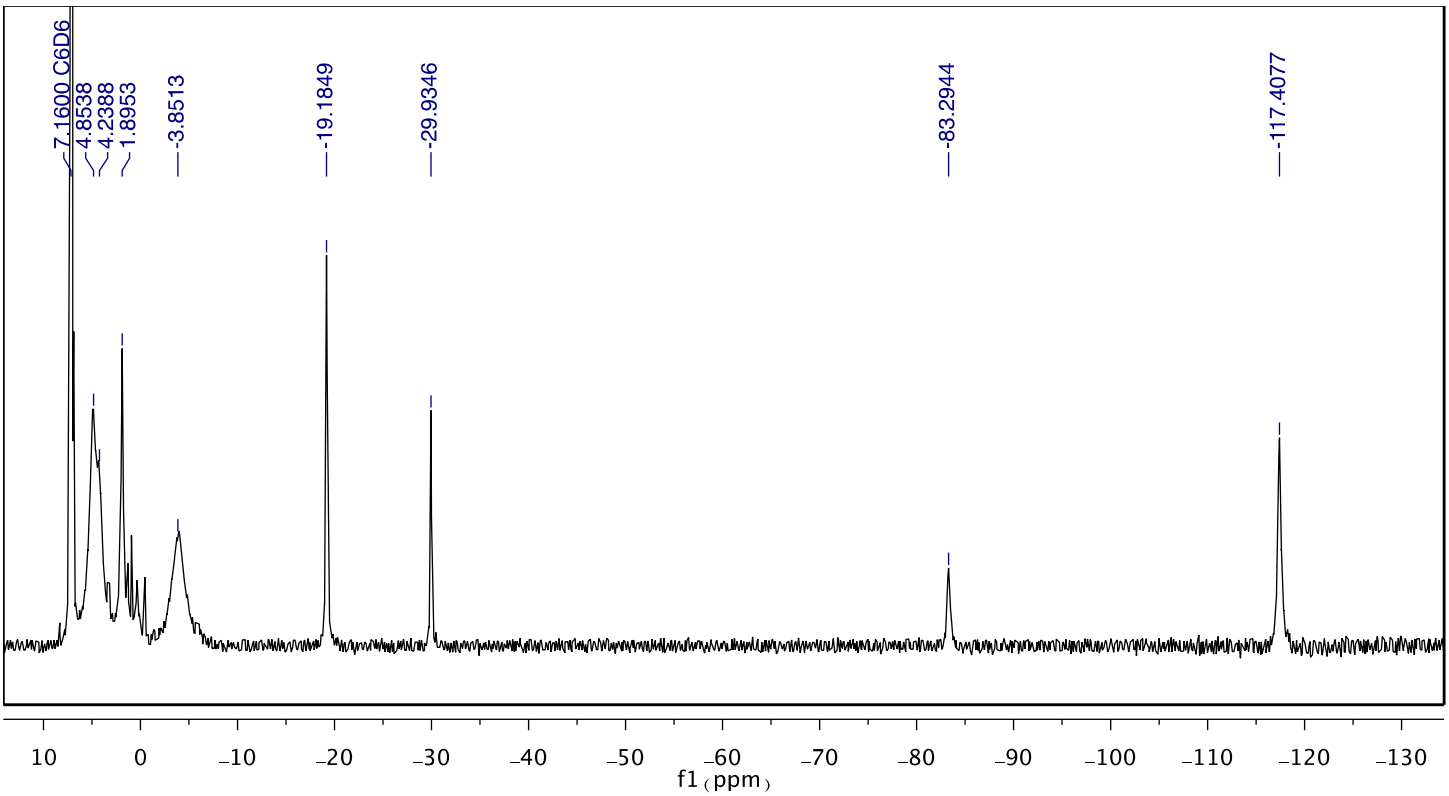



**Figure S3.** $^{1}$H NMR spectrum of [$^{i\text{-Pr}}$NDI]$Fe_2(THF)Cl_3$ (**4**) in $C_6D_6$.

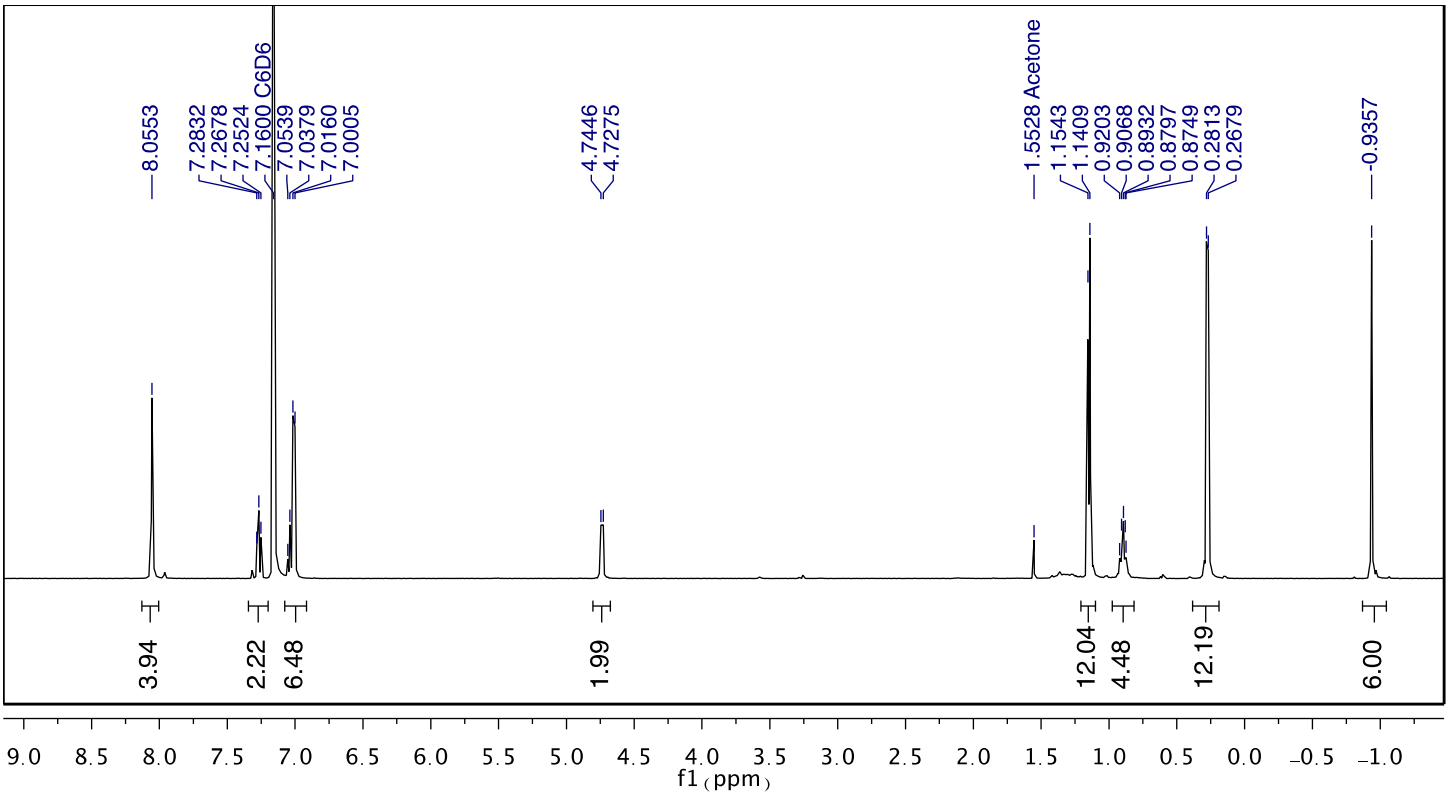



**Figure S4.** $^{1}$H NMR spectrum of [$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ (**6**) in $C_6D_6$.

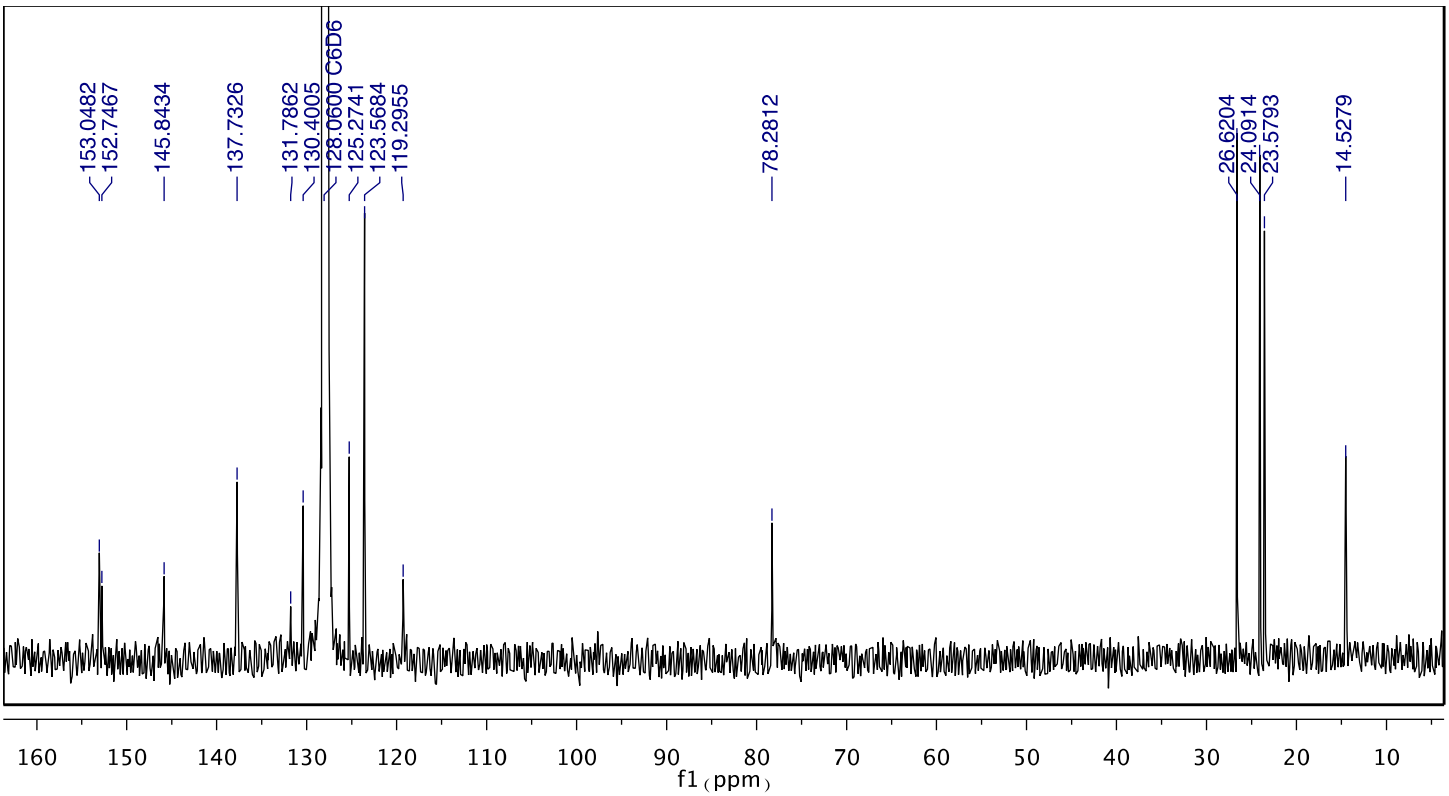



**Figure S5.** $^{13}C\{^{1}H\}$ NMR spectrum of [$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ (**6**) in $C_6D_6$.

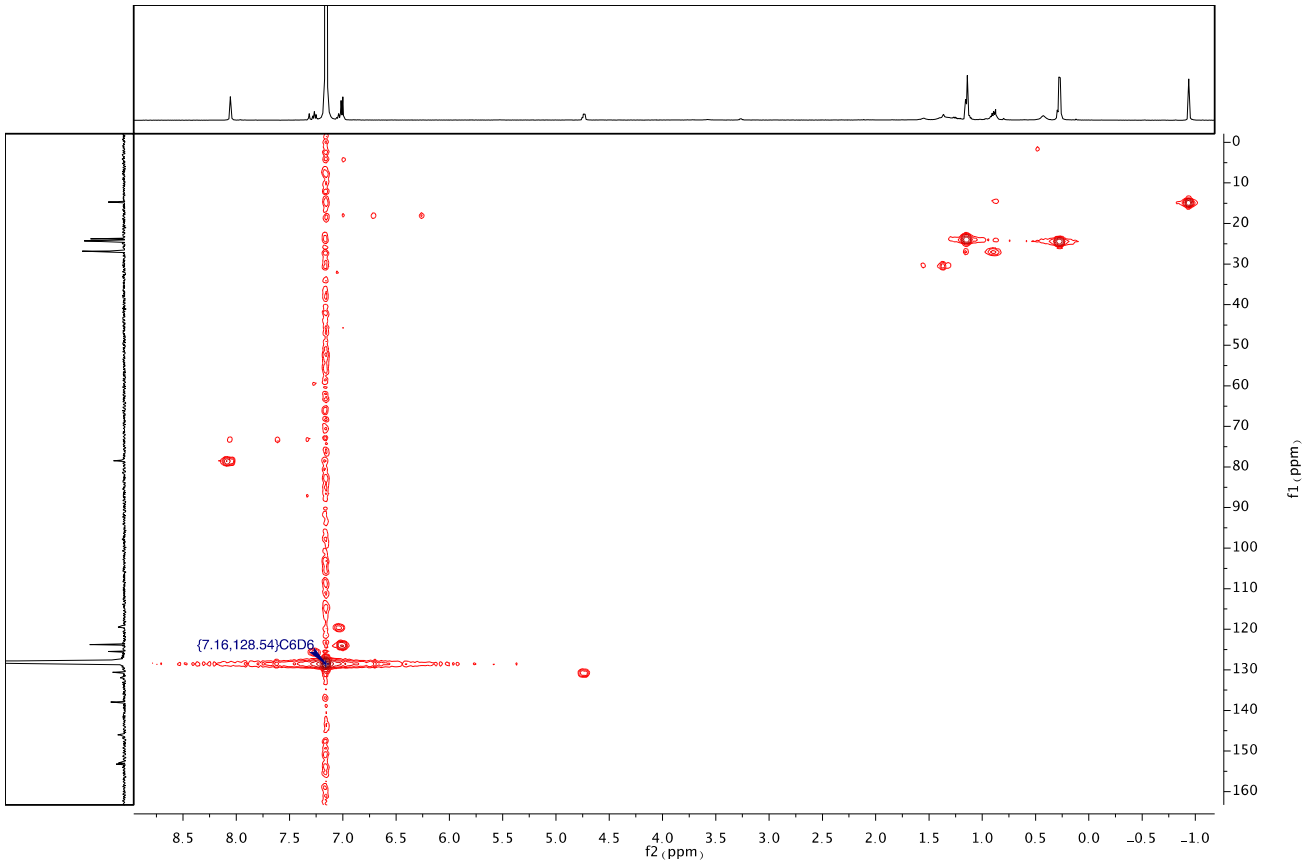



**Figure S6.** $^{1}H/^{13}C$ HMQC of [$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ (**6**) in $C_6D_6$.

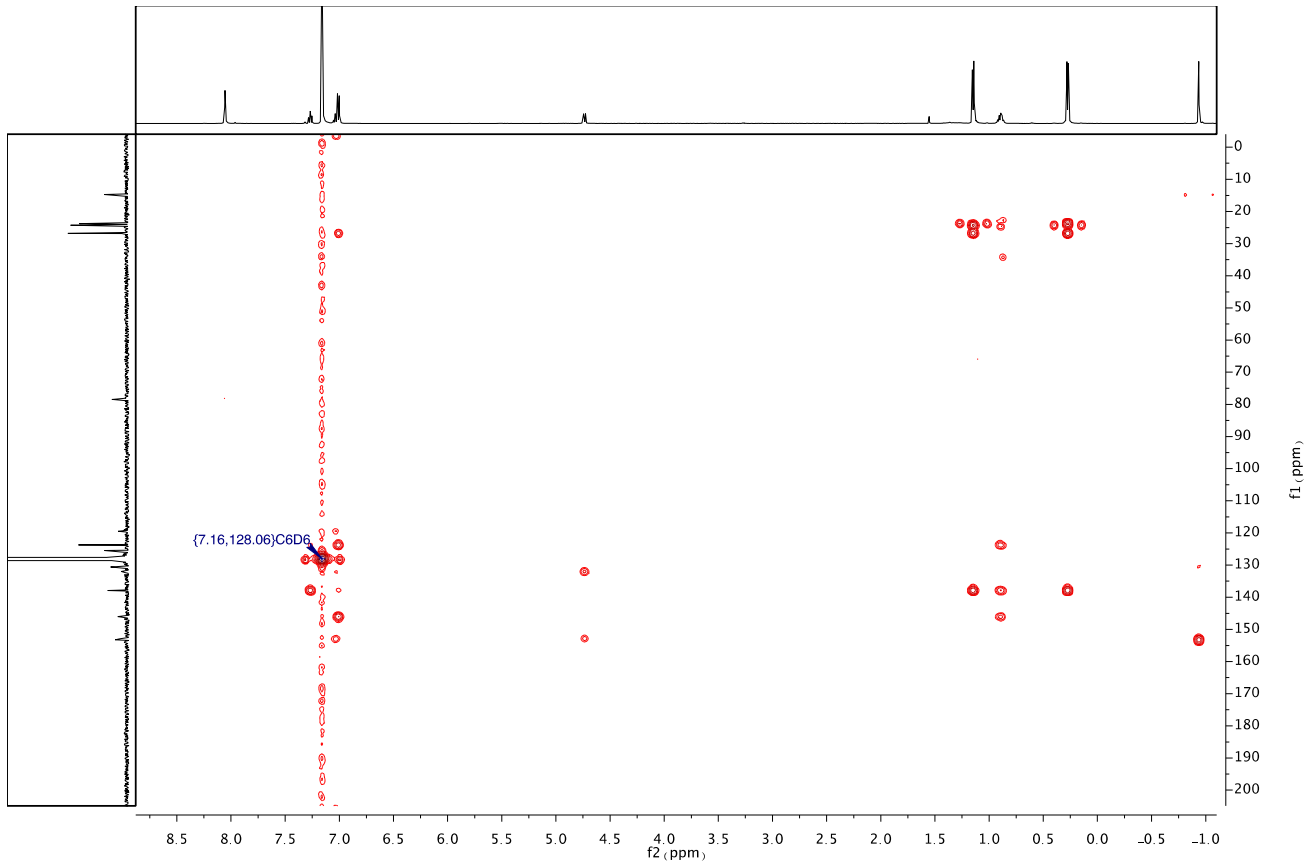



**Figure S7.** $^{1}H/^{13}C$ HMBC of [$i$-$^{Pr}$NDI]$Co_2(C_6H_6)$ (**6**) in $C_6D_6$.

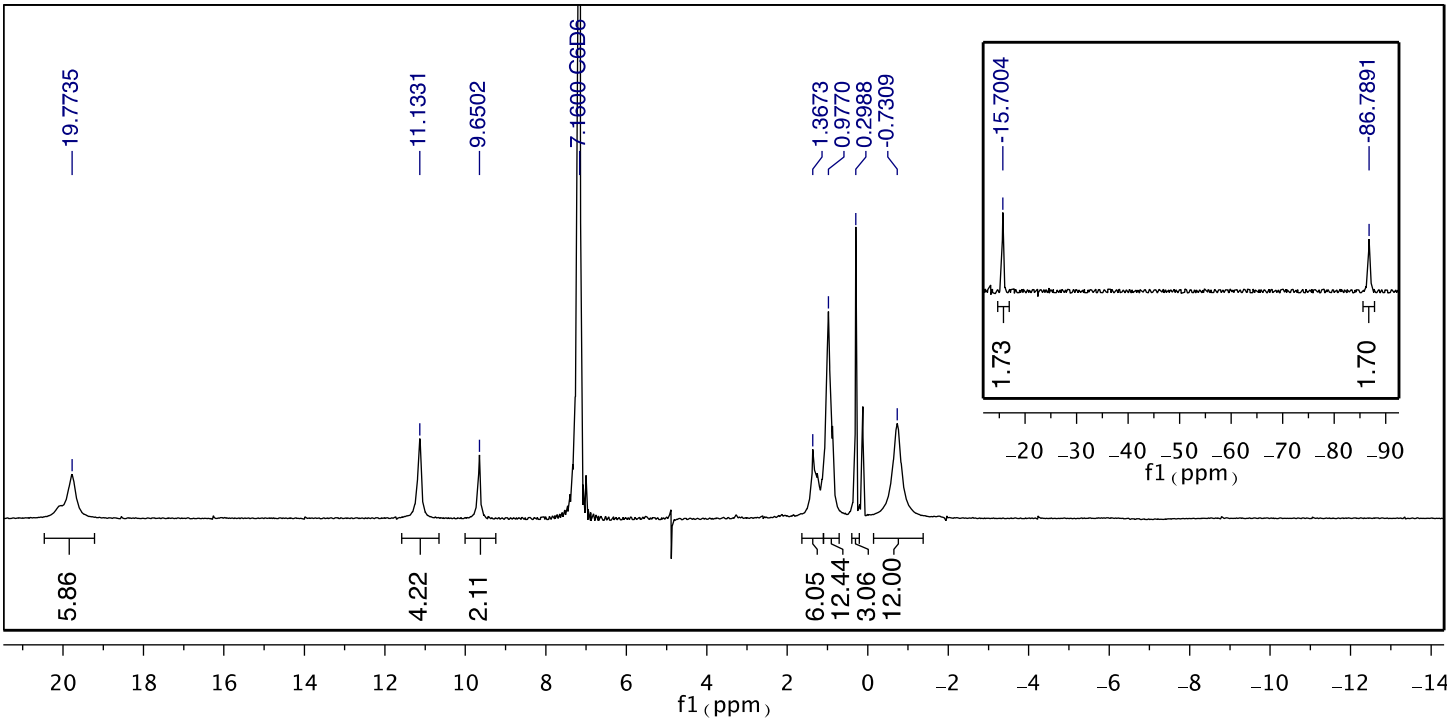



**Figure S8.** $^{1}H$ NMR spectrum of [$i$-$^{Pr}$NDI]$Fe_2(C_6H_6)$ (**7**) in $C_6D_6$.

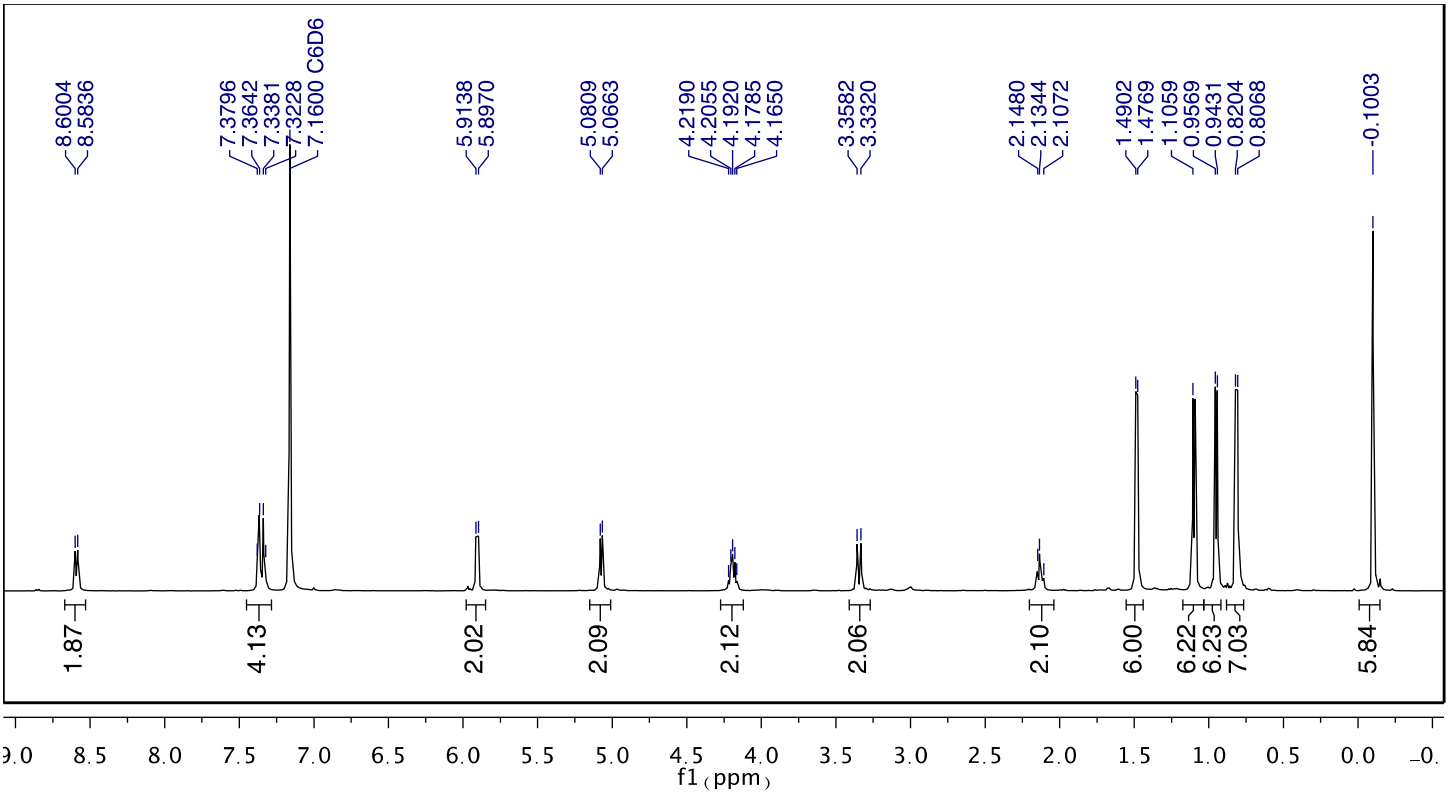



**Figure S9.** $^{1}H$ NMR spectrum of [$^{i\text{-Pr}}$NDI]$Ni_2$(allyl)Cl (**8**) in $C_6D_6$.

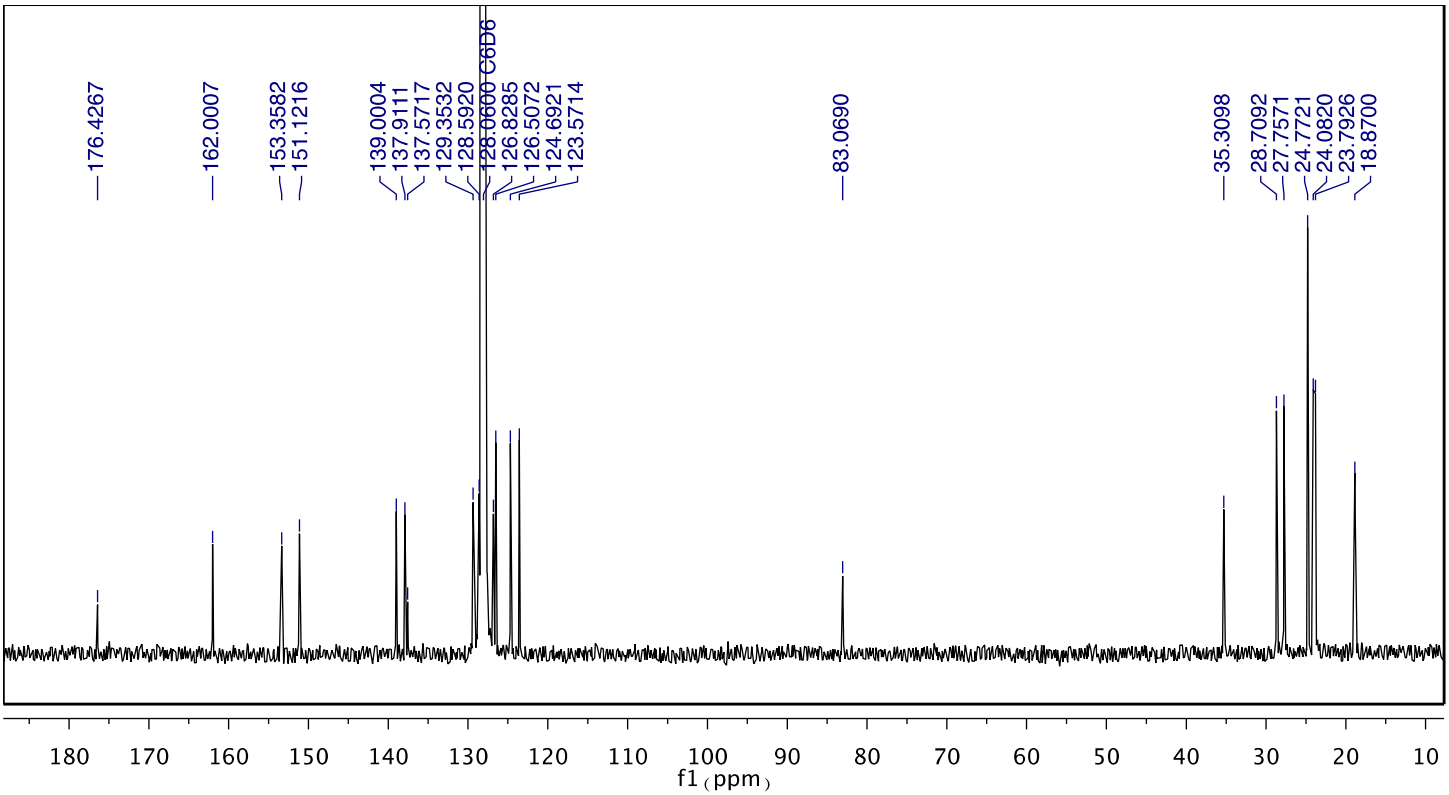



**Figure S10.** $^{13}C\{^{1}H\}$ NMR spectrum of [$^{i\text{-Pr}}$NDI]$Ni_2$(allyl)Cl (**8**) in $C_6D_6$.

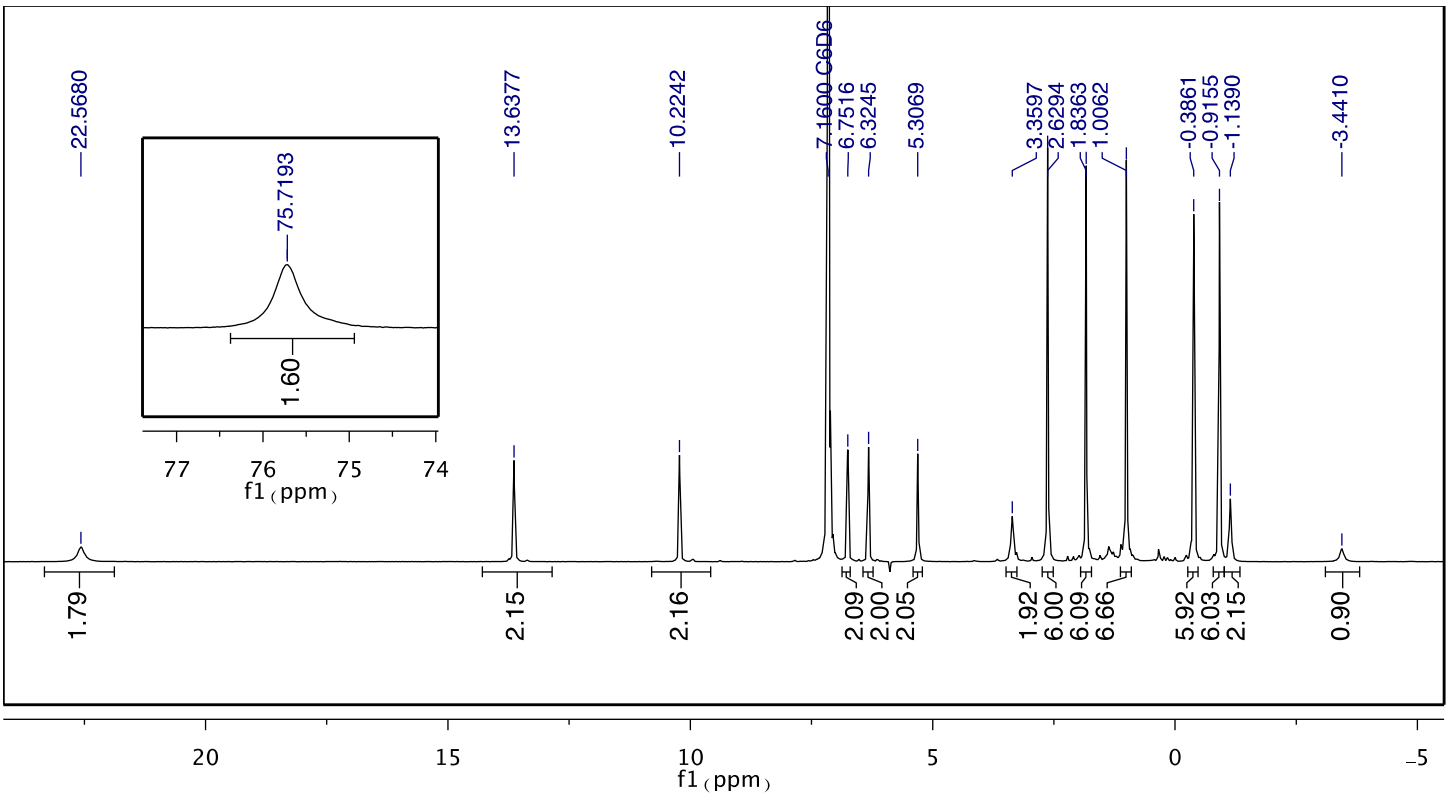



**Figure S11.** Room-temperature $^{1}$H NMR spectrum of [$^{i\text{-Pr}}$NDI]Co$_2$(allyl)Cl (**9**) in $C_6D_6$.

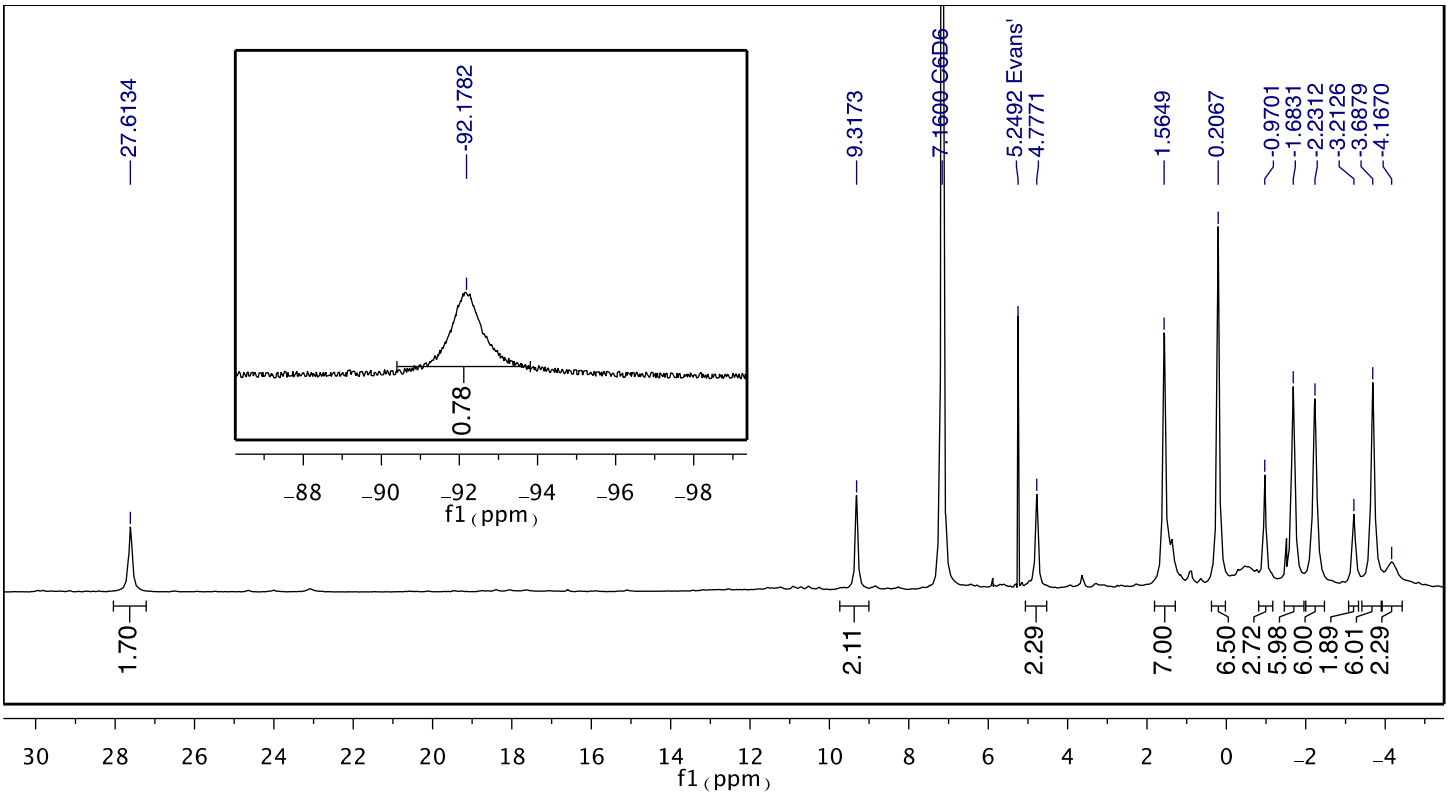



**Figure S12.** $^{1}$H NMR spectrum of [$^{i\text{-Pr}}$NDI]Fe$_2$(allyl)Cl (**10**) in $C_6D_6$.

## 4. UV–Vis–NIR Spectra

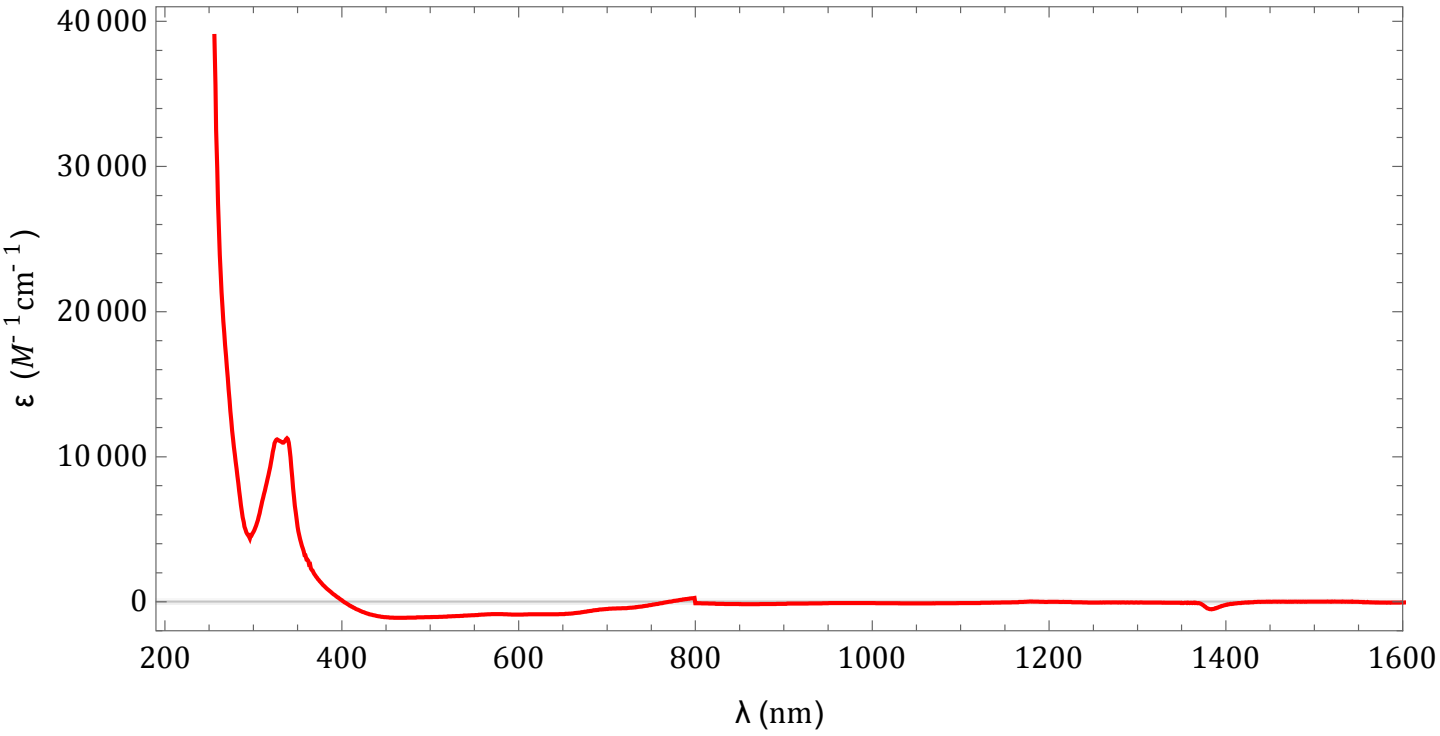



**Figure S13.** UV–Vis–NIR spectrum of [$^{i\text{-Pr}}$NDI]$Co_2(THF)Cl_3$ (**3**).

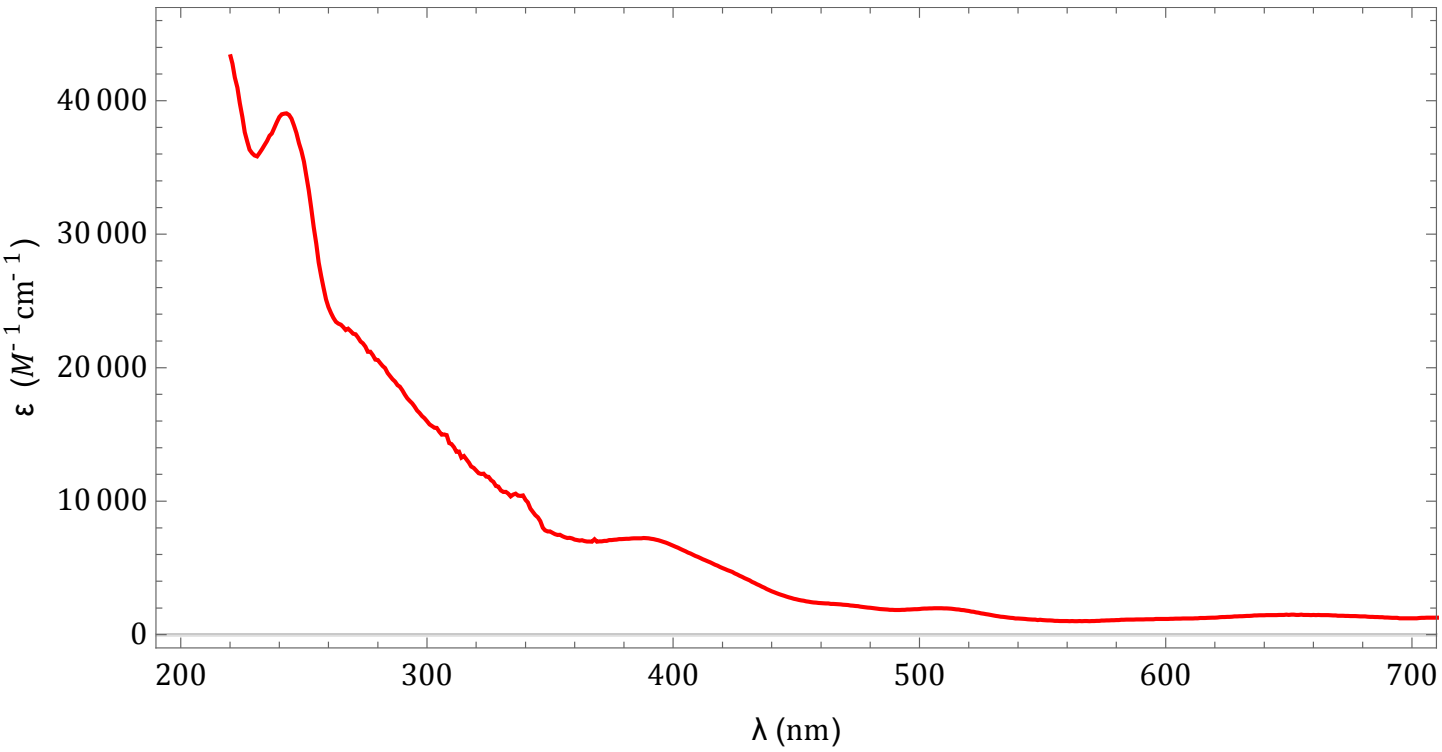



**Figure S14.** UV–Vis–NIR spectrum of [$^{i\text{-Pr}}$NDI]$Fe_2(THF)Cl_3$ (**4**).

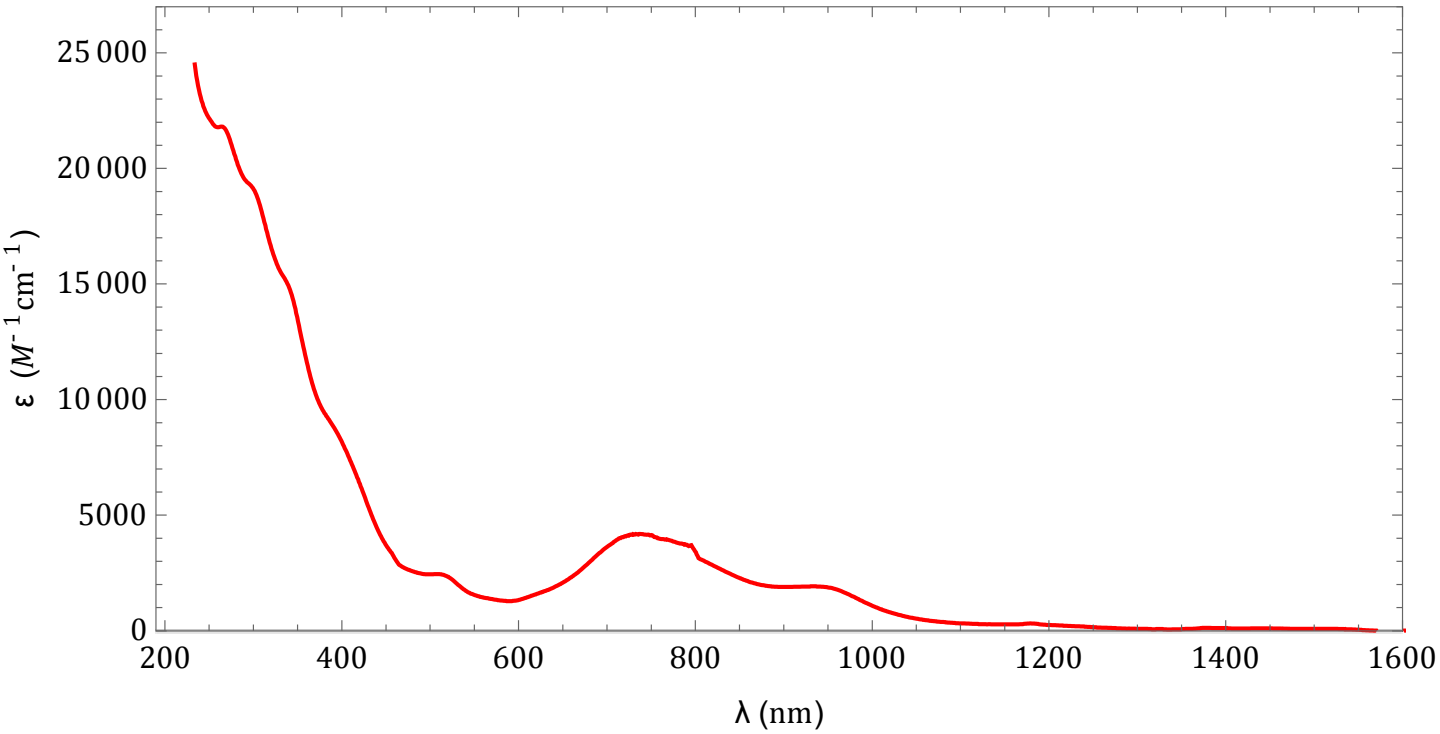



**Figure S15.** UV–Vis–NIR spectrum of [$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ (**6**).

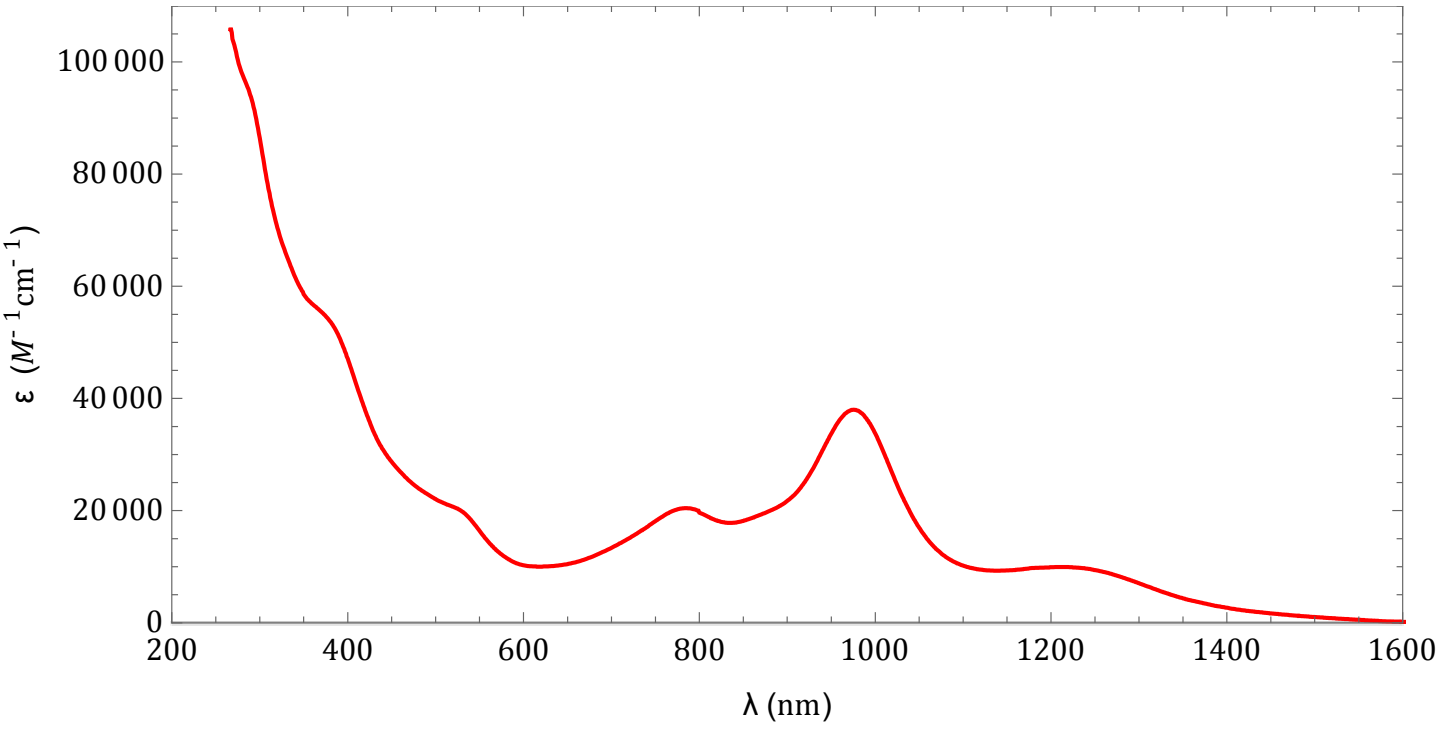



**Figure S16.** UV–Vis–NIR spectrum of [$^{i\text{-Pr}}$NDI]$Fe_2(C_6H_6)$ (**7**).

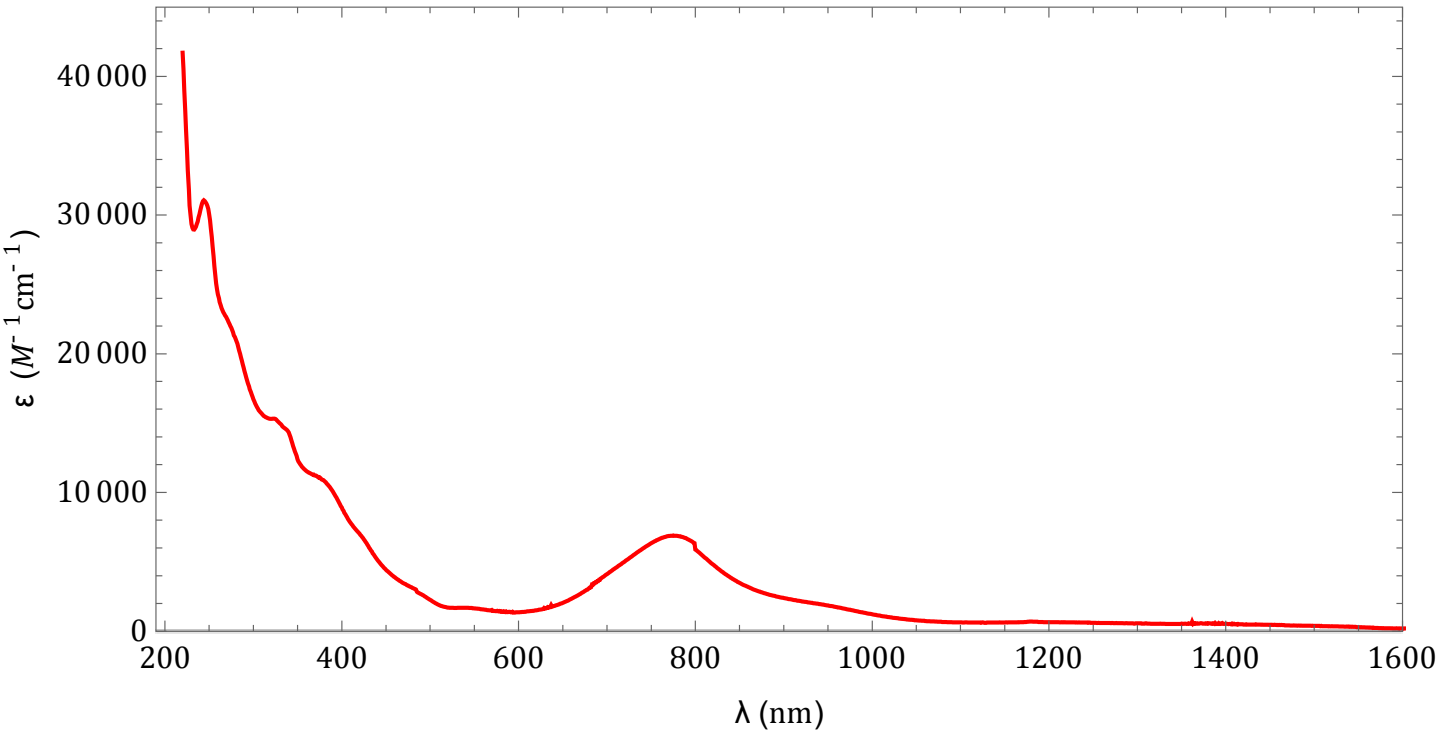



**Figure S17.** UV–Vis–NIR spectrum of [$^{i\text{-Pr}}$NDI]$Co_2(C_3H_5)Cl$ (**9**).

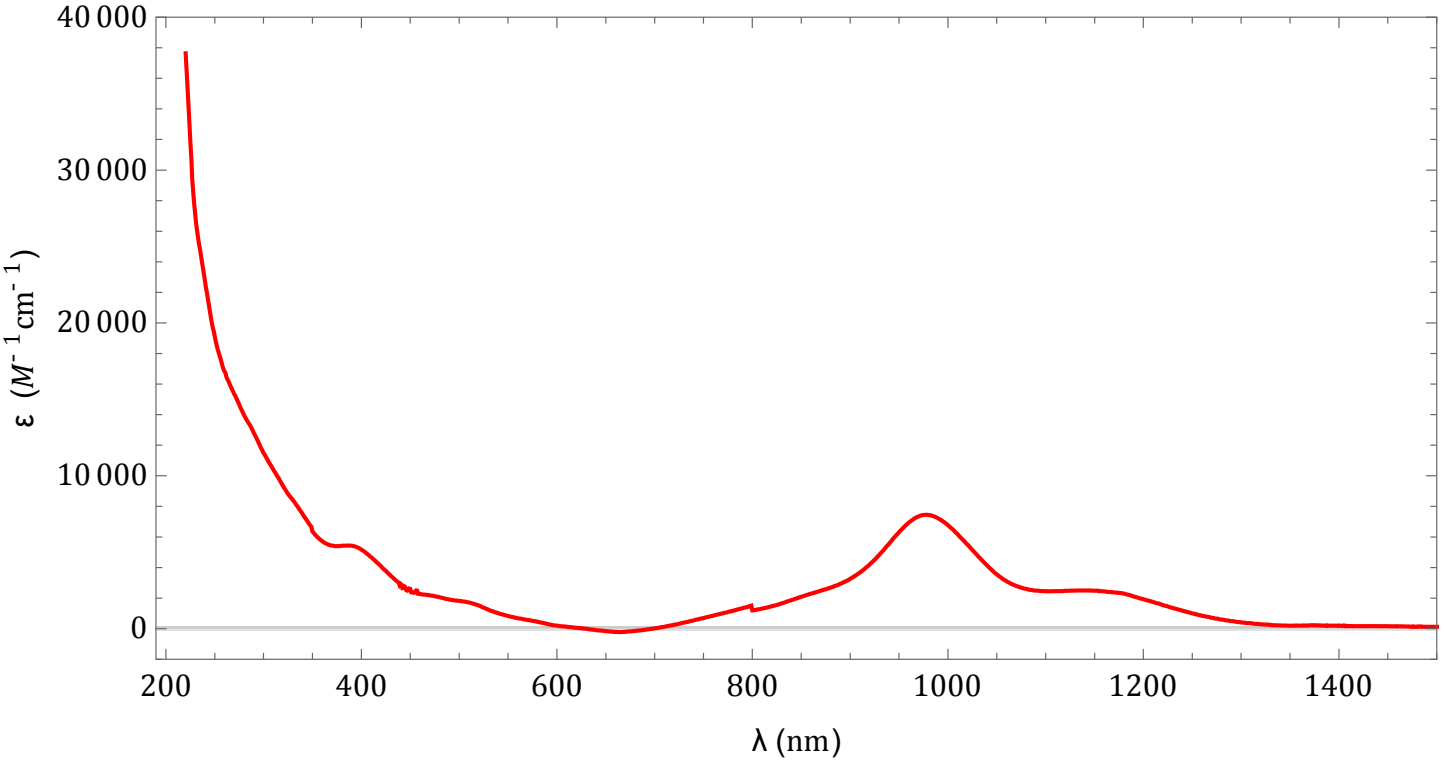



**Figure S18.** UV–Vis–NIR spectrum of [$^{i\text{-Pr}}$NDI]$Fe_2(C_3H_5)Cl$ (**10**).

## 5. IR Spectra

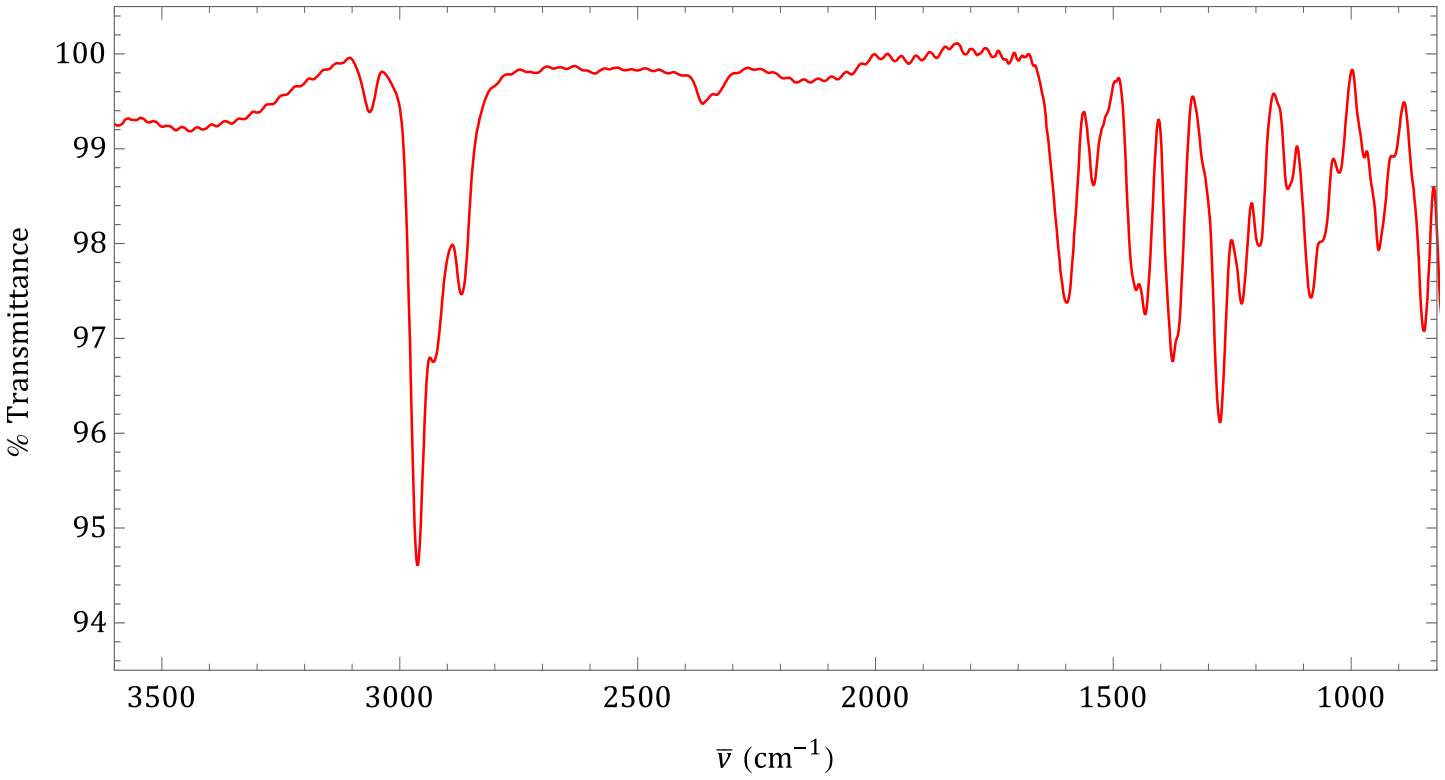



**Figure S19.** IR spectrum of [$^{i\text{-Pr}}$NDI]$Co_2$(THF)$Cl_3$ (**3**).

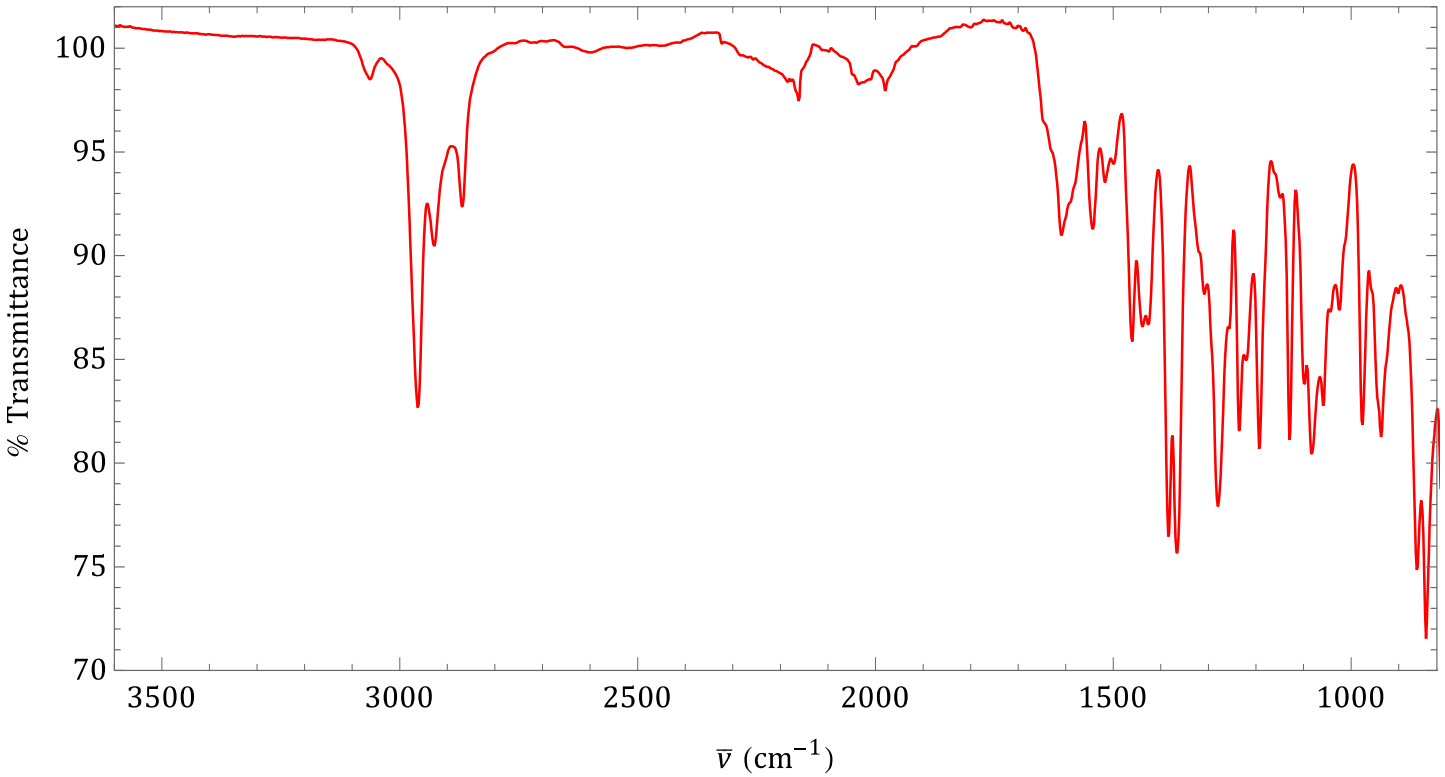



**Figure S20.** IR spectrum of [$^{i\text{-Pr}}$NDI]$Fe_2$(THF)$Cl_3$ (**4**).

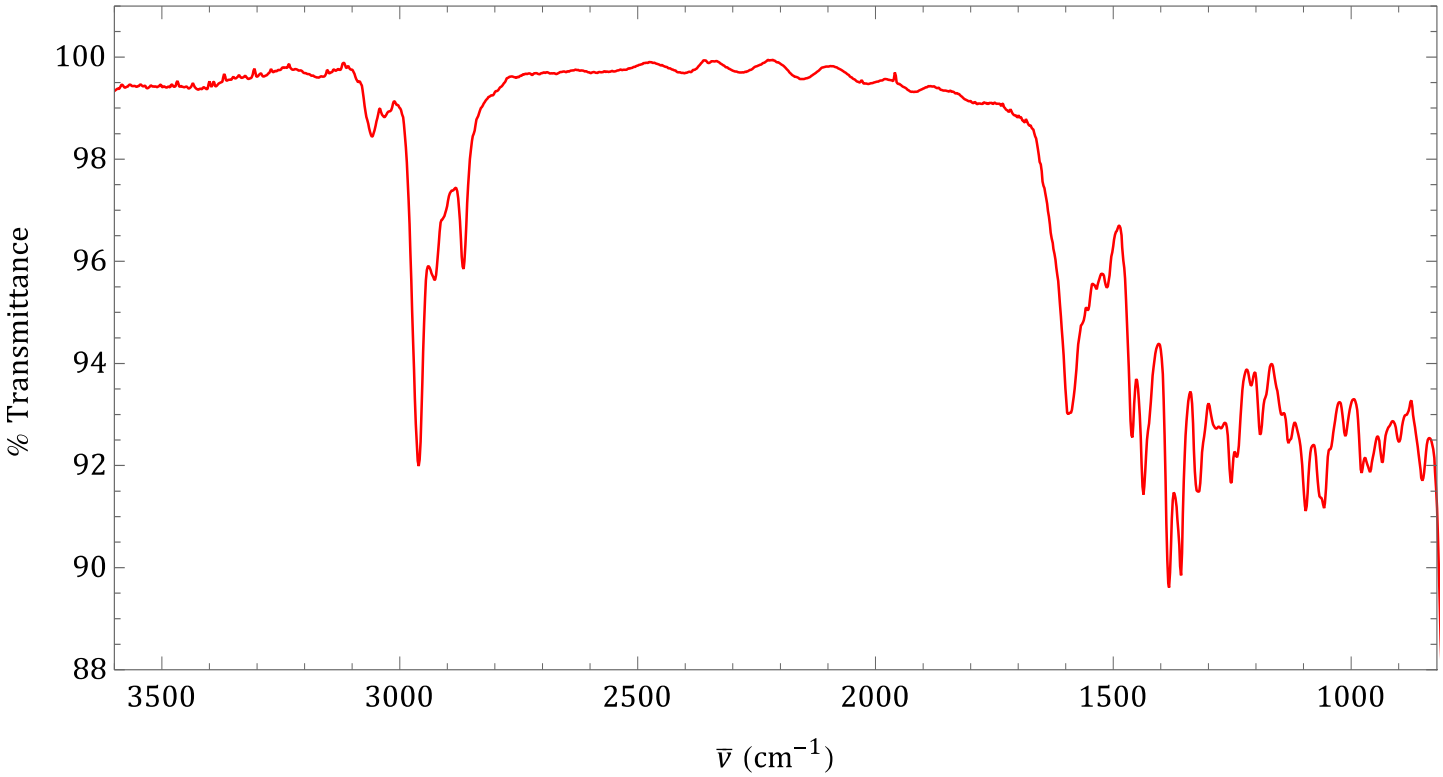



**Figure S21.** IR spectrum of [$^{i\text{-Pr}}$NDI]Co$_2$(C$_6$H$_6$) (**6**).

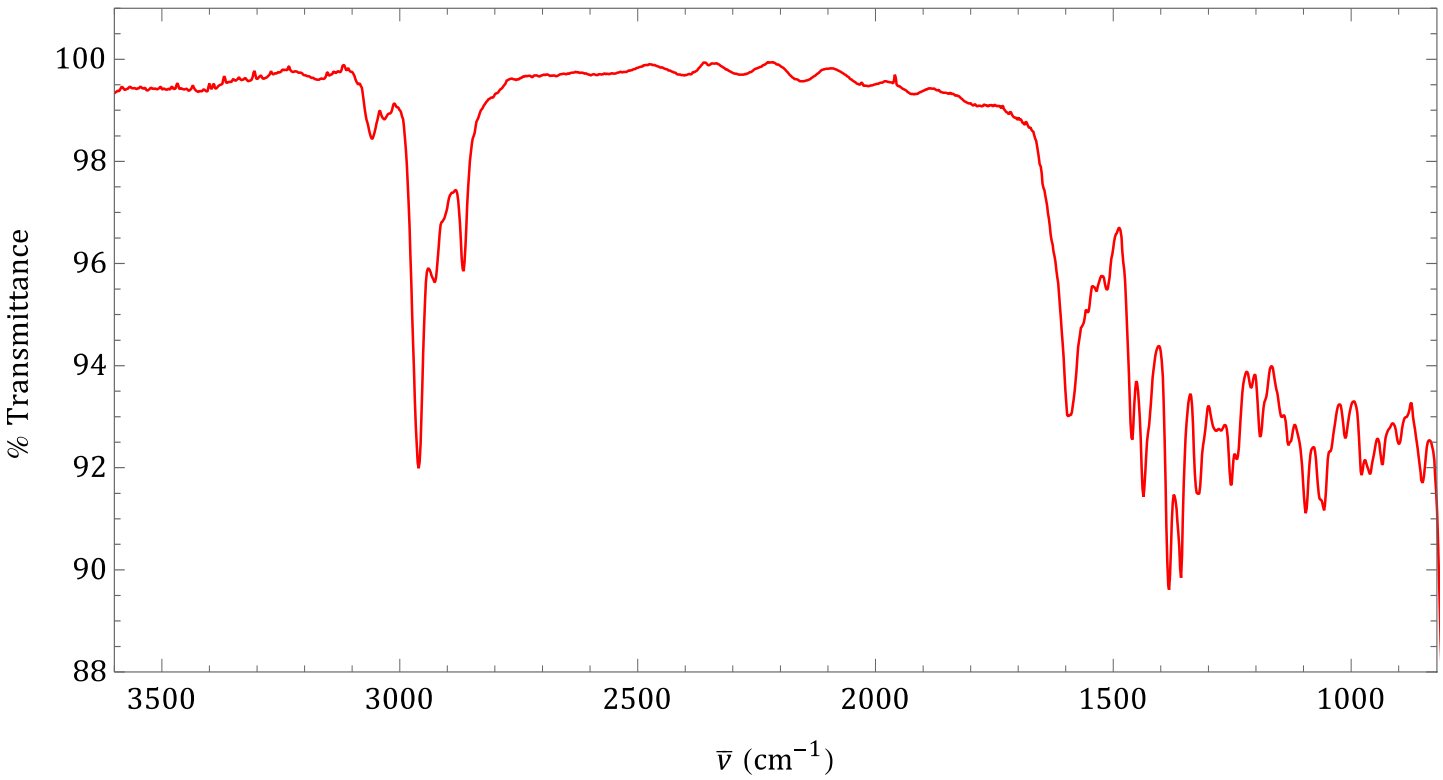



**Figure S22.** IR spectrum of [$^{i\text{-Pr}}$NDI]Fe$_2$(C$_6$H$_6$) (**7**).

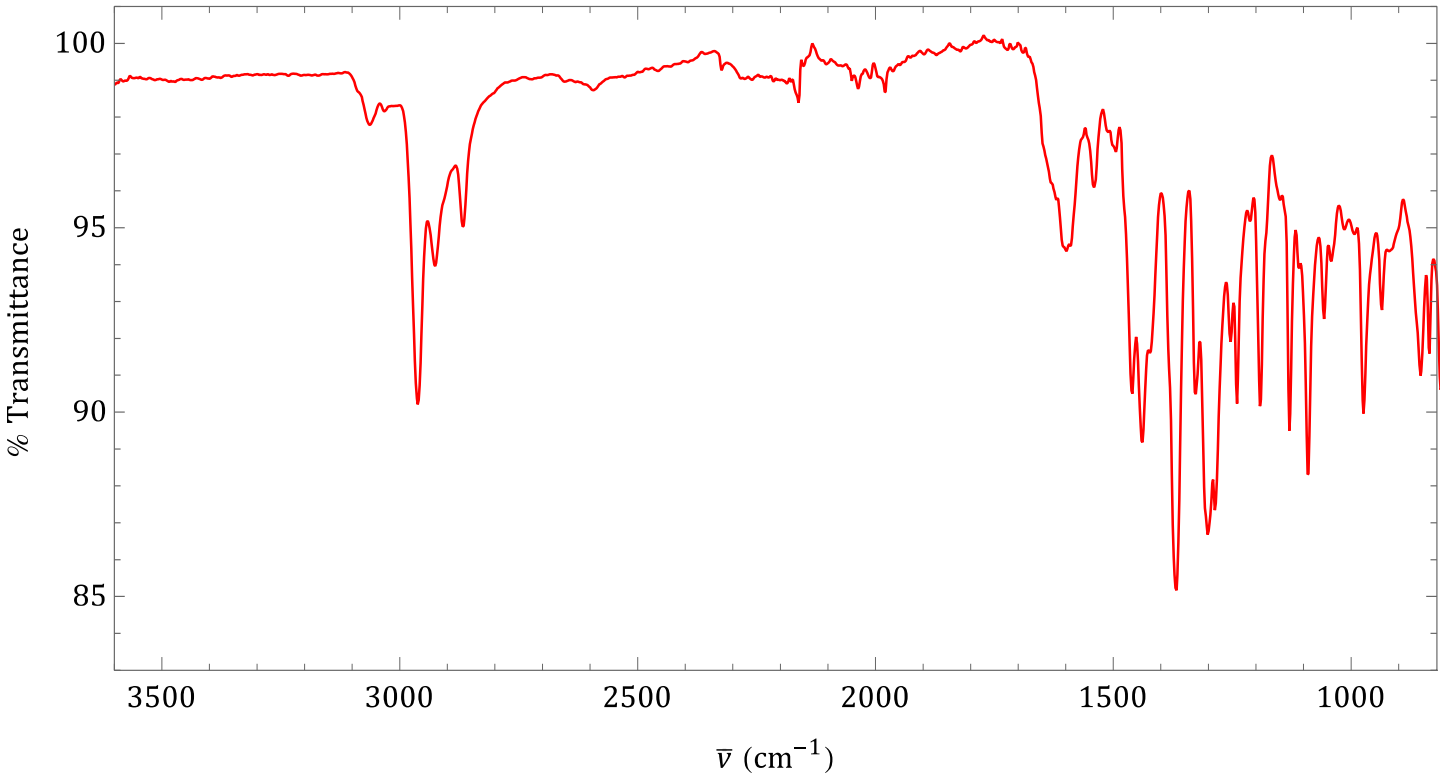



**Figure S23.** IR spectrum of [$^{i\text{-Pr}}$NDI]$Co_2(C_3H_5)Cl$ (**9**).

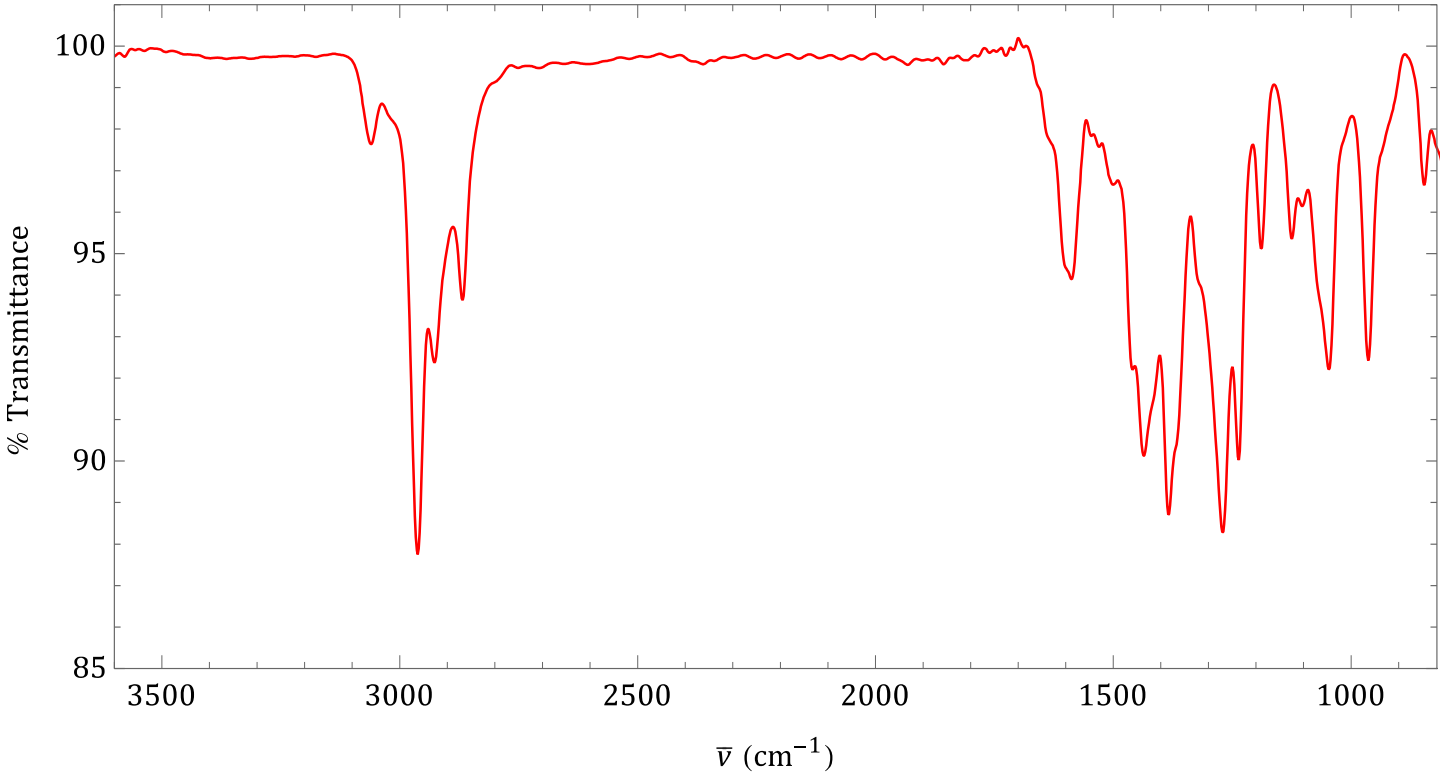



**Figure S24.** IR spectrum of [$^{i\text{-Pr}}$NDI]$Fe_2(C_3H_5)Cl$ (**10**).

## 6. Cyclic Voltammetry Data

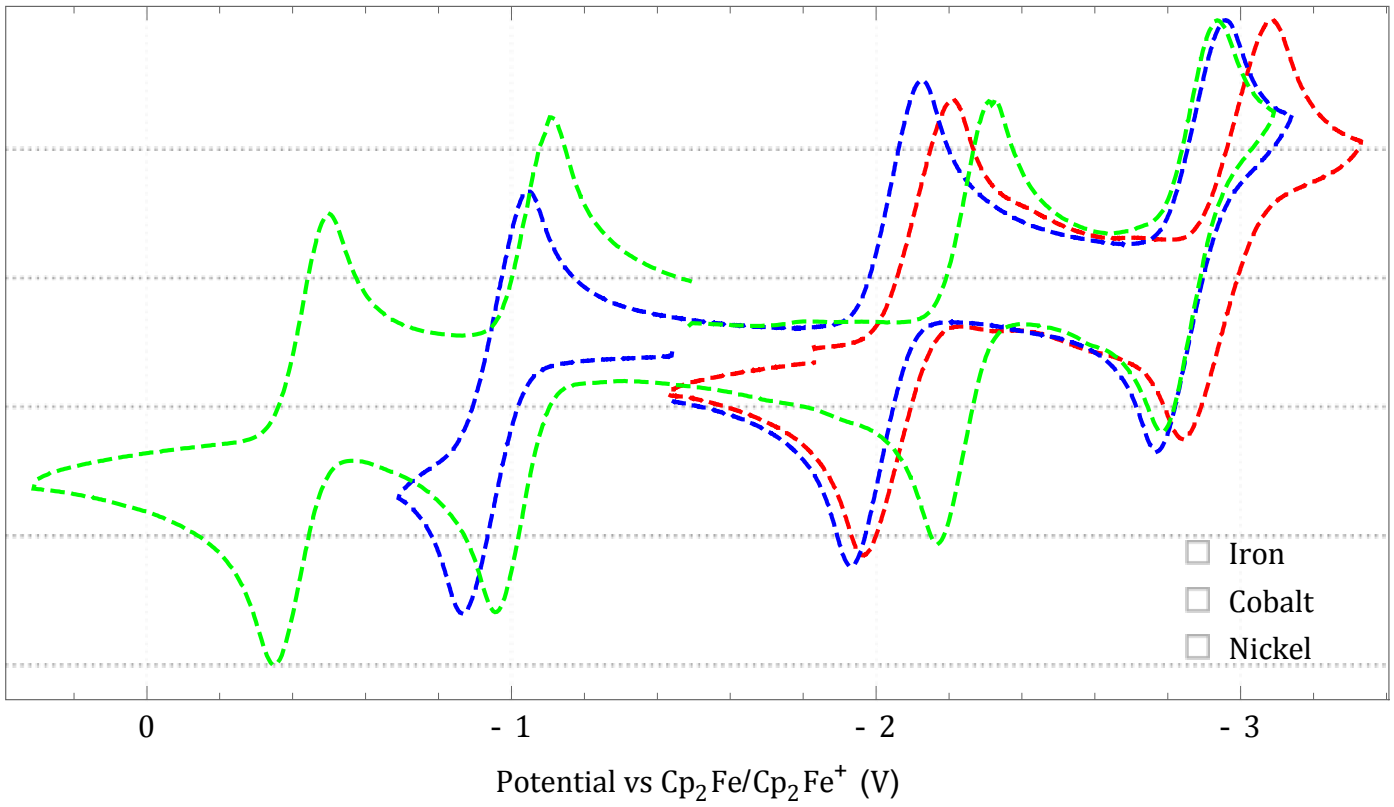



**Figure S25.** Cyclic voltammograms for [$^{i\text{-Pr}}$NDI]$M_2(C_6H_6)$ complexes (0.20 M [$n$-$Bu_4N$][$PF_6$] supporting electrolyte in THF, glassy carbon working electrode, 100 mV/s scan rate). For the $Fe_2$ and $Ni_2$ voltammograms, the scan begins at the open circuit potential and proceeds in the cathodic direction. For the $Co_2$ voltammogram, the scan begins at the open circuit potential and proceeds in the anodic direction.

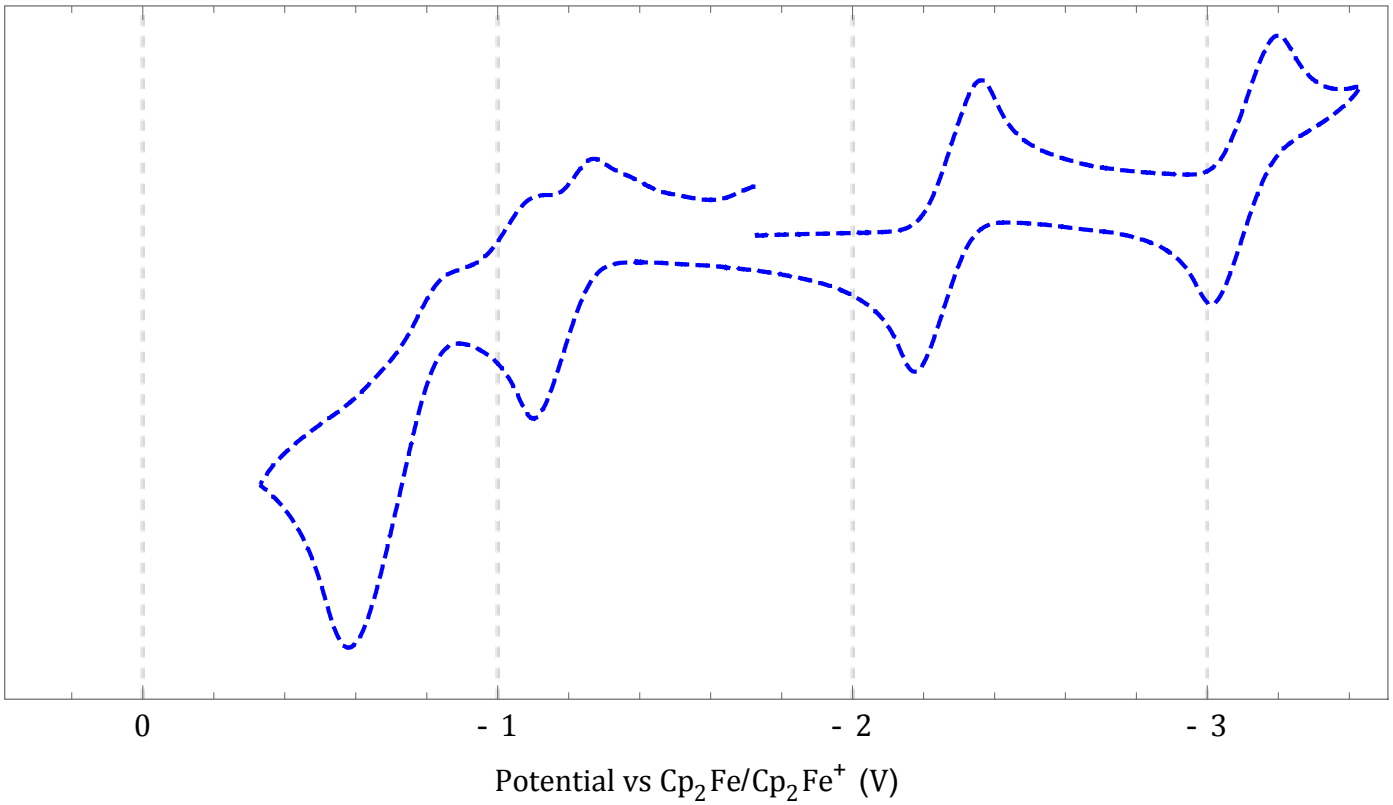



**Figure S26.** Cyclic voltammogram for [$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ (**6**) showing irreversible oxidation event.

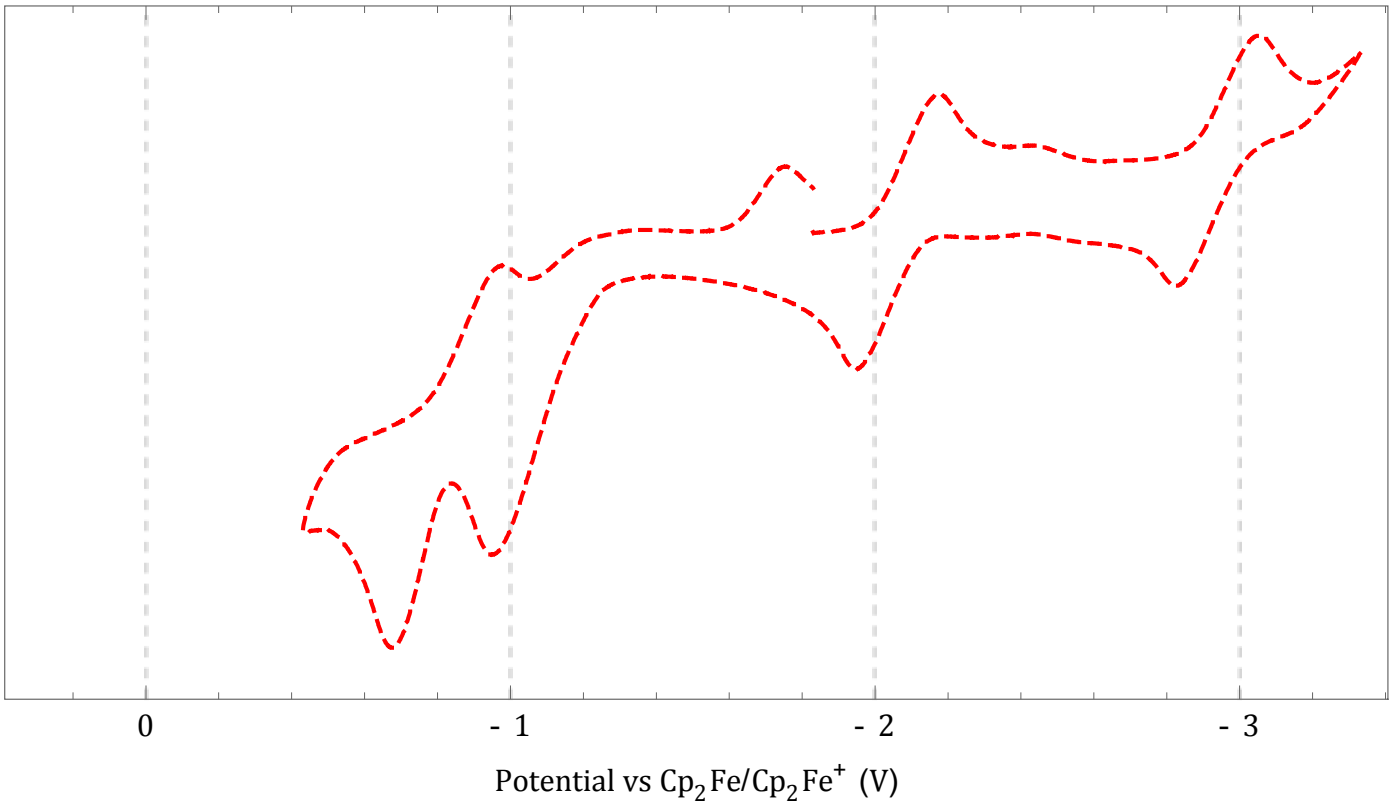



**Figure S27.** Cyclic voltammogram for [$^{i\text{-Pr}}$NDI]$Fe_2(C_6H_6)$ (**7**) showing irreversible oxidation event.

## 7. Variable Temperature $^1$H NMR Data

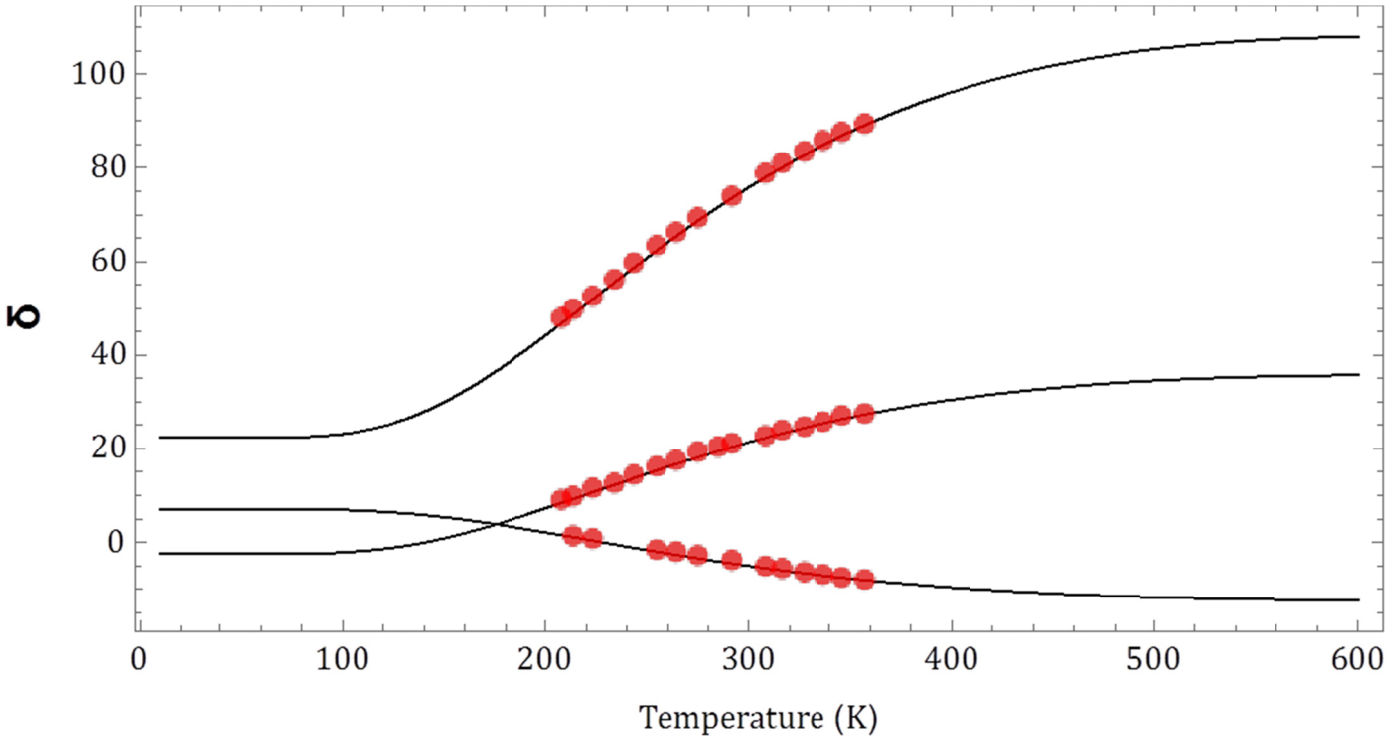



**Figure S28.** The temperature-dependence of the $^1$HNMR spectrum of $Co_2(C_3H_5)Cl(NDI)$ is consistent with thermal population of a triplet excited state. Chemical shifts for two of the allyl signals are shown here as a function of temperature.

The VT-NMR data were fit to the Boltzmann function for a singlet-triplet system shown below. The diamagnetic shift (a) and fitting constant (b) were fit individually for each curve, while the enthalpy and entropy of spin-crossover (c and d, respectively) were shared.

$$chemical\ shift = \sum_{j=1}^{3} \delta_{ij} a^j + \frac{\sum_{j=1}^{3} \delta_{ij} b^j}{T * \left(1 + e^{\left(\frac{c}{8.314*T} - \frac{d}{8.314}\right)}\right)}$$

i = curve index
$a^i$ = chemical shift for each curve in the diamagnetic state
$b^i$ = fitting constant for each curve
c = ΔH of spin-crossover in units of J/mol
d = ΔS of spin-crossover in units of J/mol•K

ΔH: 1.6 ± 0.1 kcal/mol

## 8. X-Ray Diffraction Data

**Refinement Details.** For compound **6**, [$^{i\text{-}Pr}$NDI]$Co_2(C_6H_6)$, the structure contains three independent solvent accessible voids of 2241.8 Å$^3$ combined. The residual electron density peaks are disordered around a threefold axis and were not arranged in an interpretable pattern. The hkl file was instead corrected for using reverse Fourier transform methods using the SQUEEZE routine[9] as implemented in the program Platon. The resultant files were used in the further refinement. (The FAB file with details of the Squeeze results is appended to this cif file). The Squeeze procedure corrected for 385.4 electrons within the solvent accessible voids. Positions of H atoms of the metal coordinated benzene ring were refined.

For compound **7**, [$^{i\text{-}Pr}$NDI]$Fe_2(C_6H_6)$, the structure contains three independent solvent accessible voids of 760 Å$^3$ each (located around the three fold inversion axes). The residual electron density peaks are not arranged in an interpretable pattern, indicating severe disorder around the three fold axis and inversion centers, and no meaningful solvate model could be built. The hkl file was instead corrected using reverse Fourier transform methods using the SQUEEZE routine[9] as implemented in the program Platon. The resultant files were used in the further refinement. (The FAB file with details of the Squeeze results is appended to this cif file). The Squeeze procedure corrected for three times 194 electrons within the solvent accessible voids. One of the diisopropylbenzene ligand side arms showed signs of disorder and was modeled as split over two slightly shifted orientations. The geometries of the two moieties were restrained to be similar as that of the other not disordered ligand side arm, and Uij components of ADPs of disordered atoms were restrained to be similar if closer to each other than 1.7 Å. Positions of H atoms of the metal coordinated benzene ring were refined with C-H distances restrained to 1.00(2) Å.

For compound **8**, [$^{i\text{-}Pr}$NDI]$Ni_2$(allyl)Cl, the positions of H atoms of the metal coordinated allyl fragment were refined with C-H distances restrained to 1.00(2) Å.

For compound **9**, [$^{i\text{-}Pr}$NDI]$Co_2$(allyl)Cl, the positions of the hydrogen atoms on the allyl fragment were refined, and the C-H distances were restrained to be similar to each other.

For compound **10**, [$^{i\text{-}Pr}$NDI]$Fe_2$(allyl)Cl, a methyl group was rotationally disordered. The positions of the hydrogen atoms on the allyl fragment were refined, and the C-H distances were restrained to be similar to each other.

[9] P. van der Sluis & A.L. Spek (1990). Acta Cryst. A46, 194-201.

**Crystal Structure ORTEP Diagrams.** Ellipsiods are shown at 50% probability level.

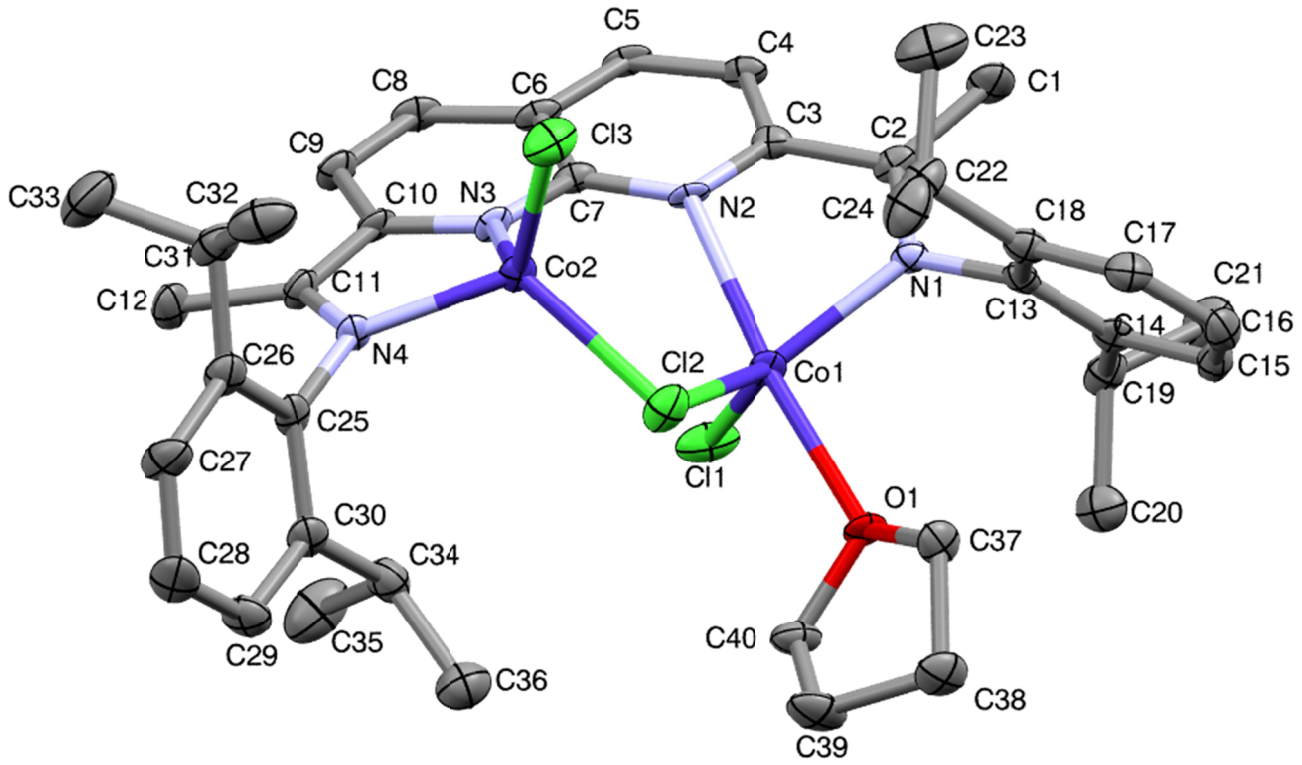



**Figure S29.** Structure of [$^{i\text{-}Pr}$NDI]$Co_2$(allyl)Cl **(3)**.

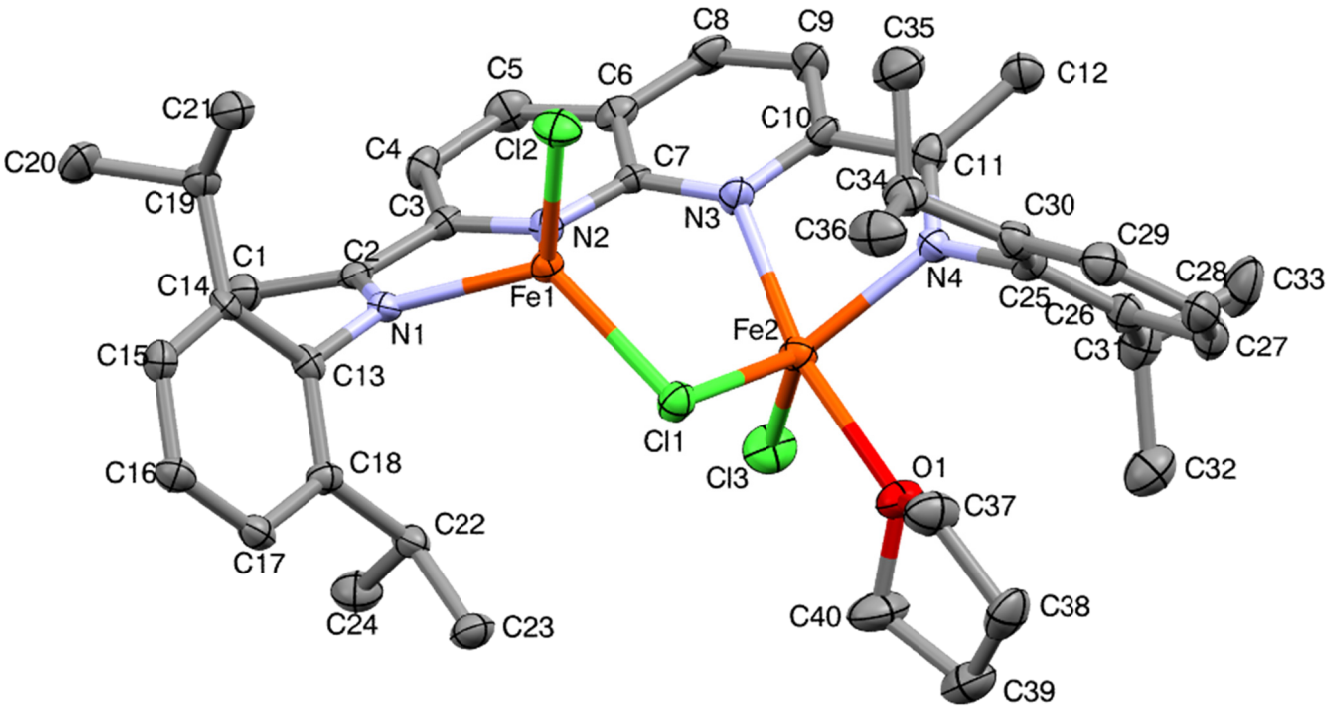



**Figure S30.** Structure of [$^{i\text{-}Pr}$NDI]$Fe_2$(allyl)Cl **(4)**.

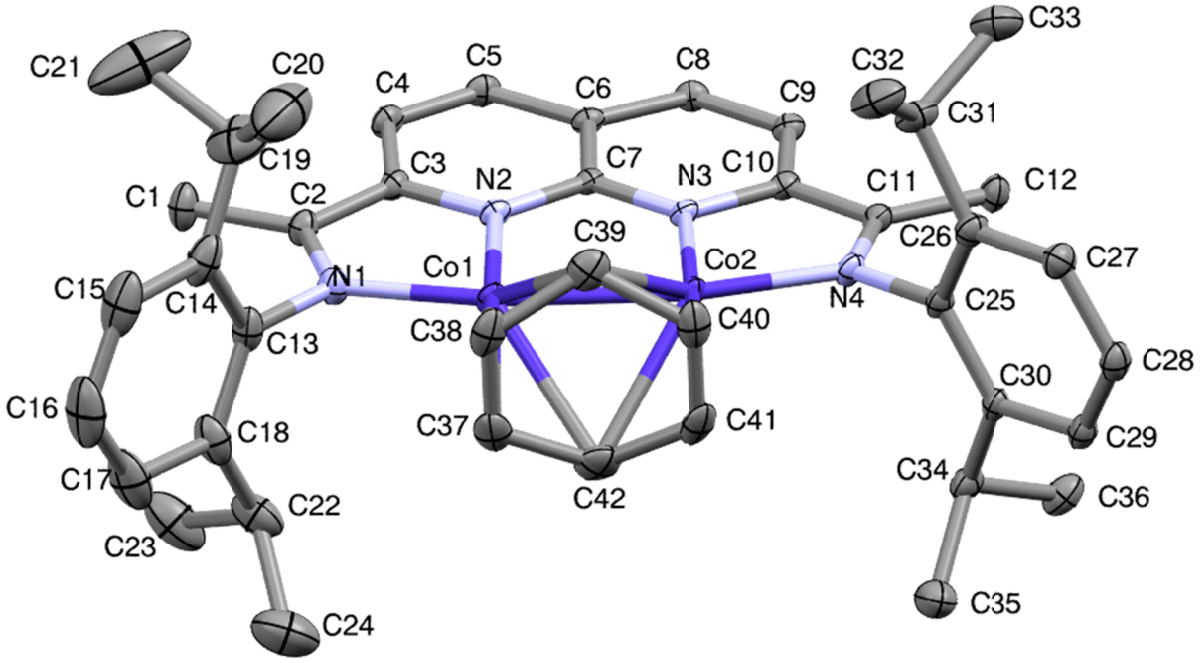



**Figure S31.** Structure of [$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$ **(6)**.

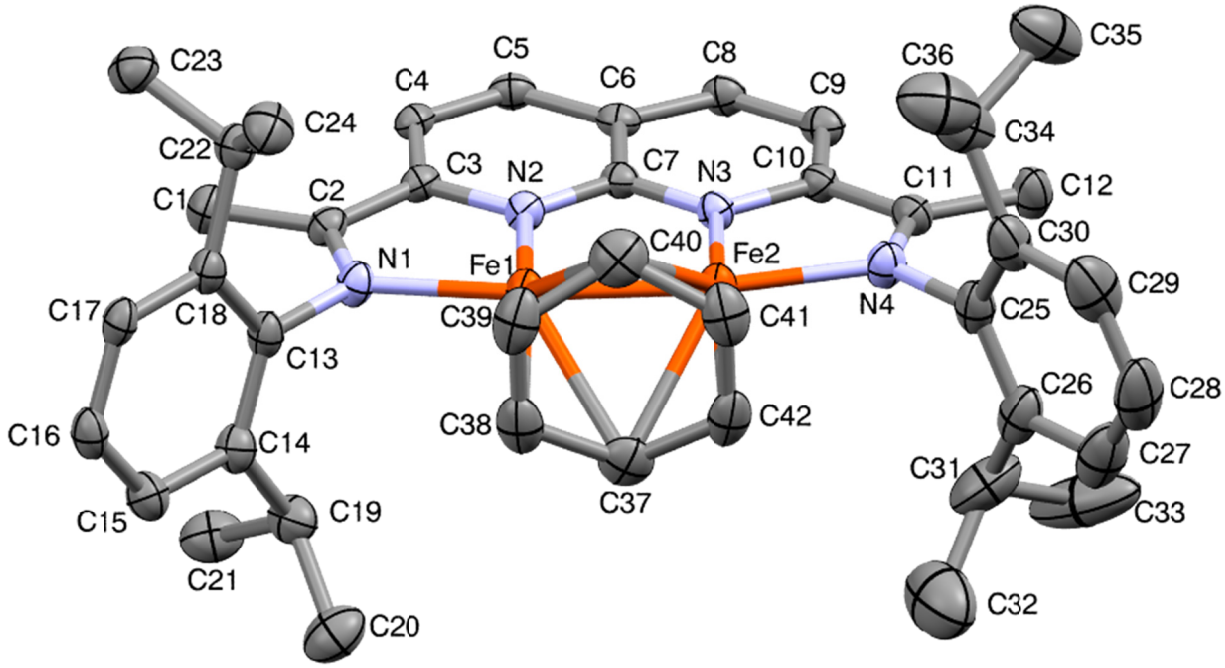



**Figure S32.** Structure of [$^{i\text{-Pr}}$NDI]$Fe_2(C_6H_6)$ **(7)**.

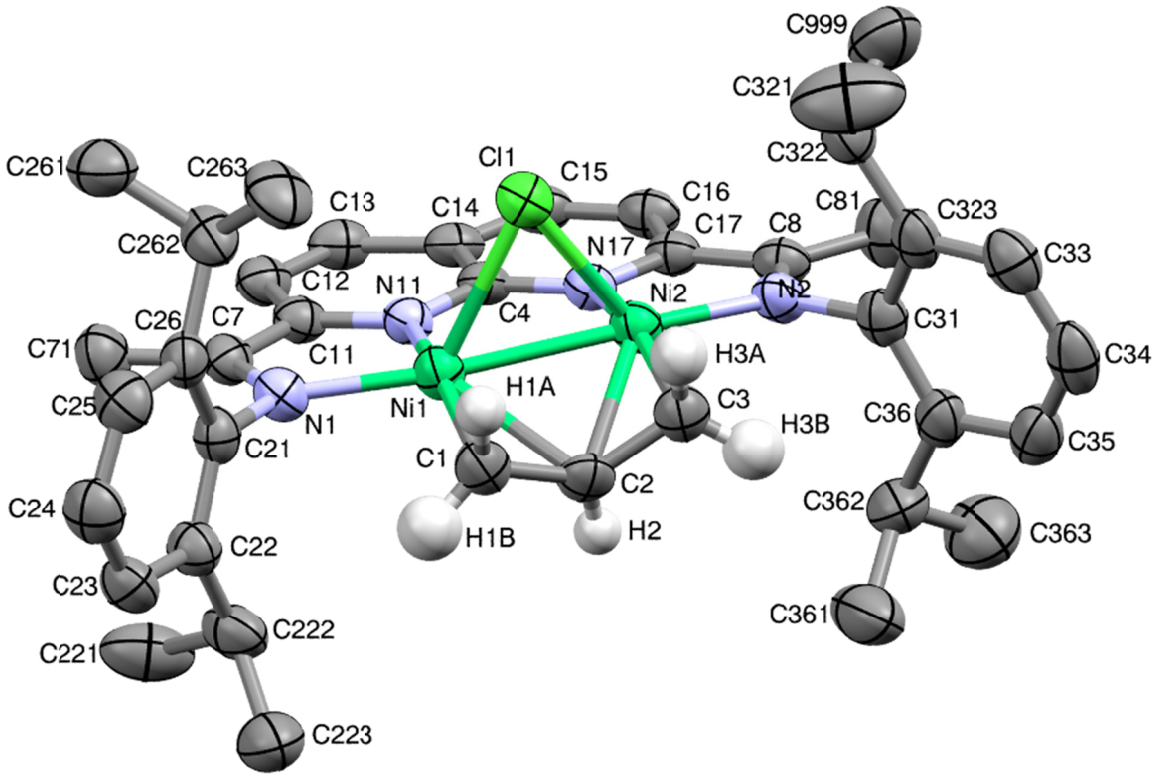



**Figure S33.** Structure of [$^{i\text{-}Pr}$NDI]$Ni_2$(allyl)Cl **(8)**.

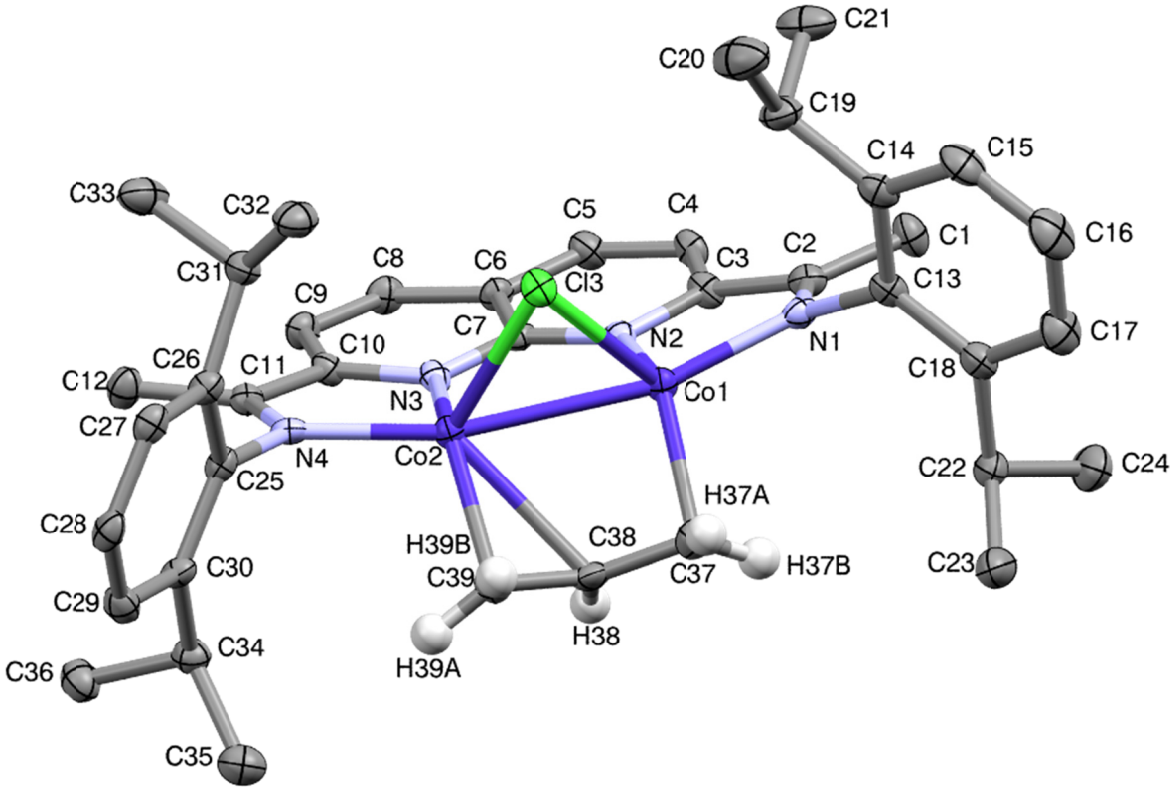



**Figure S34.** Structure of [$^{i\text{-}Pr}$NDI]$Co_2$(allyl)Cl **(9)**.

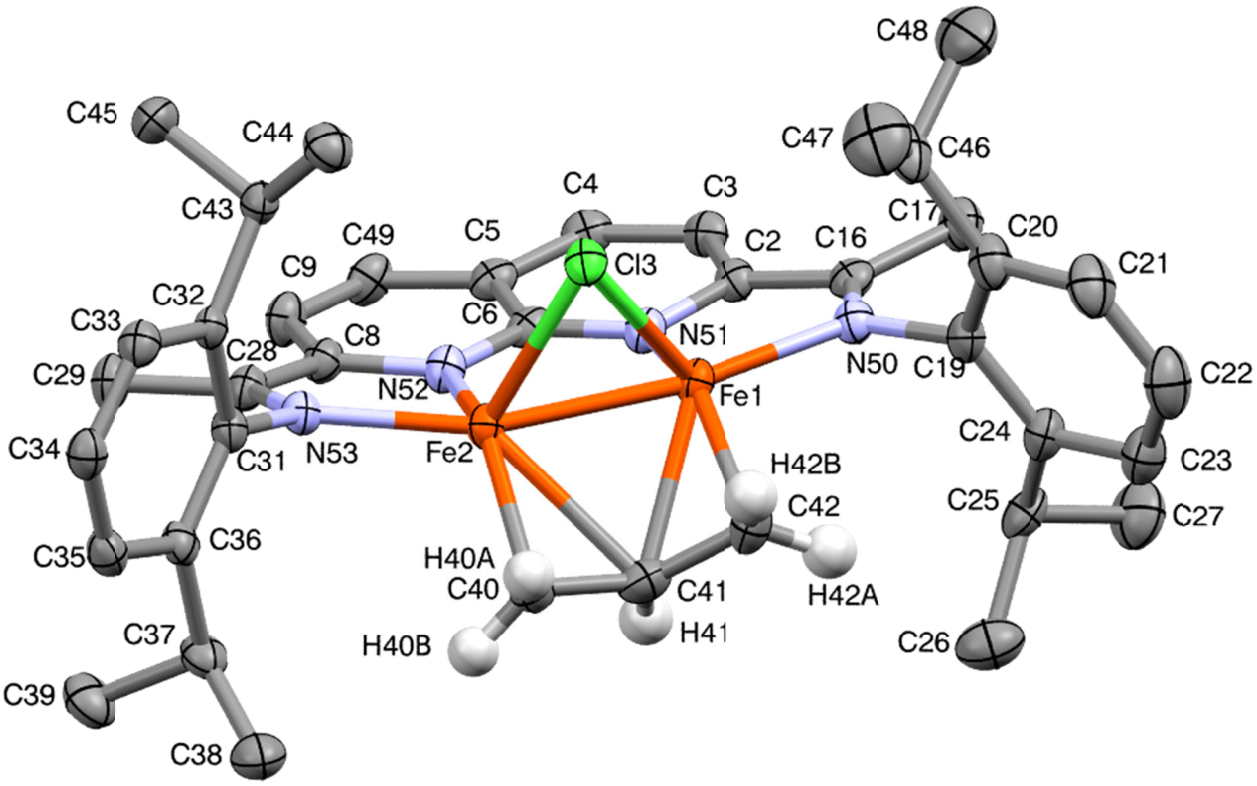



**Figure S35.** Structure of [$^{i\text{-}Pr}$NDI]$Fe_2$(allyl)Cl **(10)**.

**Table 1a.** Bond lengths and angles for [$^{i\text{-}Pr}$NDI]$Co_2(THF)Cl_3$ **(3)**.

| **Bond lengths (Å)** | | | |
|---|---|---|---|
| C1—C2 | 1.478 (6) | C22—C23 | 1.527 (7) |
| C2—N1 | 1.303 (5) | C25—C26 | 1.399 (6) |
| C2—C3 | 1.471 (6) | C25—C30 | 1.410 (6) |
| C3—N2 | 1.348 (5) | C25—N4 | 1.437 (5) |
| C3—C4 | 1.394 (5) | C26—C27 | 1.392 (6) |
| C4—C5 | 1.378 (6) | C26—C31 | 1.516 (6) |
| C5—C6 | 1.396 (6) | C27—C28 | 1.380 (7) |
| C6—C8 | 1.417 (6) | C28—C29 | 1.370 (7) |
| C6—C7 | 1.431 (5) | C29—C30 | 1.388 (6) |
| C7—N2 | 1.340 (5) | C30—C34 | 1.531 (7) |
| C7—N3 | 1.358 (5) | C31—C32 | 1.526 (7) |
| C8—C9 | 1.367 (6) | C31—C33 | 1.534 (7) |
| C9—C10 | 1.410 (5) | C34—C35 | 1.519 (7) |
| C10—N3 | 1.377 (5) | C34—C36 | 1.522 (7) |
| C10—C11 | 1.435 (6) | C37—O1 | 1.455 (5) |
| C11—N4 | 1.331 (5) | C37—C38 | 1.510 (6) |
| C11—C12 | 1.501 (6) | C38—C39 | 1.524 (7) |
| C13—C14 | 1.400 (6) | C39—C40 | 1.507 (6) |
| C13—C18 | 1.402 (6) | C40—O1 | 1.462 (5) |
| C13—N1 | 1.439 (5) | N1—Co1 | 2.047 (3) |
| C14—C15 | 1.394 (6) | N2—Co1 | 2.226 (3) |
| C14—C19 | 1.521 (6) | N3—Co2 | 1.973 (3) |
| C15—C16 | 1.382 (6) | N4—Co2 | 1.987 (4) |
| C16—C17 | 1.383 (6) | O1—Co1 | 2.184 (3) |
| C17—C18 | 1.393 (6) | Cl1—Co1 | 2.2602 (13) |
| C18—C22 | 1.513 (6) | Cl2—Co2 | 2.2687 (12) |
| C19—C20 | 1.532 (6) | Cl2—Co1 | 2.3241 (12) |
| C19—C21 | 1.538 (6) | Cl3—Co2 | 2.2212 (14) |
| C22—C24 | 1.524 (7) | | |
| **Bond Angles (°)** | | | |
| N1—C2—C3 | 115.3 (4) | C29—C28—C27 | 119.5 (4) |
| N1—C2—C1 | 124.5 (4) | C28—C29—C30 | 121.8 (5) |
| C3—C2—C1 | 120.2 (3) | C29—C30—C25 | 117.6 (4) |
| N2—C3—C4 | 122.5 (4) | C29—C30—C34 | 121.1 (4) |
| N2—C3—C2 | 115.0 (3) | C25—C30—C34 | 121.3 (4) |
| C4—C3—C2 | 122.5 (4) | C26—C31—C32 | 111.1 (4) |
| C5—C4—C3 | 119.0 (4) | C26—C31—C33 | 111.7 (4) |
| C4—C5—C6 | 119.8 (4) | C32—C31—C33 | 110.1 (4) |
| C5—C6—C8 | 125.1 (4) | C35—C34—C36 | 109.4 (4) |
| C5—C6—C7 | 117.6 (4) | C35—C34—C30 | 111.5 (4) |
| C8—C6—C7 | 117.3 (4) | C36—C34—C30 | 112.9 (4) |
| N2—C7—N3 | 116.6 (3) | O1—C37—C38 | 105.4 (4) |
| N2—C7—C6 | 121.8 (4) | C37—C38—C39 | 101.5 (4) |
| N3—C7—C6 | 121.6 (4) | C40—C39—C38 | 102.6 (4) |
| C9—C8—C6 | 120.3 (4) | O1—C40—C39 | 105.6 (4) |
| C8—C9—C10 | 120.0 (4) | C2—N1—C13 | 121.0 (4) |
| N3—C10—C9 | 120.7 (4) | C2—N1—Co1 | 116.1 (3) |
| N3—C10—C11 | 114.7 (3) | C13—N1—Co1 | 123.0 (2) |
| C9—C10—C11 | 124.6 (4) | C7—N2—C3 | 118.9 (3) |
| N4—C11—C10 | 115.6 (4) | C7—N2—Co1 | 125.2 (3) |
| N4—C11—C12 | 123.7 (4) | C3—N2—Co1 | 105.4 (3) |
| C10—C11—C12 | 120.7 (4) | C7—N3—C10 | 119.3 (3) |
| C14—C13—C18 | 123.1 (4) | C7—N3—Co2 | 128.3 (3) |
| C14—C13—N1 | 121.1 (4) | C10—N3—Co2 | 111.8 (3) |
| C18—C13—N1 | 115.6 (4) | C11—N4—C25 | 120.2 (4) |
| C15—C14—C13 | 117.0 (4) | C11—N4—Co2 | 113.0 (3) |
| C15—C14—C19 | 120.8 (4) | C25—N4—Co2 | 126.8 (3) |
| C13—C14—C19 | 122.2 (4) | C37—O1—C40 | 108.9 (3) |
| C16—C15—C14 | 121.2 (4) | C37—O1—Co1 | 123.7 (3) |
| C15—C16—C17 | 120.5 (4) | C40—O1—Co1 | 113.8 (2) |
| C16—C17—C18 | 120.8 (4) | Co2—Cl2—Co1 | 100.64 (4) |
| C17—C18—C13 | 117.3 (4) | N1—Co1—O1 | 97.88 (12) |
| C17—C18—C22 | 122.0 (4) | N1—Co1—N2 | 75.74 (13) |
| C13—C18—C22 | 120.6 (4) | O1—Co1—N2 | 173.16 (12) |
| C14—C19—C20 | 110.1 (3) | N1—Co1—Cl1 | 112.75 (10) |
| C14—C19—C21 | 111.5 (4) | O1—Co1—Cl1 | 92.52 (9) |
| C20—C19—C21 | 110.8 (4) | N2—Co1—Cl1 | 87.79 (9) |
| C18—C22—C24 | 114.2 (4) | N1—Co1—Cl2 | 125.54 (11) |
| C18—C22—C23 | 110.7 (4) | O1—Co1—Cl2 | 83.97 (8) |
| C24—C22—C23 | 110.8 (4) | N2—Co1—Cl2 | 101.69 (9) |
| C26—C25—C30 | 121.7 (4) | Cl1—Co1—Cl2 | 121.57 (5) |
| C26—C25—N4 | 120.7 (4) | N3—Co2—N4 | 81.56 (14) |
| C30—C25—N4 | 117.6 (4) | N3—Co2—Cl3 | 122.26 (11) |
| C27—C26—C25 | 117.4 (4) | N4—Co2—Cl3 | 117.63 (11) |
| C27—C26—C31 | 120.1 (4) | N3—Co2—Cl2 | 110.03 (10) |
| C25—C26—C31 | 122.4 (4) | N4—Co2—Cl2 | 117.64 (10) |
| C28—C27—C26 | 121.8 (5) | Cl3—Co2—Cl2 | 106.60 (5) |

**Table 1b.** Bond lengths and angles for [$^{i\text{-}Pr}$NDI]$Fe_2$(THF)$Cl_3$ **(3)**.

| **Bond lengths (Å)** | | | |
|---|---|---|---|
| N1—C2 | 1.314 (6) | C11—C12 | 1.499 (7) |
| N1—C13 | 1.434 (6) | C13—C14 | 1.387 (7) |
| N1—Fe1 | 2.095 (4) | C13—C18 | 1.414 (6) |
| C1—C2 | 1.492 (6) | C14—C15 | 1.391 (7) |
| O1—C37 | 1.440 (6) | C14—C19 | 1.531 (6) |
| O1—C40 | 1.440 (6) | C15—C16 | 1.403 (6) |
| O1—Fe2 | 2.307 (3) | C16—C17 | 1.380 (7) |
| Cl1—Fe1 | 2.2958 (13) | C17—C18 | 1.387 (7) |
| Cl1—Fe2 | 2.4017 (14) | C18—C22 | 1.517 (7) |
| Fe1—N2 | 2.053 (4) | C19—C21 | 1.520 (7) |
| Fe1—Cl2 | 2.2324 (13) | C19—C20 | 1.537 (7) |
| N2—C7 | 1.339 (6) | C22—C24 | 1.526 (7) |
| N2—C3 | 1.367 (6) | C22—C23 | 1.535 (6) |
| C2—C3 | 1.455 (7) | C25—C26 | 1.397 (7) |
| Fe2—N4 | 2.095 (4) | C25—C30 | 1.410 (7) |
| Fe2—N3 | 2.194 (4) | C26—C27 | 1.395 (7) |
| Fe2—Cl3 | 2.2567 (14) | C26—C31 | 1.520 (7) |
| N3—C10 | 1.357 (6) | C27—C28 | 1.382 (7) |
| N3—C7 | 1.360 (6) | C28—C29 | 1.386 (8) |
| C3—C4 | 1.387 (6) | C29—C30 | 1.397 (7) |
| N4—C11 | 1.312 (6) | C30—C34 | 1.524 (7) |
| N4—C25 | 1.444 (6) | C31—C33 | 1.532 (8) |
| C4—C5 | 1.380 (7) | C31—C32 | 1.537 (8) |
| C5—C6 | 1.408 (7) | C34—C35 | 1.520 (7) |
| C6—C8 | 1.402 (7) | C34—C36 | 1.521 (7) |
| C6—C7 | 1.439 (6) | C37—C38 | 1.510 (7) |
| C8—C9 | 1.386 (7) | C38—C39 | 1.519 (8) |
| C9—C10 | 1.405 (6) | C39—C40 | 1.533 (8) |
| C10—C11 | 1.462 (6) | | |
| **Bond Angles (°)** | | | |
| C2—N1—C13 | 121.7 (4) | C8—C9—C10 | 119.4 (4) |
| C2—N1—Fe1 | 115.3 (3) | N3—C10—C9 | 122.1 (4) |
| C13—N1—Fe1 | 122.9 (3) | N3—C10—C11 | 115.1 (4) |
| C37—O1—C40 | 103.5 (4) | C9—C10—C11 | 122.8 (5) |
| C37—O1—Fe2 | 127.1 (3) | N4—C11—C10 | 115.5 (4) |
| C40—O1—Fe2 | 119.3 (3) | N4—C11—C12 | 124.3 (4) |
| Fe1—Cl1—Fe2 | 95.28 (5) | C10—C11—C12 | 120.2 (4) |
| N2—Fe1—N1 | 77.75 (15) | C14—C13—C18 | 121.7 (4) |
| N2—Fe1—Cl2 | 118.42 (11) | C14—C13—N1 | 121.1 (4) |
| N1—Fe1—Cl2 | 114.05 (11) | C18—C13—N1 | 117.1 (4) |
| N2—Fe1—Cl1 | 111.60 (11) | C13—C14—C15 | 118.6 (4) |
| N1—Fe1—Cl1 | 121.08 (10) | C13—C14—C19 | 122.9 (4) |
| Cl2—Fe1—Cl1 | 110.70 (5) | C15—C14—C19 | 118.5 (4) |
| C7—N2—C3 | 119.5 (4) | C14—C15—C16 | 120.6 (5) |
| C7—N2—Fe1 | 123.9 (3) | C17—C16—C15 | 119.6 (4) |
| C3—N2—Fe1 | 114.3 (3) | C16—C17—C18 | 121.4 (4) |
| N1—C2—C3 | 115.6 (4) | C17—C18—C13 | 118.0 (4) |
| N1—C2—C1 | 124.3 (4) | C17—C18—C22 | 121.5 (4) |
| C3—C2—C1 | 120.1 (4) | C13—C18—C22 | 120.4 (4) |
| N4—Fe2—N3 | 75.40 (15) | C21—C19—C14 | 111.8 (4) |
| N4—Fe2—Cl3 | 119.93 (12) | C21—C19—C20 | 110.1 (4) |
| N3—Fe2—Cl3 | 94.82 (11) | C14—C19—C20 | 110.8 (4) |
| N4—Fe2—O1 | 92.32 (14) | C18—C22—C24 | 110.4 (4) |
| N3—Fe2—O1 | 167.70 (14) | C18—C22—C23 | 113.6 (4) |
| Cl3—Fe2—O1 | 92.03 (9) | C24—C22—C23 | 110.3 (4) |
| N4—Fe2—Cl1 | 124.68 (12) | C26—C25—C30 | 122.2 (4) |
| N3—Fe2—Cl1 | 104.93 (11) | C26—C25—N4 | 120.8 (4) |
| Cl3—Fe2—Cl1 | 115.19 (5) | C30—C25—N4 | 116.9 (4) |
| O1—Fe2—Cl1 | 81.21 (10) | C27—C26—C25 | 117.7 (5) |
| C10—N3—C7 | 118.9 (4) | C27—C26—C31 | 119.3 (5) |
| C10—N3—Fe2 | 108.7 (3) | C25—C26—C31 | 123.0 (4) |
| C7—N3—Fe2 | 125.5 (3) | C28—C27—C26 | 121.1 (5) |
| N2—C3—C4 | 121.5 (4) | C27—C28—C29 | 120.7 (5) |
| N2—C3—C2 | 114.9 (4) | C28—C29—C30 | 120.3 (5) |
| C4—C3—C2 | 123.4 (4) | C29—C30—C25 | 118.0 (5) |
| C11—N4—C25 | 120.5 (4) | C29—C30—C34 | 121.4 (5) |
| C11—N4—Fe2 | 116.1 (3) | C25—C30—C34 | 120.5 (4) |
| C25—N4—Fe2 | 123.4 (3) | C26—C31—C33 | 111.0 (5) |
| C5—C4—C3 | 119.9 (4) | C26—C31—C32 | 110.9 (4) |
| C4—C5—C6 | 119.8 (4) | C33—C31—C32 | 110.2 (5) |
| C8—C6—C5 | 124.9 (4) | C35—C34—C36 | 110.1 (5) |
| C8—C6—C7 | 117.9 (4) | C35—C34—C30 | 112.3 (4) |
| C5—C6—C7 | 117.2 (4) | C36—C34—C30 | 113.5 (4) |
| N2—C7—N3 | 117.1 (4) | O1—C37—C38 | 106.2 (5) |
| N2—C7—C6 | 121.6 (4) | C37—C38—C39 | 103.2 (4) |
| N3—C7—C6 | 121.3 (4) | C38—C39—C40 | 105.1 (4) |
| C9—C8—C6 | 119.7 (4) | O1—C40—C39 | 104.7 (5) |

**Table 1c.** Bond lengths and angles for [$^{i\text{-}Pr}$NDI]$Co_2(C_6H_6)$ **(6)**.

| **Bond lengths (Å)** | | | |
|---|---|---|---|
| C1—C2 | 1.504 (2) | C25—C30 | 1.4132 (19) |
| C2—N1 | 1.3417 (19) | C25—N4 | 1.4351 (18) |
| C2—C3 | 1.413 (2) | C26—C27 | 1.399 (2) |
| C3—N2 | 1.3744 (17) | C26—C31 | 1.523 (2) |
| C3—C4 | 1.416 (2) | C27—C28 | 1.387 (2) |
| C4—C5 | 1.371 (2) | C28—C29 | 1.385 (2) |
| C5—C6 | 1.4206 (19) | C29—C30 | 1.3959 (19) |
| C6—C7 | 1.4154 (19) | C30—C34 | 1.521 (2) |
| C6—C8 | 1.418 (2) | C31—C33 | 1.530 (3) |
| C7—N2 | 1.3546 (18) | C31—C32 | 1.531 (3) |
| C7—N3 | 1.3547 (17) | C34—C36 | 1.535 (2) |
| C8—C9 | 1.3708 (19) | C34—C35 | 1.537 (2) |
| C9—C10 | 1.4178 (19) | C37—C38 | 1.407 (3) |
| C10—N3 | 1.3758 (18) | C37—C42 | 1.429 (3) |
| C10—C11 | 1.4148 (19) | C37—Co1 | 2.0127 (15) |
| C11—N4 | 1.3378 (19) | C38—C39 | 1.420 (3) |
| C11—C12 | 1.498 (2) | C38—Co1 | 2.0119 (16) |
| C13—C18 | 1.406 (3) | C39—C40 | 1.429 (2) |
| C13—C14 | 1.407 (2) | C39—Co1 | 2.4380 (17) |
| C13—N1 | 1.433 (2) | C39—Co2 | 2.4564 (17) |
| C14—C15 | 1.398 (3) | C40—C41 | 1.406 (3) |
| C14—C19 | 1.506 (3) | C40—Co2 | 2.0139 (16) |
| C15—C16 | 1.369 (4) | C41—C42 | 1.420 (3) |
| C16—C17 | 1.383 (4) | C41—Co2 | 2.0089 (16) |
| C17—C18 | 1.398 (3) | C42—Co2 | 2.4231 (17) |
| C18—C22 | 1.521 (3) | C42—Co1 | 2.4441 (17) |
| C19—C21 | 1.533 (4) | N1—Co1 | 1.9362 (12) |
| C19—C20 | 1.537 (4) | N2—Co1 | 1.8946 (12) |
| C22—C23 | 1.532 (3) | N3—Co2 | 1.8980 (12) |
| C22—C24 | 1.538 (3) | N4—Co2 | 1.9446 (12) |
| C25—C26 | 1.411 (2) | Co1—Co2 | 2.4072 (3) |
| **Bond Angles (°)** | | | |
| N1—C2—C3 | 113.23 (12) | C40—C39—Co2 | 55.06 (8) |
| N1—C2—C1 | 124.48 (13) | Co1—C39—Co2 | 58.92 (4) |
| C3—C2—C1 | 122.29 (13) | C41—C40—C39 | 117.78 (16) |
| N2—C3—C2 | 112.95 (12) | C41—C40—Co2 | 69.36 (10) |
| N2—C3—C4 | 121.21 (13) | C39—C40—Co2 | 89.36 (10) |
| C2—C3—C4 | 125.82 (13) | C40—C41—C42 | 117.82 (15) |
| C5—C4—C3 | 120.08 (13) | C40—C41—Co2 | 69.73 (9) |
| C4—C5—C6 | 119.56 (13) | C42—C41—Co2 | 88.19 (10) |
| C7—C6—C8 | 117.87 (12) | C41—C42—C37 | 119.87 (18) |
| C7—C6—C5 | 117.59 (12) | C41—C42—Co2 | 55.96 (9) |
| C8—C6—C5 | 124.54 (13) | C37—C42—Co2 | 107.07 (11) |
| N2—C7—N3 | 114.17 (12) | C41—C42—Co1 | 106.92 (11) |
| N2—C7—C6 | 123.08 (12) | C37—C42—Co1 | 55.42 (8) |
| N3—C7—C6 | 122.76 (12) | Co2—C42—Co1 | 59.28 (4) |
| C9—C8—C6 | 119.64 (13) | C2—N1—C13 | 118.48 (12) |
| C8—C9—C10 | 119.92 (13) | C2—N1—Co1 | 116.48 (10) |
| N3—C10—C11 | 112.98 (12) | C13—N1—Co1 | 124.91 (10) |
| N3—C10—C9 | 121.16 (12) | C7—N2—C3 | 118.44 (12) |
| C11—C10—C9 | 125.85 (13) | C7—N2—Co1 | 124.79 (9) |
| N4—C11—C10 | 113.73 (12) | C3—N2—Co1 | 116.72 (9) |
| N4—C11—C12 | 124.19 (13) | C7—N3—C10 | 118.61 (12) |
| C10—C11—C12 | 122.05 (13) | C7—N3—Co2 | 124.99 (10) |
| C18—C13—C14 | 121.74 (15) | C10—N3—Co2 | 116.40 (9) |
| C18—C13—N1 | 119.41 (15) | C11—N4—C25 | 117.27 (12) |
| C14—C13—N1 | 118.82 (16) | C11—N4—Co2 | 115.97 (9) |
| C15—C14—C13 | 117.7 (2) | C25—N4—Co2 | 126.76 (10) |
| C15—C14—C19 | 119.77 (19) | N2—Co1—N1 | 80.61 (5) |
| C13—C14—C19 | 122.45 (16) | N2—Co1—C38 | 158.63 (7) |
| C16—C15—C14 | 121.4 (2) | N1—Co1—C38 | 99.54 (6) |
| C15—C16—C17 | 120.25 (18) | N2—Co1—C37 | 160.40 (7) |
| C16—C17—C18 | 121.2 (2) | N1—Co1—C37 | 99.94 (6) |
| C17—C18—C13 | 117.62 (19) | C38—Co1—C37 | 40.92 (8) |
| C17—C18—C22 | 119.98 (18) | N2—Co1—Co2 | 88.13 (4) |
| C13—C18—C22 | 122.33 (15) | N1—Co1—Co2 | 168.74 (4) |
| C14—C19—C21 | 110.4 (3) | C38—Co1—Co2 | 91.01 (5) |
| C14—C19—C20 | 112.7 (2) | C37—Co1—Co2 | 90.60 (5) |
| C21—C19—C20 | 108.3 (2) | N2—Co1—C39 | 129.81 (5) |
| C18—C22—C23 | 110.72 (19) | N1—Co1—C39 | 127.35 (6) |
| C18—C22—C24 | 113.32 (17) | C38—Co1—C39 | 35.63 (7) |
| C23—C22—C24 | 109.51 (19) | C37—Co1—C39 | 65.14 (7) |
| C26—C25—C30 | 120.78 (13) | Co2—Co1—C39 | 60.92 (4) |
| C26—C25—N4 | 119.22 (12) | N2—Co1—C42 | 131.07 (6) |
| C30—C25—N4 | 120.00 (13) | N1—Co1—C42 | 128.41 (6) |
| C27—C26—C25 | 118.41 (13) | C38—Co1—C42 | 65.12 (7) |
| C27—C26—C31 | 119.01 (14) | C37—Co1—C42 | 35.77 (7) |
| C25—C26—C31 | 122.50 (13) | Co2—Co1—C42 | 59.92 (4) |
| C28—C27—C26 | 121.20 (14) | C39—Co1—C42 | 68.13 (6) |

| | | | |
|---|---|---|---|
| C29—C28—C27 | 119.84 (13) | N3—Co2—N4 | 80.80 (5) |
| C28—C29—C30 | 121.27 (14) | N3—Co2—C41 | 158.89 (7) |
| C29—C30—C25 | 118.49 (13) | N4—Co2—C41 | 99.88 (6) |
| C29—C30—C34 | 118.81 (13) | N3—Co2—C40 | 160.13 (7) |
| C25—C30—C34 | 122.67 (12) | N4—Co2—C40 | 99.73 (6) |
| C26—C31—C33 | 110.06 (14) | C41—Co2—C40 | 40.91 (8) |
| C26—C31—C32 | 112.55 (14) | N3—Co2—Co1 | 87.81 (4) |
| C33—C31—C32 | 109.71 (15) | N4—Co2—Co1 | 168.58 (4) |
| C30—C34—C36 | 111.12 (13) | C41—Co2—Co1 | 91.06 (5) |
| C30—C34—C35 | 112.21 (14) | C40—Co2—Co1 | 90.68 (5) |
| C36—C34—C35 | 108.44 (13) | N3—Co2—C42 | 129.62 (6) |

| | | | |
|---|---|---|---|
| C38—C37—C42 | 117.61 (16) | N4—Co2—C42 | 128.08 (6) |
| C38—C37—Co1 | 69.51 (9) | C41—Co2—C42 | 35.85 (7) |
| C42—C37—Co1 | 88.81 (10) | C40—Co2—C42 | 65.34 (7) |
| C37—C38—C39 | 117.95 (15) | Co1—Co2—C42 | 60.79 (4) |
| C37—C38—Co1 | 69.57 (9) | N3—Co2—C39 | 130.89 (5) |
| C39—C38—Co1 | 88.78 (10) | N4—Co2—C39 | 127.78 (6) |
| C38—C39—C40 | 119.90 (16) | C41—Co2—C39 | 64.96 (7) |
| C38—C39—Co1 | 55.60 (9) | C40—Co2—C39 | 35.58 (6) |
| C40—C39—Co1 | 106.50 (11) | Co1—Co2—C39 | 60.16 (4) |
| C38—C39—Co2 | 106.32 (12) | C42—Co2—C39 | 68.17 (6) |

**Table 1d.** Bond lengths and angles for [$^{i\text{-}Pr}$NDI]$Fe_2(C_6H_6)$ **(7)**.

| **Bond lengths (Å)** | | | |
|---|---|---|---|
| C1—C2 | 1.496 (3) | C26—C27 | 1.387 (5) |
| C2—N1 | 1.337 (3) | C26—C31 | 1.510 (5) |
| C2—C3 | 1.417 (3) | C27—C28 | 1.362 (6) |
| C3—N2 | 1.389 (3) | C28—C29 | 1.375 (6) |
| C3—C4 | 1.404 (3) | C29—C30 | 1.393 (4) |
| C4—C5 | 1.378 (3) | C30—C34 | 1.513 (5) |
| C5—C6 | 1.409 (3) | C31—C32 | 1.520 (6) |
| C6—C8 | 1.413 (3) | C31—C33 | 1.526 (6) |
| C6—C7 | 1.427 (3) | C34—C36 | 1.536 (5) |
| C7—N3 | 1.342 (3) | C34—C35 | 1.542 (5) |
| C7—N2 | 1.349 (3) | C37—C38 | 1.424 (4) |
| C8—C9 | 1.379 (4) | C37—C42 | 1.425 (4) |
| C9—C10 | 1.401 (3) | C37—Fe1 | 2.456 (3) |
| C10—N3 | 1.390 (3) | C37—Fe2 | 2.461 (3) |
| C10—C11 | 1.405 (4) | C38—C39 | 1.404 (5) |
| C11—N4 | 1.334 (3) | C38—Fe1 | 2.046 (3) |
| C11—C12 | 1.511 (4) | C39—C40 | 1.419 (5) |
| C13—C18 | 1.405 (3) | C39—Fe1 | 2.037 (3) |
| C13—C14 | 1.417 (4) | C40—C41 | 1.430 (5) |
| C13—N1 | 1.435 (3) | C40—Fe1 | 2.438 (3) |
| C14—C15 | 1.392 (4) | C40—Fe2 | 2.443 (3) |
| C14—C19 | 1.522 (4) | C41—C42 | 1.404 (5) |
| C15—C16 | 1.383 (4) | C41—Fe2 | 2.039 (3) |
| C16—C17 | 1.383 (4) | C42—Fe2 | 2.043 (3) |
| C17—C18 | 1.393 (3) | C43—C44 | 1.54 (3) |
| C18—C22 | 1.525 (4) | C44—C45 | 1.40 (2) |
| C19—C21 | 1.522 (4) | C45—C46 | 1.51 (2) |
| C19—C20 | 1.532 (4) | C46—C47 | 1.489 (19) |
| C22—C24 | 1.533 (4) | N1—Fe1 | 2.048 (2) |
| C22—C23 | 1.538 (4) | N2—Fe1 | 1.944 (2) |
| C25—C30 | 1.403 (4) | N3—Fe2 | 1.941 (2) |
| C25—C26 | 1.411 (4) | N4—Fe2 | 2.039 (2) |
| C25—N4 | 1.436 (3) | Fe1—Fe2 | 2.2818 (5) |
| **Bond Angles (°)** | | | |
| N1—C2—C3 | 114.8 (2) | C39—C40—C41 | 120.1 (3) |
| N1—C2—C1 | 123.4 (2) | C39—C40—Fe1 | 56.62 (16) |
| C3—C2—C1 | 121.8 (2) | C41—C40—Fe1 | 105.0 (2) |
| N2—C3—C4 | 120.1 (2) | C39—C40—Fe2 | 105.1 (2) |
| N2—C3—C2 | 113.5 (2) | C41—C40—Fe2 | 56.51 (15) |
| C4—C3—C2 | 126.4 (2) | Fe1—C40—Fe2 | 55.74 (7) |
| C5—C4—C3 | 120.6 (2) | C42—C41—C40 | 117.9 (3) |
| C4—C5—C6 | 120.1 (2) | C42—C41—Fe2 | 70.01 (16) |
| C5—C6—C8 | 125.7 (2) | C40—C41—Fe2 | 87.70 (18) |
| C5—C6—C7 | 117.3 (2) | C41—C42—C37 | 117.9 (3) |
| C8—C6—C7 | 117.0 (2) | C41—C42—Fe2 | 69.74 (16) |
| N3—C7—N2 | 114.5 (2) | C37—C42—Fe2 | 88.53 (17) |
| N3—C7—C6 | 123.0 (2) | C45—C44—C43 | 114.6 (18) |
| N2—C7—C6 | 122.5 (2) | C44—C45—C46 | 107.0 (14) |
| C9—C8—C6 | 119.8 (2) | C47—C46—C45 | 108.4 (13) |
| C8—C9—C10 | 120.9 (2) | C2—N1—C13 | 118.0 (2) |
| N3—C10—C9 | 119.9 (2) | C2—N1—Fe1 | 115.31 (16) |
| N3—C10—C11 | 113.2 (2) | C13—N1—Fe1 | 126.66 (16) |
| C9—C10—C11 | 126.9 (2) | C7—N2—C3 | 119.4 (2) |
| N4—C11—C10 | 115.1 (2) | C7—N2—Fe1 | 123.11 (16) |
| N4—C11—C12 | 123.3 (2) | C3—N2—Fe1 | 117.45 (16) |
| C10—C11—C12 | 121.5 (2) | C7—N3—C10 | 119.4 (2) |
| C18—C13—C14 | 120.6 (2) | C7—N3—Fe2 | 122.83 (16) |
| C18—C13—N1 | 120.4 (2) | C10—N3—Fe2 | 117.70 (16) |
| C14—C13—N1 | 118.9 (2) | C11—N4—C25 | 119.7 (2) |
| C15—C14—C13 | 118.3 (2) | C11—N4—Fe2 | 115.49 (17) |
| C15—C14—C19 | 119.2 (2) | C25—N4—Fe2 | 124.63 (17) |
| C13—C14—C19 | 122.4 (2) | N2—Fe1—C39 | 159.54 (12) |
| C16—C15—C14 | 121.2 (3) | N2—Fe1—C38 | 159.98 (12) |
| C17—C16—C15 | 120.0 (2) | C39—Fe1—C38 | 40.22 (13) |
| C16—C17—C18 | 121.1 (2) | N2—Fe1—N1 | 78.74 (8) |
| C17—C18—C13 | 118.7 (2) | C39—Fe1—N1 | 98.90 (10) |
| C17—C18—C22 | 118.6 (2) | C38—Fe1—N1 | 97.90 (10) |
| C13—C18—C22 | 122.7 (2) | N2—Fe1—Fe2 | 89.43 (6) |
| C14—C19—C21 | 110.2 (2) | C39—Fe1—Fe2 | 92.64 (9) |
| C14—C19—C20 | 112.5 (2) | C38—Fe1—Fe2 | 92.79 (9) |
| C21—C19—C20 | 109.9 (3) | N1—Fe1—Fe2 | 168.10 (6) |
| C18—C22—C24 | 112.0 (2) | N2—Fe1—C40 | 132.68 (10) |
| C18—C22—C23 | 111.2 (2) | C39—Fe1—C40 | 35.55 (12) |
| C24—C22—C23 | 108.6 (2) | C38—Fe1—C40 | 64.73 (13) |
| C30—C25—C26 | 121.9 (3) | N1—Fe1—C40 | 127.46 (10) |
| C30—C25—N4 | 119.4 (3) | Fe2—Fe1—C40 | 62.24 (8) |
| C26—C25—N4 | 118.5 (3) | N2—Fe1—C37 | 133.26 (9) |
| C27—C26—C25 | 117.3 (3) | C39—Fe1—C37 | 64.45 (12) |
| C27—C26—C31 | 120.0 (3) | C38—Fe1—C37 | 35.43 (11) |

| | | | |
|---|---|---|---|
| C25—C26—C31 | 122.7 (3) | N1—Fe1—C37 | 125.56 (10) |
| C28—C27—C26 | 121.8 (4) | Fe2—Fe1—C37 | 62.45 (7) |
| C27—C28—C29 | 120.4 (3) | C40—Fe1—C37 | 68.12 (11) |
| C28—C29—C30 | 121.3 (4) | N3—Fe2—N4 | 78.51 (9) |
| C29—C30—C25 | 117.3 (3) | N3—Fe2—C41 | 161.85 (12) |
| C29—C30—C34 | 120.6 (3) | N4—Fe2—C41 | 98.28 (11) |
| C25—C30—C34 | 122.1 (3) | N3—Fe2—C42 | 157.54 (12) |
| C26—C31—C32 | 113.0 (3) | N4—Fe2—C42 | 98.09 (10) |
| C26—C31—C33 | 110.5 (4) | C41—Fe2—C42 | 40.25 (13) |
| C32—C31—C33 | 108.3 (3) | N3—Fe2—Fe1 | 89.98 (6) |
| C30—C34—C36 | 113.8 (3) | N4—Fe2—Fe1 | 168.49 (6) |
| C30—C34—C35 | 110.4 (3) | C41—Fe2—Fe1 | 92.62 (9) |
| C36—C34—C35 | 109.0 (3) | C42—Fe2—Fe1 | 92.61 (8) |

| | | | |
|---|---|---|---|
| C38—C37—C42 | 120.5 (3) | N3—Fe2—C40 | 134.64 (10) |
| C38—C37—Fe1 | 56.37 (15) | N4—Fe2—C40 | 126.77 (10) |
| C42—C37—Fe1 | 104.4 (2) | C41—Fe2—C40 | 35.79 (12) |
| C38—C37—Fe2 | 104.6 (2) | C42—Fe2—C40 | 64.84 (12) |
| C42—C37—Fe2 | 56.09 (15) | Fe1—Fe2—C40 | 62.02 (8) |
| Fe1—C37—Fe2 | 55.31 (6) | N3—Fe2—C37 | 131.76 (10) |
| C39—C38—C37 | 117.8 (3) | N4—Fe2—C37 | 126.21 (10) |
| C39—C38—Fe1 | 69.57 (17) | C41—Fe2—C37 | 64.40 (12) |
| C37—C38—Fe1 | 88.20 (18) | C42—Fe2—C37 | 35.38 (11) |
| C38—C39—C40 | 118.3 (3) | Fe1—Fe2—C37 | 62.24 (7) |
| C38—C39—Fe1 | 70.21 (16) | C40—Fe2—C37 | 67.97 (11) |
| C40—C39—Fe1 | 87.83 (18) | | |

**Table 1e.** Bond lengths and angles for [$^{i\text{-}Pr}$NDI]Ni$_2$(allyl)Cl **(8)**.

| **Bond lengths (Å)** | | | |
|---|---|---|---|
| Ni1—N1 | 1.923 (3) | C16—C17 | 1.406 (5) |
| Ni1—N11 | 1.926 (3) | C21—C22 | 1.388 (5) |
| Ni1—C1 | 1.974 (4) | C21—C26 | 1.390 (5) |
| Ni1—C2 | 2.325 (4) | C22—C23 | 1.387 (5) |
| Ni1—Ni2 | 2.4569 (9) | C22—C222 | 1.525 (6) |
| Ni1—Cl1 | 2.4840 (11) | C23—C24 | 1.381 (5) |
| Ni2—N2 | 1.925 (3) | C24—C25 | 1.367 (5) |
| Ni2—N17 | 1.931 (3) | C25—C26 | 1.386 (5) |
| Ni2—C3 | 1.973 (4) | C26—C262 | 1.519 (5) |
| Ni2—C2 | 2.307 (4) | C31—C323 | 1.402 (5) |
| Ni2—Cl1 | 2.4425 (12) | C31—C36 | 1.403 (5) |
| N1—C7 | 1.316 (4) | C33—C34 | 1.380 (6) |
| N1—C21 | 1.447 (4) | C33—C323 | 1.400 (6) |
| N2—C8 | 1.319 (4) | C34—C35 | 1.370 (6) |
| N2—C31 | 1.440 (5) | C35—C36 | 1.394 (6) |
| N11—C4 | 1.355 (4) | C36—C362 | 1.520 (6) |
| N11—C11 | 1.355 (4) | C221—C222 | 1.518 (6) |
| N17—C4 | 1.344 (4) | C222—C223 | 1.519 (6) |
| N17—C17 | 1.362 (4) | C261—C262 | 1.527 (6) |
| C1—C2 | 1.418 (6) | C262—C263 | 1.518 (5) |
| C2—C3 | 1.421 (6) | C321—C322 | 1.515 (6) |
| C4—C14 | 1.415 (5) | C322—C999 | 1.506 (6) |
| C7—C11 | 1.437 (5) | C322—C323 | 1.509 (6) |
| C7—C71 | 1.498 (5) | C361—C362 | 1.546 (6) |
| C8—C17 | 1.442 (5) | C362—C363 | 1.521 (6) |
| C8—C81 | 1.501 (5) | C1—H1B | 0.97 (4) |
| C11—C12 | 1.416 (5) | C1—H1A | 1.05 (3) |
| C12—C13 | 1.365 (5) | C2—H2 | 0.88 (3) |
| C13—C14 | 1.416 (5) | C3—H3B | 1.00 (4) |
| C14—C15 | 1.409 (5) | C3—H3A | 1.03 (4) |
| C15—C16 | 1.367 (5) | | |
| **Bond Angles (°)** | | | |
| N1—Ni1—N11 | 81.34 (13) | C12—C11—C7 | 125.7 (4) |
| N1—Ni1—C1 | 100.58 (16) | C13—C12—C11 | 120.1 (4) |
| N11—Ni1—C1 | 162.83 (18) | C12—C13—C14 | 119.6 (4) |
| N1—Ni1—C2 | 132.55 (14) | C15—C14—C4 | 117.3 (4) |
| N11—Ni1—C2 | 131.54 (15) | C15—C14—C13 | 125.2 (4) |
| C1—Ni1—C2 | 37.41 (16) | C4—C14—C13 | 117.5 (4) |
| N1—Ni1—Ni2 | 168.11 (10) | C16—C15—C14 | 119.5 (4) |
| N11—Ni1—Ni2 | 86.83 (9) | C15—C16—C17 | 120.5 (4) |
| C1—Ni1—Ni2 | 91.07 (14) | N17—C17—C16 | 120.8 (4) |
| C2—Ni1—Ni2 | 57.61 (10) | N17—C17—C8 | 112.6 (3) |
| N1—Ni1—Cl1 | 121.32 (10) | C16—C17—C8 | 126.7 (4) |
| N11—Ni1—Cl1 | 98.64 (9) | C22—C21—C26 | 122.4 (4) |
| C1—Ni1—Cl1 | 94.88 (15) | C22—C21—N1 | 119.2 (4) |
| C2—Ni1—Cl1 | 90.38 (12) | C26—C21—N1 | 118.4 (3) |
| Ni2—Ni1—Cl1 | 59.25 (3) | C23—C22—C21 | 117.7 (4) |
| N2—Ni2—N17 | 80.69 (13) | C23—C22—C222 | 119.9 (4) |
| N2—Ni2—C3 | 99.47 (17) | C21—C22—C222 | 122.4 (4) |
| N17—Ni2—C3 | 163.26 (18) | C24—C23—C22 | 121.1 (4) |
| N2—Ni2—C2 | 127.04 (15) | C25—C24—C23 | 119.6 (4) |
| N17—Ni2—C2 | 130.47 (15) | C24—C25—C26 | 121.7 (4) |
| C3—Ni2—C2 | 37.77 (16) | C25—C26—C21 | 117.4 (4) |
| N2—Ni2—Cl1 | 126.69 (10) | C25—C26—C262 | 120.2 (4) |
| N17—Ni2—Cl1 | 101.74 (10) | C21—C26—C262 | 122.3 (4) |
| C3—Ni2—Cl1 | 91.62 (16) | C323—C31—C36 | 123.1 (4) |
| C2—Ni2—Cl1 | 91.86 (13) | C323—C31—N2 | 117.5 (4) |
| N2—Ni2—Ni1 | 166.97 (10) | C36—C31—N2 | 119.2 (4) |
| N17—Ni2—Ni1 | 87.42 (9) | C34—C33—C323 | 121.4 (4) |
| C3—Ni2—Ni1 | 90.37 (14) | C35—C34—C33 | 120.1 (4) |
| C2—Ni2—Ni1 | 58.32 (11) | C34—C35—C36 | 121.9 (4) |
| Cl1—Ni2—Ni1 | 60.93 (3) | C35—C36—C31 | 116.7 (4) |
| Ni2—Cl1—Ni1 | 59.82 (3) | C35—C36—C362 | 121.0 (4) |
| C7—N1—C21 | 118.9 (3) | C31—C36—C362 | 122.2 (4) |
| C7—N1—Ni1 | 116.0 (3) | C221—C222—C223 | 110.0 (4) |
| C21—N1—Ni1 | 124.7 (2) | C221—C222—C22 | 111.5 (4) |
| C8—N2—C31 | 119.8 (3) | C223—C222—C22 | 112.3 (4) |
| C8—N2—Ni2 | 117.1 (3) | C263—C262—C26 | 112.2 (4) |
| C31—N2—Ni2 | 123.1 (2) | C263—C262—C261 | 110.8 (4) |
| C4—N11—C11 | 118.8 (3) | C26—C262—C261 | 111.0 (3) |
| C4—N11—Ni1 | 126.0 (3) | C999—C322—C323 | 111.9 (4) |
| C11—N11—Ni1 | 115.1 (2) | C999—C322—C321 | 110.2 (4) |
| C4—N17—C17 | 118.9 (3) | C323—C322—C321 | 113.5 (4) |
| C4—N17—Ni2 | 125.3 (2) | C33—C323—C31 | 116.7 (4) |
| C17—N17—Ni2 | 115.7 (3) | C33—C323—C322 | 121.8 (4) |
| C2—C1—Ni1 | 84.9 (3) | C31—C323—C322 | 121.5 (4) |
| C1—C2—C3 | 124.2 (5) | C36—C362—C363 | 111.7 (4) |
| C1—C2—Ni2 | 115.1 (3) | C36—C362—C361 | 110.9 (4) |
| C3—C2—Ni2 | 58.3 (2) | C363—C362—C361 | 109.8 (4) |

| | | | |
|---|---|---|---|
| C1—C2—Ni1 | 57.7 (2) | Ni1—C1—H1B | 104 (2) |
| C3—C2—Ni1 | 112.9 (3) | Ni1—C1—H1A | 103.3 (19) |
| Ni2—C2—Ni1 | 64.07 (10) | H1A—C1—H1B | 119 (3) |
| C2—C3—Ni2 | 84.0 (3) | C2—C1—H1B | 119 (3) |
| N17—C4—N11 | 114.2 (3) | C2—C1—H1A | 116.4 (19) |
| N17—C4—C14 | 123.1 (3) | Ni1—C2—H2 | 105 (2) |
| N11—C4—C14 | 122.7 (4) | Ni2—C2—H2 | 98 (2) |
| N1—C7—C11 | 114.2 (3) | C1—C2—H2 | 121 (2) |

| | | | |
|---|---|---|---|
| N1—C7—C71 | 124.8 (4) | C3—C2—H2 | 114 (2) |
| C11—C7—C71 | 121.0 (4) | Ni2—C3—H3B | 107 (2) |
| N2—C8—C17 | 113.8 (3) | Ni2—C3—H3A | 105 (2) |
| N2—C8—C81 | 125.1 (4) | H3A—C3—H3B | 119 (3) |
| C17—C8—C81 | 121.1 (3) | C2—C3—H3B | 114 (2) |
| N11—C11—C12 | 121.3 (4) | C2—C3—H3A | 119 (2) |
| N11—C11—C7 | 113.0 (3) | | |

**Table 1f.** Bond lengths and angles for [$^{i\text{-}Pr}$NDI]$Co_2$(allyl)Cl **(9)**.

| **Bond lengths (Å)** | | | |
|---|---|---|---|
| Co1—N2 | 1.942 (4) | C13—C14 | 1.409 (7) |
| Co1—N1 | 1.943 (4) | C14—C15 | 1.392 (7) |
| Co1—C37 | 2.023 (5) | C14—C19 | 1.523 (7) |
| Co1—Cl3 | 2.3218 (13) | C15—C16 | 1.379 (8) |
| Co1—C38 | 2.477 (5) | C16—C17 | 1.391 (8) |
| Co1—Co2 | 2.6212 (10) | C17—C18 | 1.394 (7) |
| Co2—N3 | 1.928 (4) | C18—C22 | 1.518 (7) |
| Co2—N4 | 1.942 (4) | C19—C20 | 1.528 (8) |
| Co2—C39 | 2.025 (5) | C19—C21 | 1.543 (7) |
| Co2—Cl3 | 2.3179 (13) | C22—C24 | 1.525 (7) |
| Co2—C38 | 2.436 (5) | C22—C23 | 1.530 (7) |
| N1—C2 | 1.338 (6) | C25—C30 | 1.402 (6) |
| N1—C13 | 1.443 (6) | C25—C26 | 1.416 (6) |
| N2—C7 | 1.349 (6) | C26—C27 | 1.397 (7) |
| N2—C3 | 1.385 (6) | C26—C31 | 1.518 (6) |
| N3—C7 | 1.366 (6) | C27—C28 | 1.388 (7) |
| N3—C10 | 1.382 (6) | C28—C29 | 1.383 (7) |
| N4—C11 | 1.331 (6) | C29—C30 | 1.393 (7) |
| N4—C25 | 1.441 (6) | C30—C34 | 1.522 (6) |
| C1—C2 | 1.496 (6) | C31—C32 | 1.525 (7) |
| C2—C3 | 1.437 (7) | C31—C33 | 1.529 (7) |
| C3—C4 | 1.401 (7) | C34—C35 | 1.527 (7) |
| C4—C5 | 1.371 (7) | C34—C36 | 1.532 (7) |
| C5—C6 | 1.419 (6) | C37—C38 | 1.401 (7) |
| C6—C8 | 1.415 (6) | C38—C39 | 1.389 (7) |
| C6—C7 | 1.420 (7) | C37—H37B | 0.98 (3) |
| C8—C9 | 1.371 (7) | C37—H37A | 0.97 (3) |
| C9—C10 | 1.402 (7) | C38—H38 | 0.99 (5) |
| C10—C11 | 1.431 (6) | C39—H39B | 0.97 (3) |
| C11—C12 | 1.496 (6) | C39—H39A | 0.98 (3) |
| C13—C18 | 1.404 (7) | | |
| **Bond Angles (°)** | | | |
| N2—Co1—N1 | 82.64 (16) | N4—C11—C10 | 114.5 (4) |
| N2—Co1—C37 | 128.76 (19) | N4—C11—C12 | 123.9 (4) |
| N1—Co1—C37 | 107.96 (19) | C10—C11—C12 | 121.5 (4) |
| N2—Co1—Cl3 | 103.17 (12) | C18—C13—C14 | 121.0 (4) |
| N1—Co1—Cl3 | 117.59 (12) | C18—C13—N1 | 122.2 (4) |
| C37—Co1—Cl3 | 113.87 (16) | C14—C13—N1 | 116.7 (4) |
| N2—Co1—C38 | 106.09 (17) | C15—C14—C13 | 118.6 (5) |
| N1—Co1—C38 | 136.90 (17) | C15—C14—C19 | 119.9 (5) |
| C37—Co1—C38 | 34.44 (18) | C13—C14—C19 | 121.5 (5) |
| Cl3—Co1—C38 | 101.68 (13) | C16—C15—C14 | 120.9 (5) |
| N2—Co1—Co2 | 85.12 (11) | C15—C16—C17 | 120.1 (5) |
| N1—Co1—Co2 | 163.95 (12) | C16—C17—C18 | 121.0 (5) |
| C37—Co1—Co2 | 87.81 (15) | C17—C18—C13 | 118.3 (5) |
| Cl3—Co1—Co2 | 55.53 (3) | C17—C18—C22 | 118.9 (5) |
| C38—Co1—Co2 | 57.01 (12) | C13—C18—C22 | 122.8 (4) |
| N3—Co2—N4 | 82.35 (16) | C14—C19—C20 | 113.9 (5) |
| N3—Co2—C39 | 130.4 (2) | C14—C19—C21 | 111.3 (4) |
| N4—Co2—C39 | 106.04 (18) | C20—C19—C21 | 110.3 (4) |
| N3—Co2—Cl3 | 102.86 (11) | C18—C22—C24 | 111.9 (4) |
| N4—Co2—Cl3 | 118.24 (12) | C18—C22—C23 | 111.2 (4) |
| C39—Co2—Cl3 | 114.07 (16) | C24—C22—C23 | 110.3 (5) |
| N3—Co2—C38 | 107.10 (17) | C30—C25—C26 | 121.4 (4) |
| N4—Co2—C38 | 134.66 (16) | C30—C25—N4 | 120.9 (4) |
| C39—Co2—C38 | 34.77 (18) | C26—C25—N4 | 117.5 (4) |
| Cl3—Co2—C38 | 103.02 (12) | C27—C26—C25 | 117.8 (4) |
| N3—Co2—Co1 | 85.30 (11) | C27—C26—C31 | 120.5 (4) |
| N4—Co2—Co1 | 164.45 (12) | C25—C26—C31 | 121.6 (4) |
| C39—Co2—Co1 | 89.17 (15) | C28—C27—C26 | 121.0 (4) |
| Cl3—Co2—Co1 | 55.67 (4) | C29—C28—C27 | 120.2 (4) |
| C38—Co2—Co1 | 58.51 (12) | C28—C29—C30 | 121.1 (4) |
| Co2—Cl3—Co1 | 68.80 (4) | C29—C30—C25 | 118.4 (4) |
| C2—N1—C13 | 119.8 (4) | C29—C30—C34 | 118.9 (4) |
| C2—N1—Co1 | 114.3 (3) | C25—C30—C34 | 122.7 (4) |
| C13—N1—Co1 | 125.8 (3) | C26—C31—C32 | 114.8 (4) |
| C7—N2—C3 | 119.3 (4) | C26—C31—C33 | 109.2 (4) |
| C7—N2—Co1 | 126.9 (3) | C32—C31—C33 | 109.4 (4) |
| C3—N2—Co1 | 113.5 (3) | C30—C34—C35 | 112.0 (4) |
| C7—N3—C10 | 118.9 (4) | C30—C34—C36 | 111.8 (4) |
| C7—N3—Co2 | 127.0 (3) | C35—C34—C36 | 109.0 (4) |
| C10—N3—Co2 | 113.8 (3) | C38—C37—Co1 | 90.8 (3) |
| C11—N4—C25 | 122.2 (4) | C39—C38—C37 | 128.7 (5) |
| C11—N4—Co2 | 115.2 (3) | C39—C38—Co2 | 56.2 (3) |
| C25—N4—Co2 | 122.5 (3) | C37—C38—Co2 | 112.9 (3) |
| N1—C2—C3 | 115.2 (4) | C39—C38—Co1 | 113.6 (3) |
| N1—C2—C1 | 123.9 (4) | C37—C38—Co1 | 54.8 (3) |
| C3—C2—C1 | 120.9 (4) | Co2—C38—Co1 | 64.48 (12) |
| N2—C3—C4 | 120.8 (4) | C38—C39—Co2 | 89.0 (3) |

| | | | |
|---|---|---|---|
| N2—C3—C2 | 113.6 (4) | H37A—C37—H37B | 117 (5) |
| C4—C3—C2 | 125.3 (4) | Co1—C37—H37B | 102 (3) |
| C5—C4—C3 | 119.9 (4) | Co1—C37—H37A | 107 (3) |
| C4—C5—C6 | 120.2 (5) | C38—C37—H37B | 118 (3) |
| C8—C6—C5 | 125.1 (4) | C38—C37—H37A | 116 (3) |
| C8—C6—C7 | 117.4 (4) | Co1—C38—H38 | 103 (3) |
| C5—C6—C7 | 117.5 (4) | Co2—C38—H38 | 104 (3) |
| N2—C7—N3 | 115.7 (4) | C37—C38—H38 | 114 (3) |
| N2—C7—C6 | 122.1 (4) | C39—C38—H38 | 117 (3) |
| N3—C7—C6 | 122.2 (4) | H39A—C39—H39B | 108 (4) |
| C9—C8—C6 | 120.2 (5) | Co2—C39—H39B | 105 (3) |
| C8—C9—C10 | 120.3 (5) | Co2—C39—H39A | 107 (3) |
| N3—C10—C9 | 120.7 (4) | C38—C39—H39B | 118 (3) |
| N3—C10—C11 | 114.1 (4) | C38—C39—H39A | 124 (3) |
| C9—C10—C11 | 125.2 (4) | | |

**Table 1g.** Bond lengths and angles for [$^{i\text{-}Pr}$NDI]$Fe_2$(allyl)Cl **(10)**.

| **Bond lengths (Å)** | | | |
|---|---|---|---|
| Fe1—N51 | 1.975 (2) | C19—N50 | 1.431 (4) |
| Fe1—N50 | 2.020 (2) | C20—C21 | 1.389 (4) |
| Fe1—C42 | 2.045 (3) | C20—C46 | 1.516 (5) |
| Fe1—C41 | 2.357 (3) | C21—C22 | 1.384 (5) |
| Fe1—Cl3 | 2.3601 (8) | C22—C23 | 1.387 (5) |
| Fe1—Fe2 | 2.4086 (6) | C23—C24 | 1.389 (4) |
| Fe2—N52 | 1.989 (2) | C24—C25 | 1.524 (4) |
| Fe2—N53 | 2.037 (2) | C25—C26 | 1.529 (5) |
| Fe2—C40 | 2.040 (3) | C25—C27 | 1.529 (4) |
| Fe2—Cl3 | 2.3642 (8) | C28—N53 | 1.330 (3) |
| Fe2—C41 | 2.444 (3) | C28—C29 | 1.505 (4) |
| C2—C3 | 1.392 (4) | C31—C32 | 1.407 (4) |
| C2—N51 | 1.393 (4) | C31—C36 | 1.411 (4) |
| C2—C16 | 1.430 (4) | C31—N53 | 1.444 (3) |
| C4—C3 | 1.377 (4) | C32—C33 | 1.400 (4) |
| C4—C5 | 1.417 (4) | C32—C43 | 1.515 (4) |
| C5—C49 | 1.409 (4) | C33—C34 | 1.381 (4) |
| C5—C6 | 1.428 (4) | C34—C35 | 1.381 (4) |
| C6—N51 | 1.350 (4) | C35—C36 | 1.393 (4) |
| C6—N52 | 1.354 (4) | C36—C37 | 1.511 (4) |
| C8—N52 | 1.384 (4) | C37—C39 | 1.528 (4) |
| C8—C9 | 1.391 (4) | C37—C38 | 1.529 (4) |
| C8—C28 | 1.427 (4) | C40—C41 | 1.420 (4) |
| C9—C49 | 1.376 (4) | C41—C42 | 1.410 (5) |
| C10—C15 | 1.375 (5) | C43—C44 | 1.522 (4) |
| C10—C11 | 1.377 (5) | C43—C45 | 1.531 (4) |
| C11—C12 | 1.373 (6) | C46—C47 | 1.511 (5) |
| C12—C13 | 1.379 (5) | C46—C48 | 1.528 (5) |
| C13—C14 | 1.388 (5) | C40—H40B | 0.98 (2) |
| C14—C15 | 1.372 (5) | C40—H40A | 0.98 (2) |
| C16—N50 | 1.329 (4) | C41—H41 | 1.00 (3) |
| C16—C17 | 1.503 (4) | C42—H42B | 0.99 (2) |
| C19—C24 | 1.410 (4) | C42—H42A | 0.98 (2) |
| C19—C20 | 1.413 (4) | | |
| **Bond Angles (°)** | | | |
| N51—Fe1—N50 | 78.96 (10) | C19—C24—C25 | 122.6 (3) |
| N51—Fe1—C42 | 143.94 (12) | C24—C25—C26 | 113.0 (3) |
| N50—Fe1—C42 | 100.96 (11) | C24—C25—C27 | 111.0 (3) |
| N51—Fe1—C41 | 116.89 (11) | C26—C25—C27 | 109.3 (3) |
| N50—Fe1—C41 | 127.76 (10) | N53—C28—C8 | 116.3 (2) |
| C42—Fe1—C41 | 36.50 (12) | N53—C28—C29 | 123.6 (3) |
| N51—Fe1—Cl3 | 107.56 (7) | C8—C28—C29 | 120.1 (2) |
| N50—Fe1—Cl3 | 120.17 (7) | C32—C31—C36 | 121.0 (2) |
| C42—Fe1—Cl3 | 103.45 (10) | C32—C31—N53 | 118.1 (2) |
| C41—Fe1—Cl3 | 102.65 (8) | C36—C31—N53 | 120.9 (2) |
| N51—Fe1—Fe2 | 89.05 (7) | C33—C32—C31 | 117.9 (3) |
| N50—Fe1—Fe2 | 167.29 (7) | C33—C32—C43 | 118.9 (2) |
| C42—Fe1—Fe2 | 91.20 (9) | C31—C32—C43 | 123.2 (2) |
| C41—Fe1—Fe2 | 61.70 (8) | C34—C33—C32 | 121.7 (3) |
| Cl3—Fe1—Fe2 | 59.43 (2) | C33—C34—C35 | 119.5 (3) |
| N52—Fe2—N53 | 79.60 (9) | C34—C35—C36 | 121.4 (3) |
| N52—Fe2—C40 | 135.30 (11) | C35—C36—C31 | 118.3 (3) |
| N53—Fe2—C40 | 106.41 (11) | C35—C36—C37 | 118.8 (3) |
| N52—Fe2—Cl3 | 105.62 (8) | C31—C36—C37 | 122.8 (3) |
| N53—Fe2—Cl3 | 112.40 (7) | C36—C37—C39 | 112.1 (3) |
| C40—Fe2—Cl3 | 111.96 (9) | C36—C37—C38 | 110.4 (3) |
| N52—Fe2—Fe1 | 87.37 (7) | C39—C37—C38 | 110.6 (3) |
| N53—Fe2—Fe1 | 162.04 (7) | C41—C40—Fe2 | 87.99 (19) |
| C40—Fe2—Fe1 | 91.55 (9) | C42—C41—C40 | 126.8 (3) |
| Cl3—Fe2—Fe1 | 59.27 (2) | C42—C41—Fe1 | 59.61 (17) |
| N52—Fe2—C41 | 115.72 (10) | C40—C41—Fe1 | 113.4 (2) |
| N53—Fe2—C41 | 139.16 (11) | C42—C41—Fe2 | 108.8 (2) |
| C40—Fe2—C41 | 35.50 (11) | C40—C41—Fe2 | 56.51 (16) |
| Cl3—Fe2—C41 | 99.96 (8) | Fe1—C41—Fe2 | 60.18 (7) |
| Fe1—Fe2—C41 | 58.12 (8) | C41—C42—Fe1 | 83.89 (19) |
| C3—C2—N51 | 120.1 (3) | C32—C43—C44 | 112.4 (2) |
| C3—C2—C16 | 126.8 (3) | C32—C43—C45 | 109.8 (2) |
| N51—C2—C16 | 113.1 (2) | C44—C43—C45 | 111.0 (2) |
| Fe1—Cl3—Fe2 | 61.30 (2) | C47—C46—C20 | 113.9 (3) |
| C3—C4—C5 | 120.2 (3) | C47—C46—C48 | 109.9 (3) |
| C49—C5—C4 | 126.1 (3) | C20—C46—C48 | 111.0 (3) |
| C49—C5—C6 | 117.1 (3) | C9—C49—C5 | 119.9 (3) |
| C4—C5—C6 | 116.8 (3) | C16—N50—C19 | 121.5 (2) |
| N51—C6—N52 | 115.3 (2) | C16—N50—Fe1 | 116.45 (19) |
| N51—C6—C5 | 122.6 (3) | C19—N50—Fe1 | 121.75 (18) |
| N52—C6—C5 | 122.1 (3) | C6—N51—C2 | 119.3 (2) |
| N52—C8—C9 | 119.7 (3) | C6—N51—Fe1 | 123.60 (18) |
| N52—C8—C28 | 113.9 (2) | C2—N51—Fe1 | 116.41 (19) |
| C9—C8—C28 | 126.1 (3) | C6—N52—C8 | 119.7 (2) |

| | | | |
|---|---|---|---|
| C49—C9—C8 | 121.2 (3) | C6—N52—Fe2 | 124.60 (19) |
| C15—C10—C11 | 120.1 (4) | C8—N52—Fe2 | 115.27 (18) |
| C12—C11—C10 | 120.0 (3) | C28—N53—C31 | 119.1 (2) |
| C11—C12—C13 | 120.4 (4) | C28—N53—Fe2 | 114.43 (18) |
| C12—C13—C14 | 119.2 (4) | C31—N53—Fe2 | 126.51 (17) |
| C15—C14—C13 | 120.3 (3) | C4—C3—C2 | 120.8 (3) |
| C14—C15—C10 | 120.0 (3) | H40A—C40—H40B | 110 (3) |
| N50—C16—C2 | 115.0 (3) | Fe2—C40—H40B | 111 (2) |
| N50—C16—C17 | 123.0 (3) | Fe2—C40—H40A | 106 (2) |
| C2—C16—C17 | 121.8 (3) | C41—C40—H40B | 119 (2) |
| C24—C19—C20 | 121.2 (3) | C41—C40—H40A | 120 (2) |

| | | | |
|---|---|---|---|
| C24—C19—N50 | 120.3 (3) | Fe1—C41—H41 | 98 (2) |
| C20—C19—N50 | 118.3 (3) | Fe2—C41—H41 | 105 (2) |
| C21—C20—C19 | 118.0 (3) | C40—C41—H41 | 115 (2) |
| C21—C20—C46 | 121.4 (3) | C42—C41—H41 | 118 (2) |
| C19—C20—C46 | 120.6 (3) | H42A—C42—H42B | 118 (3) |
| C22—C21—C20 | 121.7 (3) | Fe1—C42—H42B | 106 (2) |
| C21—C22—C23 | 119.5 (3) | Fe1—C42—H42A | 106 (2) |
| C22—C23—C24 | 121.6 (3) | C41—C42—H42B | 116 (2) |
| C23—C24—C19 | 118.0 (3) | C41—C42—H42A | 119 (2) |
| C23—C24—C25 | 119.4 (3) | | |

**Table 2.** Crystal, Data Collection and Refinement Parameters.

| **Compound** | **(3)** | **(4)** | **(6)** |
|---|---|---|---|
| **Crystal data** | | | |
| **Chemical formula** | $C_{40}H_{52}Cl_3Co_2N_4O$ | $C_{40}H_{52}Cl_3Fe_2N_4O$ | $C_{42}H_{50}Co_2N_4$ |
| $M_r$ | 829.06 | 822.90 | 728.72 |
| **Crystal system, space group** | Monoclinic, $P2_1/c$ | Monoclinic, $P2_1/c$ | Trigonal, $R\bar{3}:H$ |
| **Temperature (K)** | 100 | 100 | 100 |
| ***a*, *b*, *c* (Å)** | 15.3397 (4), 16.7127 (8), 17.2810 (6) | 17.933 (2), 12.679 (2), 18.838 (2) | 37.5514 (11), 37.5514 (11), 14.5525 (4) |
| **α, β, γ (°)** | 90, 112.992 (2), 90 | 90, 109.745 (3), 90 | 90, 90, 120 |
| ***V* (Å$^3$)** | 4078.3 (3) | 4031.4 (9) | 17771.3 (12) |
| ***Z*** | 4 | 4 | 18 |
| ***F*(000)** | 1732 | 1724 | 6912 |
| **$D_x$ (Mg m$^{-3}$)** | 1.350 | 1.356 | 1.226 |
| **Radiation type** | Cu *K*α | Cu *K*α | Mo *K*α |
| **No. of reflections for cell measurement** | 34879 | 39795 | 9964 |
| **θ range (°) for cell measurement** | 5.3–68.2 | 5.2–72.2 | 2.7–35.6 |
| **μ (mm$^{-1}$)** | 8.45 | 7.87 | 0.87 |
| **Crystal shape** | Block | Fragment | Block |
| **Colour** | Black | Black | Black |
| **Crystal size (mm)** | 0.31 × 0.27 × 0.21 | 0.22 × 0.20 × 0.17 | 0.41 × 0.39 × 0.27 |
| **Data collection** | | | |
| **Diffractometer** | Rigaku Rapid II curved image plate diffractometer | Rigaku Rapid II curved image plate diffractometer | Bruker AXS D8 Quest CMOS diffractometer |
| **Radiation source** | microfocus X-ray tube | microfocus X-ray tube | I-mu-S microsource X-ray tube |
| **Monochromator** | Laterally graded multilayer (Goebel) mirror | Laterally graded multilayer (Goebel) mirror | Laterally graded multilayer (Goebel) mirror |
| **Scan method** | ω scans | ω scans | ω and phi scans |
| **Absorption correction** | Multi-scan *SCALEPACK* (Otwinowski & Minor, 1997) | Multi-scan *SCALEPACK* (Otwinowski & Minor, 1997) | Multi-scan Apex2 v2014.11 (Bruker, 2014) |
| **$T_{min}$, $T_{max}$** | 0.226, 0.270 | 0.145, 0.348 | 0.595, 0.747 |
| **No. of measured, independent and observed [$I > 2\sigma(I)$] reflections** | 34879, 7300, 5970 | 39795, 7516, 6207 | 27455, 16913, 12607 |
| **$R_{int}$** | 0.179 | 0.077 | 0.023 |
| **θ values (°)** | $\theta_{max}$ = 68.2, $\theta_{min}$ = 5.3 | $\theta_{max}$ = 72.2, $\theta_{min}$ = 5.2 | $\theta_{max}$ = 35.6, $\theta_{min}$ = 2.7 |
| **$(\sin\theta/\lambda)_{max}$ (Å$^{-1}$)** | 0.602 | 0.618 | 0.819 |

| **Range of *h*, *k*, *l*** | $h$ = -18→18, $k$ = -20→20, $l$ = -20→20 | $h$ = -21→21, $k$ = -14→14, $l$ = -23→23 | $h$ = -61→27, $k$ = -44→61, $l$ = -16→22 |
|---|---|---|---|
| **Refinement** | | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.068, 0.158, 1.03 | 0.065, 0.190, 1.09 | 0.045, 0.113, 1.04 |
| **No. of reflections** | 7300 | 7516 | 16913 |
| **No. of parameters** | 461 | 461 | 463 |
| **No. of restraints** | 0 | 0 | 0 |
| **H-atom treatment** | H-atom parameters constrained | H-atom parameters constrained | H atoms treated by a mixture of independent and constrained refinement |
| | $w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 11.0238P]$ where $P = (F_o^2 + 2F_c^2)/3$ | $w = 1/[\sigma^2(F_o^2) + (0.0902P)^2 + 14.9634P]$ where $P = (F_o^2 + 2F_c^2)/3$ | $w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 50.3464P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $(\Delta/\sigma)_{max}$ | < 0.001 | < 0.001 | 0.003 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.91, -0.78 | 0.66, -0.91 | 0.67, -1.08 |
| **Extinction method** | None | None | None |
| **Extinction coefficient** | ? | ? | ? |

| **Compound** | (7) | (8) | (9) |
|---|---|---|---|
| **Crystal data** | | | |
| **Chemical formula** | $C_{42}H_{50}Fe_2N_4$ | $C_{39}H_{49}ClN_4Ni_2$ | $C_{39}H_{49}ClCo_2N_4$ |
| $M_r$ | 722.56 | 726.69 | 727.13 |
| **Crystal system, space group** | Trigonal, $R\bar{3}$:*H* | Orthorhombic, *Pbca* | Monoclinic, $P2_1/n$ |
| **Temperature (K)** | 200 | 150 | 100 |
| ***a*, *b*, *c* (Å)** | 37.8082 (8), 37.8082 (8), 14.6373 (5) | 15.0650 (6), 16.6481 (6), 29.4529 (10) | 8.7910 (4), 45.9431 (19), 9.9343 (4) |
| **α, β, γ (°)** | 90, 90, 120 | 90, 90, 90 | 90, 115.797 (3), 90 |
| $V$ (Å$^3$) | 18120.2 (10) | 7386.9 (5) | 3612.5 (3) |
| $Z$ | 18 | 8 | 4 |
| $F$(000) | 6876 | 3072 | 1528 |
| $D_x$ (Mg m$^{-3}$) | 1.192 | 1.307 | 1.337 |
| **Radiation type** | Mo *K*α | Cu *K*α | Cu *K*α |
| **No. of reflections for cell measurement** | 24184 | 34784 | 50530 |
| **θ range (°) for cell measurement** | 1.5–26.4 | 4.2–72.2 | 5.6–72.0 |
| **μ (mm$^{-1}$)** | 0.75 | 2.17 | 8.11 |
| **Crystal shape** | Needle | Platelet | Plate |
| **Colour** | Green | Green | Black |
| **Crystal size (mm)** | 0.50 × 0.30 × 0.20 | 0.20 × 0.20 × 0.05 | 0.15 × 0.15 × 0.05 |
| **Data collection** | | | |

| **Diffractometer** | Nonius Kappa CCD diffractometer | Rigaku Rapid II curved image plate diffractometer | Rigaku Rapid II curved image plate diffractometer |
|---|---|---|---|
| **Radiation source** | fine focus X-ray tube | microfocus X-ray tube | microfocus X-ray tube |
| **Monochromator** | Graphite | Laterally graded multilayer (Goebel) mirror | Laterally graded multilayer (Goebel) mirror |
| **Scan method** | ω and ϕ scans | ω scans | ω scans |
| **Absorption correction** | Multi-scan *SCALEPACK* (Otwinowski & Minor, 1997) | Multi-scan *SCALEPACK* (Otwinowski & Minor, 1997) | Multi-scan *SCALEPACK* (Otwinowski & Minor, 1997) |
| $T_{min}$, $T_{max}$ | 0.693, 0.864 | 0.120, 0.899 | 0.425, 0.687 |
| **No. of measured, independent and observed [$I > 2\sigma(I)$] reflections** | 24184, 8225, 5639 | 34784, 7043, 4182 | 50530, 6803, 5009 |
| $R_{int}$ | 0.040 | 0.071 | 0.090 |
| **θ values (°)** | $\theta_{max}$ = 26.4, $\theta_{min}$ = 1.5 | $\theta_{max}$ = 72.2, $\theta_{min}$ = 4.2 | $\theta_{max}$ = 72.0, $\theta_{min}$ = 5.6 |
| **$(\sin\theta/\lambda)_{max}$ (Å$^{-1}$)** | 0.625 | 0.618 | 0.617 |
| **Range of *h*, *k*, *l*** | $h$ = -47→45, $k$ = -36→47, $l$ = -18→15 | $h$ = -18→18, $k$ = -20→19, $l$ = -36→31 | $h$ = -10→10, $k$ = -56→56, $l$ = -11→12 |
| **Refinement** | | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.048, 0.111, 1.00 | 0.058, 0.151, 1.07 | 0.066, 0.153, 1.06 |
| **No. of reflections** | 8225 | 7043 | 6803 |
| **No. of parameters** | 574 | 441 | 440 |
| **No. of restraints** | 456 | 5 | 6 |
| **H-atom treatment** | H atoms treated by a mixture of independent and constrained refinement | H atoms treated by a mixture of independent and constrained refinement | H atoms treated by a mixture of independent and constrained refinement |
| | $w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 38.4426P]$ where $P = (F_o^2 + 2F_c^2)/3$ | $w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 11.0436P]$ where $P = (F_o^2 + 2F_c^2)/3$ | $w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 19.7181P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $(\Delta/\sigma)_{max}$ | 0.001 | 0.001 | < 0.001 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.33, -0.26 | 0.38, -0.48 | 0.74, -0.79 |
| **Extinction method** | None | *SHELXL2014*/7 (Sheldrick 2014, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ | None |
| **Extinction coefficient** | ? | 0.000119 (19) | ? |

| **Compound** | (10) |
|---|---|
| **Crystal data** | |
| **Chemical formula** | $C_{39}H_{49}ClFe_2N_4 \cdot C_6H_6$ |
| $M_r$ | 799.08 |
| **Crystal system, space group** | Triclinic, $P\bar{1}$ |

| | |
|---|---|
| **Temperature (K)** | 100 |
| ***a*, *b*, *c* (Å)** | 9.3766 (5), 9.8778 (8), 23.678 (2) |
| **α, β, γ (°)** | 94.489 (5), 98.981 (5), 107.591 (5) |
| ***V* (Å$^3$)** | 2046.5 (3) |
| ***Z*** | 2 |
| ***F*(000)** | 844 |
| ***D*$_x$ (Mg m$^{-3}$)** | 1.297 |
| **Radiation type** | Cu *K*α |
| **No. of reflections for cell measurement** | 58270 |
| **θ range (°) for cell measurement** | 4.9–72.1 |
| **μ (mm$^{-1}$)** | 6.55 |
| **Crystal shape** | Plate |
| **Colour** | Black |
| **Crystal size (mm)** | 0.10 × 0.10 × 0.05 |
| **Data collection** | |
| **Diffractometer** | Rigaku Rapid II curved image plate diffractometer |
| **Radiation source** | microfocus X-ray tube |
| **Monochromator** | Laterally graded multilayer (Goebel) mirror |
| **Scan method** | ω scans |
| **Absorption correction** | Multi-scan *SCALEPACK* (Otwinowski & Minor, 1997) |
| ***T*$_{min}$, *T*$_{max}$** | 0.433, 0.735 |
| **No. of measured, independent and observed [*I* > 2σ(*I*)] reflections** | 58270, 7767, 6589 |
| ***R*$_{int}$** | 0.073 |
| **θ values (°)** | $\theta_{max}$ = 72.1, $\theta_{min}$ = 4.9 |
| **(sin θ/λ)$_{max}$ (Å$^{-1}$)** | 0.617 |
| **Range of *h*, *k*, *l*** | *h* = -11→11, *k* = -11→11, *l* = -28→29 |
| **Refinement** | |
| ***R*[*F*$^2$ > 2σ(*F*$^2$)], *wR*(*F*$^2$), *S*** | 0.046, 0.116, 1.04 |
| **No. of reflections** | 7767 |
| **No. of parameters** | 495 |

| | |
|---|---|
| **No. of restraints** | 6 |
| **H-atom treatment** | H atoms treated by a mixture of independent and constrained refinement |
| | $w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 3.2586P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $(\Delta/\sigma)_{max}$ | 0.001 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.50, -0.45 |
| **Extinction method** | None |
| **Extinction coefficient** | ? |

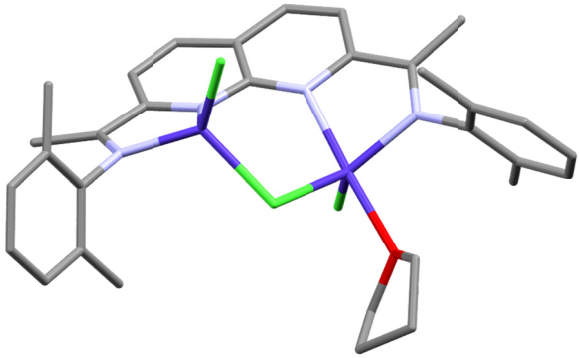
Computer programs: *CrystalClear*-SM Expert 2.1 b32 (Rigaku, 2014), Apex2 v2014.11 (Bruker, 2014), Nonius Collect (Nonius, 1998), *HKL-3000* (Otwinowski & Minor, 1997), *SAINT* V8.34A (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014*/7 (Sheldrick, 2014), SHELXLE Rev794 (Hübschle *et al.*, 2011), SHELXLE Rev714 (Hübschle *et al.*, 2011), SHELXLE Rev816 (Hübschle *et al.*, 2011).

## 9. Computational Methods and Optimized Structures

**Computational Methods.** DFT calculations were performed with the Gaussian09/D.01 package,[10] using the BP86 functional and the 6-311G(d,p) basis set. Stationary points and saddle points were confirmed by frequency analysis, and wavefunction stability by stability analysis. Starting geometries for each complex were obtained from the corresponding crystallographic data. To simplify the calculations, isopropyl groups were truncated to methyl groups in the trichloride structures. No other modifications or constraints were necessary to obtain reasonable geometries. Geometries are reported as cartesian coordinates.

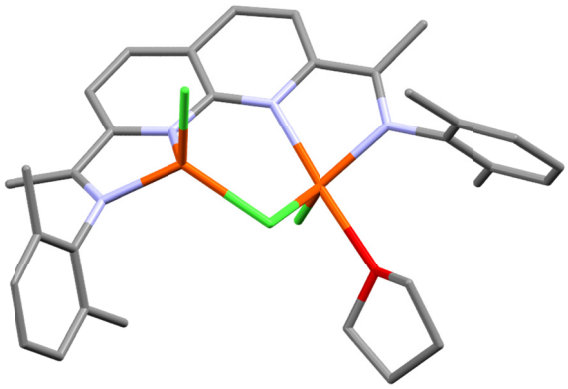
[10] Gaussian 09, Revision **D.01**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

**Optimized Structures.**



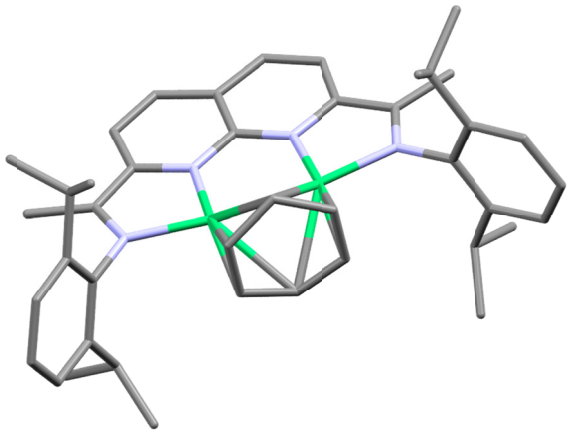
**[$^{i\text{-Pr}}$NDI]$Co_2$(THF)$Cl_3$**
**ZPVE: -5681.972259 $E_h$**
**Charge: 0**
**Multiplicity: 6**

| | | | |
|---|---|---|---|
| Co | 1.51383721 | -0.01838774 | -0.67298791 |
| Co | -1.82590978 | 0.04645179 | 0.80917733 |
| Cl | 1.55359519 | 0.82950028 | -2.76942970 |
| Cl | -1.56243324 | 0.08873414 | 2.99104302 |
| Cl | -0.31244213 | -1.39138393 | -0.11785352 |
| O | 2.41921877 | -1.90792401 | -1.31276929 |
| N | 3.02922565 | 0.66549363 | 0.40146741 |
| N | -3.59755890 | 0.08817636 | 0.01667097 |
| N | 0.73686992 | 1.85800923 | -0.02023840 |
| N | -1.56735633 | 1.65794154 | -0.27852273 |
| C | 2.67427687 | -2.96714269 | -0.32401598 |
| H | 1.91917819 | -2.87444822 | 0.47393131 |
| H | 3.67756716 | -2.80115361 | 0.09166454 |
| C | 2.52471864 | -4.28914996 | -1.08123881 |
| H | 2.20158042 | -5.10601787 | -0.41881024 |
| H | 3.47972624 | -4.58204800 | -1.54873050 |
| C | 1.48367550 | -3.92939026 | -2.15600957 |
| H | 0.47395897 | -3.90915105 | -1.71589210 |
| H | 1.48478049 | -4.62138754 | -3.01169599 |
| C | 1.90843737 | -2.51761238 | -2.55022509 |
| H | 2.72869491 | -2.51919279 | -3.28861672 |
| H | 1.09664308 | -1.88264738 | -2.92532098 |
| C | 3.03686653 | 1.97243713 | 0.57918047 |
| C | -3.88233630 | 1.22269845 | -0.61893427 |
| C | 1.81614388 | 2.66847614 | 0.17886219 |
| C | 1.76352598 | 4.07011312 | 0.00350543 |
| H | 2.65025217 | 4.67693726 | 0.19097608 |
| C | 0.59721326 | 4.65031147 | -0.46510862 |
| H | 0.54525701 | 5.72221579 | -0.67296528 |
| C | -0.55123139 | 3.84497038 | -0.65655879 |
| C | -1.79906328 | 4.33357976 | -1.12970516 |
| H | -1.88368741 | 5.37900863 | -1.43667117 |
| C | -2.88991474 | 3.48305459 | -1.19098307 |
| H | -3.85207885 | 3.84238834 | -1.56019276 |
| C | -2.77037043 | 2.15453061 | -0.72441604 |
| C | -0.45248643 | 2.44531401 | -0.32735659 |
| C | 4.11387128 | -0.14888517 | 0.86755380 |
| C | 5.20601517 | -0.42358068 | 0.01119518 |
| C | 6.21027100 | -1.28505215 | 0.48468662 |
| H | 7.06128840 | -1.50904421 | -0.16533027 |
| C | 6.13401280 | -1.85495625 | 1.76061684 |
| H | 6.92380624 | -2.52589198 | 2.10835037 |
| C | 5.04203875 | -1.57028443 | 2.58794752 |
| H | 4.97721604 | -2.01797591 | 3.58394379 |
| C | 4.01108378 | -0.71673171 | 2.16089427 |
| C | -4.56659273 | -0.95716067 | 0.15686795 |
| C | -4.60821184 | -1.98264705 | -0.81890741 |
| C | -5.52423667 | -3.03149352 | -0.63835609 |
| H | -5.56192695 | -3.83206907 | -1.38327796 |
| C | -6.37508987 | -3.06513434 | 0.47118211 |
| H | -7.07867753 | -3.89204706 | 0.59744440 |
| C | -6.31550742 | -2.04326774 | 1.42421293 |
| H | -6.97464171 | -2.06971812 | 2.29685122 |
| C | -5.41604786 | -0.97306468 | 1.28991305 |
| C | 4.19807447 | 2.73571202 | 1.15784408 |
| H | 4.97632995 | 2.05125632 | 1.51880861 |
| H | 3.87058114 | 3.37645498 | 1.99182390 |
| H | 4.64703257 | 3.39406204 | 0.39449260 |
| C | -5.23615143 | 1.55220444 | -1.18975137 |
| H | -5.91935004 | 0.69970191 | -1.07991079 |
| H | -5.16538928 | 1.80761391 | -2.25979958 |
| H | -5.68529616 | 2.41853293 | -0.67418302 |
| C | -3.68119784 | -1.95181194 | -2.01177159 |
| H | -3.90866051 | -1.10904733 | -2.68715407 |
| H | -2.63147107 | -1.83166695 | -1.69860704 |
| H | -3.76712485 | -2.88072402 | -2.59406805 |
| C | -5.34274559 | 0.11836267 | 2.33084512 |
| H | -4.32778802 | 0.19775551 | 2.75546640 |
| H | -5.59194516 | 1.10672019 | 1.90759473 |
| H | -6.04545970 | -0.08129329 | 3.15289780 |
| C | 5.28525775 | 0.18925432 | -1.36626954 |
| H | 6.06230050 | -0.30467603 | -1.96764958 |
| H | 4.32445751 | 0.10877084 | -1.89742155 |
| H | 5.53615242 | 1.26362678 | -1.31919399 |
| C | 2.82907609 | -0.41110311 | 3.05050780 |
| H | 2.86748121 | 0.62246457 | 3.43619085 |
| H | 1.87042187 | -0.50404199 | 2.51602460 |
| H | 2.80424849 | -1.08671075 | 3.91726874 |



**[$^{i\text{-Pr}}$NDI]$Fe_2$(THF)$Cl_3$**
**ZPVE: -5443.853266 $E_h$**
**Charge: 0**
**Multiplicity: 8**

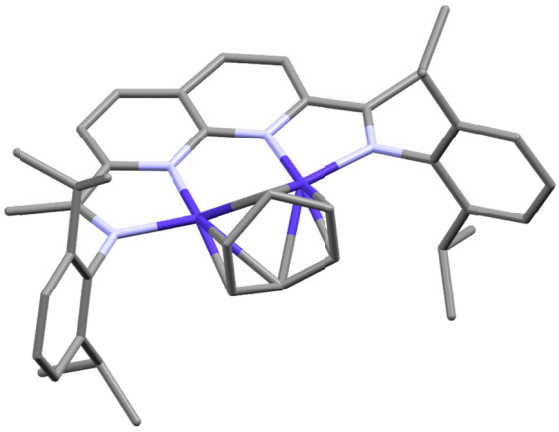
| | | | |
|---|---|---|---|
| N | -3.59549776 | -0.00130735 | 0.00944384 |
| C | -5.28065934 | 1.34888572 | -1.26226126 |
| H | -5.20627847 | 1.57668472 | -2.33805873 |
| H | -5.77412602 | 2.20952132 | -0.77849554 |
| H | -5.92494180 | 0.46872046 | -1.13627982 |
| O | 2.28929003 | -2.09335165 | -1.01138918 |
| Cl | -0.17741277 | -1.38524284 | 0.59671121 |
| Fe | -1.86435457 | 0.14595331 | 0.98741746 |
| N | -1.62777989 | 1.64287762 | -0.34690453 |
| C | -3.92043238 | 1.10117719 | -0.66576852 |
| Cl | -1.88463847 | 0.89202037 | 3.06469409 |
| Fe | 1.40278268 | -0.03197721 | -0.62333716 |
| N | 0.67522799 | 1.91138749 | -0.16089887 |
| Cl | 1.22897013 | 0.32635284 | -2.84330289 |
| C | -2.85336171 | 2.07540025 | -0.80115745 |
| N | 3.00820920 | 0.77731007 | 0.27359888 |
| C | -3.02630610 | 3.37595291 | -1.33450833 |
| H | -4.00877880 | 3.69276193 | -1.68792878 |
| C | -1.95280665 | 4.24717662 | -1.36096315 |
| H | -2.07024242 | 5.26974954 | -1.72913084 |
| C | -0.67540726 | 3.81599211 | -0.90908100 |
| C | -0.53625288 | 2.45231957 | -0.47487618 |
| C | 0.47115650 | 4.64997176 | -0.84600147 |
| H | 0.38826166 | 5.70034463 | -1.13729078 |
| C | 1.67323438 | 4.12622827 | -0.40913244 |
| H | 2.56061181 | 4.75676309 | -0.34165190 |
| C | 1.76471796 | 2.74607454 | -0.10008397 |
| C | 3.01334151 | 2.10767867 | 0.27900123 |
| C | 4.21720599 | 2.93726178 | 0.64392054 |
| H | 4.59997118 | 3.48297673 | -0.23604613 |
| H | 5.02636126 | 2.30248028 | 1.02797426 |
| H | 3.96419328 | 3.68753503 | 1.40992820 |
| C | -4.48465596 | -1.12024212 | 0.10697912 |
| C | -5.42834811 | -1.19399073 | 1.16092134 |
| C | -6.23062517 | -2.34417695 | 1.24846117 |
| H | -6.96093152 | -2.41444592 | 2.06006356 |
| C | -6.10657316 | -3.38843664 | 0.32663598 |
| H | -6.73762798 | -4.27634389 | 0.41656389 |
| C | -5.16639560 | -3.29712780 | -0.70463051 |
| H | -5.06206804 | -4.11354907 | -1.42538108 |
| C | -4.34198526 | -2.16832072 | -0.83582606 |
| C | 4.13088851 | 0.04109761 | 0.77210541 |
| C | 5.15342030 | -0.36971050 | -0.11768665 |
| C | 6.19924961 | -1.15498886 | 0.39605041 |
| H | 6.99720032 | -1.47701233 | -0.27973955 |
| C | 6.23147836 | -1.52685593 | 1.74487518 |
| H | 7.05111073 | -2.14275272 | 2.12392605 |
| C | 5.20860690 | -1.11390976 | 2.60569287 |
| H | 5.22694737 | -1.40788741 | 3.65933039 |
| C | 4.14261682 | -0.32499888 | 2.14095846 |
| C | 2.71055918 | -3.02758702 | 0.02461217 |
| H | 1.83606591 | -3.29124581 | 0.64825318 |
| H | 3.46247184 | -2.51719075 | 0.63879461 |
| C | 3.23746463 | -4.22611756 | -0.76356291 |
| H | 3.23249697 | -5.14998257 | -0.16599177 |
| H | 4.27143158 | -4.03276135 | -1.08709131 |
| C | 2.28190548 | -4.29210555 | -1.98641372 |
| H | 1.53330063 | -5.09000064 | -1.86865312 |
| H | 2.83451959 | -4.48882149 | -2.91653674 |
| C | 1.59456942 | -2.90607645 | -2.01057068 |
| H | 1.67451529 | -2.36533457 | -2.96072048 |
| H | 0.53083412 | -2.97337595 | -1.72215885 |
| C | 5.11060923 | 0.02096193 | -1.57508428 |
| H | 5.91533316 | -0.47595633 | -2.13636759 |
| H | 4.14492640 | -0.25029085 | -2.03009197 |
| H | 5.22950492 | 1.10964493 | -1.70955280 |
| C | 3.02898855 | 0.10662255 | 3.06621818 |
| H | 3.05034950 | 1.19390193 | 3.25338107 |
| H | 2.03753721 | -0.11650985 | 2.64085416 |
| H | 3.10869844 | -0.40095009 | 4.03815932 |
| C | -3.32327407 | -2.07108576 | -1.94717534 |
| H | -3.58690608 | -1.28823164 | -2.67878860 |
| H | -2.32689527 | -1.81082132 | -1.55589429 |
| H | -3.24567350 | -3.02423247 | -2.49018876 |
| C | -5.56552631 | -0.07693971 | 2.16849137 |
| H | -4.60637316 | 0.14688541 | 2.66388923 |
| H | -5.90415577 | 0.86176215 | 1.69712632 |
| H | -6.29825386 | -0.34447506 | 2.94356795 |



**[$^{i\text{-Pr}}$NDI]Ni$_2$(C$_6$H$_6$)**
**ZPVE: -4866.380350 E$_h$**
**Charge: 0**
**Multiplicity: 1**

| | | | |
|---|---|---|---|
| Ni | 1.25900000 | 0.00000000 | 0.00100000 |
| Ni | -1.26000000 | 0.00000000 | 0.00000000 |
| N | 3.17300000 | 0.32700000 | 0.00000000 |
| N | -3.17300000 | 0.32700000 | 0.00100000 |
| N | 1.14800000 | 1.85300000 | -0.00100000 |
| N | -1.14800000 | 1.85300000 | -0.00300000 |
| C | 1.24000000 | -1.86700000 | 0.71300000 |
| C | 1.23400000 | -1.86500000 | -0.72200000 |
| C | -0.00500000 | -1.64700000 | -1.39000000 |
| C | -1.23900000 | -1.86800000 | -0.71200000 |
| C | -1.23400000 | -1.86400000 | 0.72200000 |
| C | 0.00600000 | -1.64000000 | 1.38900000 |
| C | 3.49800000 | 1.63800000 | -0.00200000 |
| C | -3.49800000 | 1.63800000 | -0.00100000 |
| C | 2.38500000 | 2.51800000 | -0.00200000 |
| C | 2.43400000 | 3.92000000 | -0.00200000 |

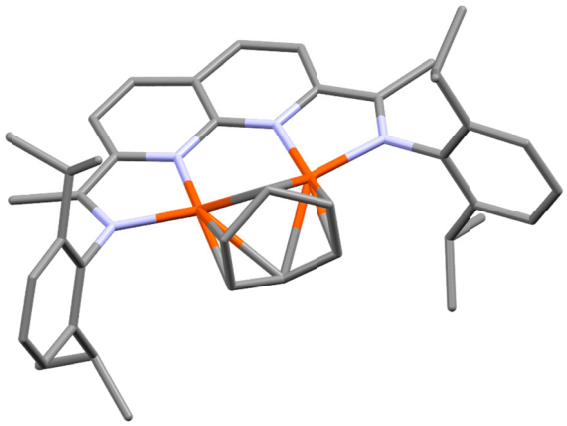
| | | | |
|---|---|---|---|
| C | 1.26000000 | 4.66800000 | -0.00200000 |
| C | 0.00000000 | 4.01300000 | -0.00200000 |
| C | -1.26000000 | 4.66800000 | -0.00200000 |
| C | -2.43400000 | 3.92000000 | -0.00200000 |
| C | -2.38500000 | 2.51800000 | -0.00200000 |
| C | 0.00000000 | 2.57100000 | -0.00200000 |
| C | 4.19500000 | -0.67200000 | 0.00100000 |
| C | 4.68100000 | -1.18200000 | 1.23900000 |
| C | 5.67300000 | -2.17700000 | 1.21100000 |
| C | 6.17300000 | -2.67200000 | 0.00400000 |
| C | 5.67500000 | -2.17900000 | -1.20500000 |
| C | 4.68300000 | -1.18400000 | -1.23600000 |
| C | -4.19500000 | -0.67200000 | 0.00000000 |
| C | -4.68300000 | -1.18200000 | 1.23800000 |
| C | -5.67500000 | -2.17800000 | 1.20800000 |
| C | -6.17300000 | -2.67200000 | 0.00000000 |
| C | -5.67300000 | -2.17900000 | -1.20800000 |
| C | -4.68100000 | -1.18300000 | -1.23700000 |
| C | 4.91600000 | 2.15500000 | -0.00200000 |
| C | -4.91600000 | 2.15500000 | -0.00200000 |
| H | 2.14700000 | -2.10600000 | 1.26700000 |
| H | 2.13800000 | -2.10200000 | -1.28300000 |
| H | -0.01000000 | -1.58600000 | -2.48100000 |
| H | -2.14700000 | -2.10800000 | -1.26600000 |
| H | -2.13800000 | -2.10000000 | 1.28400000 |
| H | 0.01000000 | -1.57600000 | 2.47900000 |
| H | 3.40500000 | 4.42100000 | -0.00200000 |
| H | 1.29300000 | 5.76000000 | -0.00200000 |
| H | -1.29300000 | 5.76000000 | -0.00200000 |
| H | -3.40500000 | 4.42100000 | -0.00200000 |
| H | 6.06000000 | -2.57100000 | 2.15500000 |
| H | 6.94500000 | -3.44600000 | 0.00500000 |
| H | 6.06400000 | -2.57500000 | -2.14700000 |
| H | -6.06400000 | -2.57200000 | 2.15100000 |
| H | -6.94500000 | -3.44600000 | -0.00100000 |
| H | -6.06000000 | -2.57400000 | -2.15100000 |
| H | 5.64200000 | 1.33200000 | -0.00100000 |
| H | 5.10700000 | 2.78400000 | 0.88300000 |
| H | 5.10800000 | 2.78100000 | -0.88900000 |
| H | -5.64200000 | 1.33200000 | -0.00100000 |
| H | -5.10800000 | 2.78100000 | -0.89000000 |
| H | -5.10800000 | 2.78400000 | 0.88300000 |
| C | 4.18000000 | -0.65100000 | -2.57900000 |
| H | 3.26000000 | -0.07700000 | -2.37400000 |
| C | 4.17500000 | -0.64600000 | 2.58000000 |
| H | 3.25600000 | -0.07200000 | 2.37200000 |
| C | -4.17400000 | -0.65000000 | -2.57900000 |
| H | -3.25500000 | -0.07600000 | -2.37200000 |
| C | -4.18000000 | -0.64700000 | 2.58000000 |
| H | -3.26000000 | -0.07300000 | 2.37400000 |
| C | -5.20700000 | 0.31300000 | 3.22300000 |
| H | -6.14300000 | -0.21900000 | 3.46100000 |
| H | -4.80800000 | 0.73500000 | 4.16100000 |
| H | -5.45800000 | 1.15000000 | 2.55500000 |
| C | -3.82500000 | -1.76900000 | 3.57900000 |
| H | -3.36600000 | -1.33900000 | 4.48400000 |
| H | -4.72000000 | -2.32700000 | 3.90200000 |
| H | -3.11700000 | -2.49800000 | 3.15400000 |
| C | 3.81700000 | -1.76800000 | 3.57900000 |
| H | 4.71100000 | -2.32700000 | 3.90300000 |
| H | 3.35600000 | -1.33800000 | 4.48300000 |
| H | 3.10900000 | -2.49600000 | 3.15100000 |
| C | 5.20000000 | 0.31400000 | 3.22500000 |
| H | 6.13600000 | -0.21900000 | 3.46500000 |
| H | 5.45300000 | 1.15000000 | 2.55700000 |
| H | 4.80000000 | 0.73500000 | 4.16200000 |
| C | 5.20600000 | 0.30900000 | -3.22300000 |
| H | 6.14300000 | -0.22300000 | -3.46000000 |
| H | 4.80800000 | 0.72900000 | -4.16200000 |
| H | 5.45700000 | 1.14700000 | -2.55600000 |
| C | 3.82600000 | -1.77400000 | -3.57700000 |
| H | 3.36600000 | -1.34500000 | -4.48200000 |
| H | 4.72100000 | -2.33200000 | -3.89900000 |
| H | 3.11800000 | -2.50200000 | -3.15100000 |
| C | -5.20000000 | 0.31000000 | -3.22500000 |
| H | -4.79900000 | 0.73000000 | -4.16300000 |
| H | -6.13600000 | -0.22300000 | -3.46500000 |
| H | -5.45200000 | 1.14700000 | -2.55900000 |
| C | -3.81800000 | -1.77400000 | -3.57600000 |
| H | -4.71200000 | -2.33200000 | -3.90000000 |
| H | -3.35700000 | -1.34500000 | -4.48100000 |
| H | -3.11000000 | -2.50100000 | -3.14800000 |



**[$^{i\text{-Pr}}$NDI]$Co_2(C_6H_6)$**
**ZPVE: -4615.259429 $E_h$**
**Charge: 0**
**Multiplicity: 1**

| | | | |
|---|---|---|---|
| Co | -1.21794200 | -0.03779200 | 0.00000800 |
| Co | 1.21789200 | -0.03779300 | 0.00003000 |
| C | 2.42343900 | 3.93622400 | 0.00175300 |
| C | 1.26332700 | 4.67931600 | 0.00179500 |
| C | -0.00002000 | 4.01266800 | 0.00130500 |
| C | -0.00002100 | 2.59237800 | 0.00084300 |
| C | 2.35564400 | 2.51432400 | 0.00119100 |
| H | -1.29260900 | 5.77214600 | 0.00156700 |
| H | 3.40082400 | 4.42221000 | 0.00215400 |
| H | 1.29257300 | 5.77214400 | 0.00220300 |
| C | -1.26336700 | 4.67931800 | 0.00126700 |
| C | -2.35568200 | 2.51432200 | 0.00052000 |
| C | -2.42347800 | 3.93622500 | 0.00087200 |
| H | -3.40086700 | 4.42220200 | 0.00081400 |

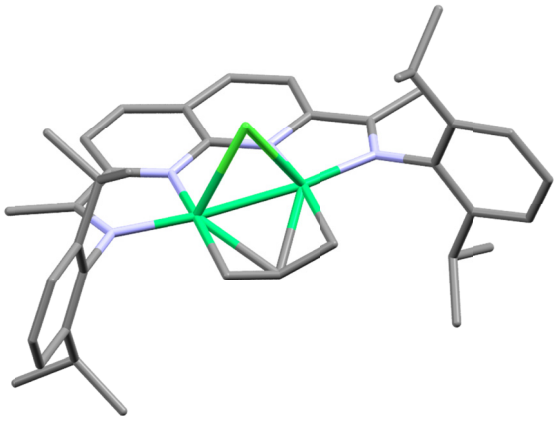
| | | | |
|---|---|---|---|
| N | -1.14352300 | 1.84790500 | 0.00048600 |
| N | 1.14348700 | 1.84790400 | 0.00076600 |
| C | 3.46585900 | 1.62646300 | 0.00093600 |
| C | -3.46589800 | 1.62646100 | 0.00024700 |
| C | 4.88703900 | 2.12557500 | 0.00146400 |
| H | 5.09011100 | 2.75282200 | -0.88413900 |
| H | 5.09012900 | 2.75091400 | 0.88842900 |
| H | 5.60495600 | 1.29529800 | 0.00061600 |
| C | -4.88707700 | 2.12556300 | 0.00022700 |
| H | -5.09012700 | 2.75194100 | -0.88600600 |
| H | -5.60498300 | 1.29526700 | 0.00011300 |
| H | -5.09019700 | 2.75177200 | 0.88656300 |
| N | 3.08481900 | 0.32638700 | 0.00031200 |
| N | -3.08483900 | 0.32638500 | 0.00004900 |
| C | 4.11672700 | -0.67613400 | -0.00024800 |
| C | 4.60684800 | -1.17712600 | 1.23742500 |
| C | 4.60690400 | -1.17556200 | -1.23853500 |
| C | 5.60959200 | -2.16169400 | 1.20647800 |
| C | 5.60963100 | -2.16018900 | -1.20882100 |
| C | 6.11482000 | -2.64882300 | -0.00147100 |
| H | 6.00174700 | -2.55250100 | 2.14950300 |
| H | 6.00179200 | -2.54978800 | -2.15234400 |
| H | 6.89621800 | -3.41347100 | -0.00191600 |
| C | -4.11671900 | -0.67616100 | -0.00015500 |
| C | -4.60674800 | -1.17669000 | 1.23774100 |
| C | -4.60692200 | -1.17610900 | -1.23821700 |
| C | -5.60940400 | -2.16136400 | 1.20725000 |
| C | -5.60954900 | -2.16082400 | -1.20805500 |
| C | -6.11463400 | -2.64902400 | -0.00048400 |
| H | -6.00147900 | -2.55180200 | 2.15045800 |
| H | -6.00171500 | -2.55086500 | -2.15139500 |
| H | -6.89594700 | -3.41376000 | -0.00061400 |
| C | -4.09524300 | -0.64848700 | -2.58122800 |
| H | -3.16594700 | -0.09015900 | -2.37591000 |
| C | -4.09478200 | -0.64977000 | 2.58091700 |
| H | -3.16533200 | -0.09166000 | 2.37570800 |
| C | 4.09509300 | -0.64746300 | -2.58131800 |
| H | 3.16564300 | -0.08949000 | -2.37572100 |
| C | 4.09488500 | -0.65087300 | 2.58085800 |
| H | 3.16544300 | -0.09264600 | 2.37594300 |
| C | -1.23934900 | -1.88676900 | 0.70984700 |
| C | -1.23966300 | -1.88627500 | -0.71086600 |
| C | 0.00033600 | -1.50257700 | 1.35041900 |
| C | -0.00033100 | -1.50123500 | -1.35164100 |
| H | -2.11551100 | -2.19269100 | -1.28339000 |
| C | 1.23966800 | -1.88692000 | 0.70926100 |
| H | 0.00059300 | -1.37495000 | 2.43496400 |
| C | 1.23935900 | -1.88610200 | -0.71144800 |
| H | -0.00058400 | -1.37256000 | -2.43606400 |
| H | 2.11555100 | -2.19375700 | 1.28150900 |
| H | 2.11496300 | -2.19235400 | -1.28443700 |
| H | -2.11496600 | -2.19355400 | 1.28254500 |
| C | 5.10712300 | 0.32646300 | -3.22688200 |
| H | 6.05134800 | -0.19254000 | -3.46441400 |
| H | 4.70155100 | 0.73783900 | -4.16631400 |
| H | 5.34634400 | 1.16961400 | -2.56307600 |
| C | 3.75775800 | -1.77522500 | -3.58057100 |
| H | 3.29166700 | -1.35109100 | -4.48494200 |
| H | 4.66153000 | -2.31862600 | -3.90343400 |
| H | 3.05978800 | -2.51291100 | -3.15536800 |
| C | 3.75749900 | -1.78001400 | 3.57855600 |
| H | 4.66126100 | -2.32385900 | 3.90069800 |
| H | 3.29138000 | -1.35710700 | 4.48348500 |
| H | 3.05953700 | -2.51711800 | 3.15232400 |
| C | 5.10677900 | 0.32221900 | 3.22791100 |
| H | 6.05102300 | -0.19705200 | 3.46478100 |
| H | 5.34600100 | 1.16636400 | 2.56535600 |
| H | 4.70108400 | 0.73220400 | 4.16789400 |
| C | -3.75738800 | -1.77840400 | 3.57916800 |
| H | -3.29124400 | -1.35505800 | 4.48387800 |
| H | -4.66113900 | -2.32209400 | 3.90160400 |
| H | -3.05944000 | -2.51570900 | 3.15326100 |
| C | -5.10666900 | 0.32369100 | 3.22742200 |
| H | -5.34586700 | 1.16744700 | 2.56436800 |
| H | -6.05092000 | -0.19542400 | 3.46460300 |
| H | -4.70096600 | 0.73422300 | 4.16716700 |
| C | -3.75759200 | -1.77659600 | -3.57998500 |
| H | -4.66121400 | -2.32041900 | -3.90255000 |
| H | -3.29166800 | -1.35273500 | -4.48456600 |
| H | -3.05937800 | -2.51386800 | -3.15446800 |
| C | -5.10754700 | 0.32489200 | -3.22720100 |
| H | -6.05162100 | -0.19447000 | -3.46454300 |
| H | -5.34702700 | 1.16822300 | -2.56370900 |
| H | -4.70208200 | 0.73603300 | -4.16678200 |



**[$^{i\text{-Pr}}$NDI]$Fe_2(C_6H_6)$**
**ZPVE: -4377.099548 $E_h$**
**Charge: 0**
**Multiplicity: 5**

| | | | |
|---|---|---|---|
| Fe | 1.27900000 | -0.07800000 | -0.01500000 |
| Fe | -1.27900000 | -0.07800000 | 0.01700000 |
| N | 3.18600000 | 0.33100000 | 0.06600000 |
| N | -3.18700000 | 0.33100000 | -0.06700000 |
| N | 1.14900000 | 1.84800000 | 0.04900000 |
| N | -1.14900000 | 1.84800000 | -0.05000000 |
| C | -0.02900000 | -1.52800000 | 1.33400000 |
| H | -0.04700000 | -1.38100000 | 2.41700000 |
| C | 1.23700000 | -1.93200000 | 0.73500000 |
| H | 2.07500000 | -2.28400000 | 1.33800000 |
| C | 1.26400000 | -1.95500000 | -0.68800000 |
| H | 2.12600000 | -2.32200000 | -1.25000000 |

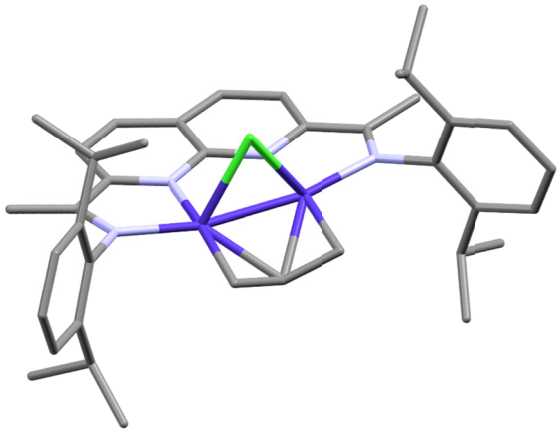
| | | | |
|---|---|---|---|
| C | 0.02900000 | -1.52900000 | -1.33200000 |
| H | 0.04700000 | -1.38200000 | -2.41600000 |
| C | -1.23700000 | -1.93300000 | -0.73300000 |
| H | -2.07500000 | -2.28400000 | -1.33700000 |
| C | -1.26400000 | -1.95500000 | 0.69000000 |
| H | -2.12600000 | -2.32100000 | 1.25200000 |
| C | 3.50200000 | 1.64700000 | 0.10200000 |
| C | -3.50200000 | 1.64700000 | -0.10300000 |
| C | 2.37800000 | 2.51900000 | 0.09600000 |
| C | 2.42900000 | 3.92300000 | 0.10800000 |
| H | 3.39900000 | 4.42400000 | 0.15300000 |
| C | 1.25700000 | 4.66900000 | 0.05800000 |
| H | 1.28800000 | 5.76100000 | 0.06100000 |
| C | 0.00000000 | 4.01200000 | -0.00100000 |
| C | -1.25700000 | 4.66900000 | -0.05900000 |
| H | -1.28800000 | 5.76100000 | -0.06300000 |
| C | -2.42900000 | 3.92300000 | -0.10900000 |
| H | -3.39900000 | 4.42400000 | -0.15400000 |
| C | -2.37800000 | 2.51900000 | -0.09600000 |
| C | 0.00000000 | 2.56800000 | 0.00000000 |
| C | 4.22600000 | -0.65500000 | -0.01500000 |
| C | 4.74800000 | -1.23600000 | 1.17400000 |
| C | 5.74900000 | -2.21600000 | 1.05400000 |
| H | 6.16600000 | -2.66600000 | 1.95900000 |
| C | 6.22000000 | -2.62800000 | -0.19500000 |
| H | 6.99900000 | -3.39200000 | -0.26300000 |
| C | 5.68500000 | -2.06500000 | -1.35500000 |
| H | 6.05200000 | -2.39400000 | -2.33200000 |
| C | 4.68500000 | -1.07900000 | -1.29400000 |
| C | -4.22600000 | -0.65600000 | 0.01500000 |
| C | -4.74800000 | -1.23700000 | -1.17400000 |
| C | -5.74800000 | -2.21700000 | -1.05400000 |
| H | -6.16500000 | -2.66700000 | -1.96000000 |
| C | -6.22000000 | -2.62900000 | 0.19400000 |
| H | -6.99900000 | -3.39300000 | 0.26300000 |
| C | -5.68500000 | -2.06400000 | 1.35500000 |
| H | -6.05200000 | -2.39400000 | 2.33100000 |
| C | -4.68600000 | -1.07900000 | 1.29400000 |
| C | 4.91400000 | 2.17600000 | 0.14000000 |
| H | 5.64700000 | 1.36100000 | 0.08100000 |
| H | 5.10200000 | 2.73900000 | 1.07000000 |
| H | 5.10200000 | 2.86800000 | -0.69900000 |
| C | -4.91400000 | 2.17600000 | -0.14000000 |
| H | -5.64700000 | 1.36100000 | -0.08100000 |
| H | -5.10200000 | 2.73900000 | -1.07100000 |
| H | -5.10200000 | 2.86800000 | 0.69700000 |
| C | -4.14300000 | -0.46200000 | 2.58500000 |
| H | -3.24000000 | 0.11000000 | 2.31500000 |
| C | -4.27000000 | -0.79800000 | -2.55900000 |
| H | -3.33000000 | -0.23900000 | -2.41300000 |
| C | 4.14200000 | -0.46300000 | -2.58600000 |
| H | 3.23900000 | 0.10900000 | -2.31500000 |
| C | 4.27100000 | -0.79800000 | 2.55900000 |
| H | 3.33100000 | -0.23900000 | 2.41300000 |
| C | 5.15900000 | 0.52000000 | -3.20800000 |
| H | 5.44800000 | 1.31100000 | -2.50100000 |
| H | 6.07800000 | -0.01100000 | -3.51100000 |
| H | 4.73500000 | 1.00200000 | -4.10500000 |
| C | 3.73200000 | -1.52200000 | -3.63100000 |
| H | 3.25800000 | -1.03400000 | -4.49900000 |
| H | 4.60400000 | -2.08200000 | -4.00800000 |
| H | 3.01800000 | -2.25300000 | -3.22100000 |
| C | 5.29000000 | 0.15000000 | 3.23300000 |
| H | 6.24800000 | -0.37000000 | 3.40600000 |
| H | 5.49700000 | 1.03600000 | 2.61700000 |
| H | 4.91100000 | 0.49500000 | 4.21000000 |
| C | 3.97500000 | -1.98800000 | 3.49700000 |
| H | 4.89500000 | -2.53200000 | 3.76700000 |
| H | 3.52200000 | -1.62700000 | 4.43500000 |
| H | 3.28200000 | -2.71200000 | 3.04200000 |
| C | -5.16100000 | 0.52100000 | 3.20700000 |
| H | -5.45000000 | 1.31100000 | 2.49900000 |
| H | -6.08000000 | -0.01000000 | 3.51000000 |
| H | -4.73700000 | 1.00300000 | 4.10300000 |
| C | -3.73400000 | -1.52000000 | 3.63200000 |
| H | -3.26000000 | -1.03200000 | 4.49900000 |
| H | -4.60600000 | -2.08100000 | 4.00800000 |
| H | -3.01900000 | -2.25100000 | 3.22300000 |
| C | -5.28900000 | 0.14900000 | -3.23400000 |
| H | -6.24700000 | -0.37100000 | -3.40700000 |
| H | -5.49600000 | 1.03500000 | -2.61700000 |
| H | -4.90900000 | 0.49400000 | -4.21000000 |
| C | -3.97400000 | -1.98800000 | -3.49700000 |
| H | -4.89400000 | -2.53300000 | -3.76800000 |
| H | -3.52100000 | -1.62800000 | -4.43500000 |
| H | -3.28100000 | -2.71300000 | -3.04200000 |



**[$^{i\text{-Pr}}$NDI]Ni$_2$(allyl)Cl**
**ZPVE: -5211.735279 $E_h$**
**Charge: 0**
**Multiplicity: 1**

| | | | |
|---|---|---|---|
| Ni | 1.25453400 | -0.07567200 | 0.03420700 |
| Ni | -1.24205400 | -0.05386000 | 0.09013600 |
| Cl | -0.09398400 | -0.75795500 | -1.96671100 |
| N | 3.12612400 | 0.26599100 | -0.03856600 |
| N | -3.10439500 | 0.31616100 | 0.08835400 |
| N | 1.15831900 | 1.80614200 | -0.30709200 |
| N | -1.12879800 | 1.82888900 | -0.24181400 |
| C | 1.27515100 | -1.81646500 | 0.84963100 |
| C | 0.02152500 | -1.36576700 | 1.39346800 |
| C | -1.26159200 | -1.79455800 | 0.90363100 |

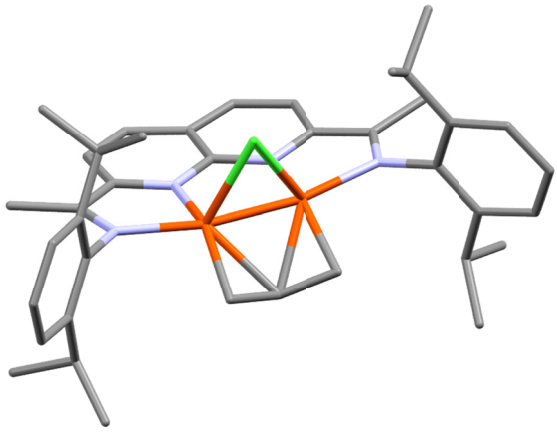
| | | | |
|---|---|---|---|
| C | 0.01670900 | 2.53003600 | -0.44967000 |
| C | 3.48284000 | 1.51485800 | -0.35085800 |
| C | -3.45674800 | 1.57565700 | -0.18892200 |
| C | 2.36316200 | 2.41912700 | -0.50974700 |
| C | 2.44541100 | 3.79873700 | -0.83340800 |
| C | 1.28703600 | 4.54634400 | -0.95842800 |
| C | 0.02112400 | 3.92183600 | -0.77820800 |
| C | -1.24152500 | 4.57063300 | -0.89125200 |
| C | -2.40476900 | 3.84477500 | -0.70558100 |
| C | -2.33204400 | 2.46382900 | -0.38273600 |
| C | 4.14792400 | -0.72537700 | 0.17038600 |
| C | 4.84399000 | -0.77788200 | 1.40586300 |
| C | 5.81143800 | -1.78521300 | 1.57451000 |
| C | 6.08275300 | -2.70924200 | 0.56405400 |
| C | 5.36706400 | -2.65458700 | -0.63647500 |
| C | 4.38369900 | -1.67741800 | -0.85704000 |
| C | -4.13373700 | -0.67486200 | 0.26522200 |
| C | -5.53317500 | -2.41990100 | -0.65645100 |
| C | -6.11401000 | -2.62590400 | 0.59790000 |
| C | -5.68361200 | -1.87029400 | 1.69116700 |
| C | -4.68527800 | -0.88980600 | 1.55537400 |
| C | 4.89839300 | 1.99180100 | -0.52881100 |
| C | -4.87146900 | 2.06784500 | -0.32843800 |
| C | -4.53373100 | -1.45199000 | -0.85184800 |
| H | 0.04625700 | -0.90776000 | 2.38913600 |
| H | 3.42276000 | 4.25934700 | -0.98703400 |
| H | 1.33181900 | 5.61132400 | -1.20076300 |
| H | -1.27882600 | 5.63590500 | -1.13344600 |
| H | -3.38024800 | 4.32189400 | -0.81478800 |
| H | 1.22820300 | -2.61148600 | 0.09440200 |
| H | 2.11791800 | -1.90605600 | 1.54393900 |
| H | 6.35828400 | -1.84639700 | 2.52004700 |
| H | 6.84198500 | -3.48117600 | 0.71569500 |
| H | 5.56961800 | -3.39310900 | -1.41629900 |
| H | -5.86084500 | -3.02405200 | -1.50735000 |
| H | -6.89286000 | -3.38240100 | 0.72563700 |
| H | -6.12808100 | -2.04592300 | 2.67503600 |
| H | -1.26091400 | -2.59269000 | 0.15103500 |
| H | -2.07465600 | -1.86495400 | 1.63360800 |
| H | 5.60446900 | 1.15188900 | -0.52197600 |
| H | 5.18766900 | 2.69031700 | 0.27611300 |
| H | 5.00881200 | 2.53289800 | -1.48317500 |
| H | -5.59282800 | 1.26954500 | -0.11408100 |
| H | -5.05819200 | 2.43202500 | -1.35351500 |
| H | -5.06749300 | 2.91036500 | 0.35650800 |
| C | -4.22987500 | -0.09128700 | 2.77817700 |
| H | -3.35524600 | 0.50700700 | 2.47259100 |
| C | -3.91066700 | -1.26047200 | -2.23372000 |
| H | -3.08652700 | -0.53707400 | -2.13614600 |
| C | 3.58978500 | -1.62658700 | -2.15940600 |
| H | 2.62959300 | -1.13468300 | -1.93035000 |
| C | 4.55037800 | 0.18397300 | 2.55909600 |
| H | 3.81015400 | 0.91958200 | 2.20578000 |
| C | 4.30862100 | -0.76831700 | -3.22404000 |
| H | 4.49210000 | 0.25615000 | -2.86459200 |
| H | 5.28226000 | -1.21123200 | -3.49564000 |
| H | 3.69402400 | -0.69895700 | -4.13622500 |
| C | 3.25593200 | -3.01940200 | -2.72358400 |
| H | 2.53554300 | -2.91773500 | -3.54998000 |
| H | 4.14852900 | -3.53438500 | -3.11859100 |
| H | 2.79840500 | -3.66436400 | -1.95750500 |
| C | 5.80933900 | 0.95799100 | 3.00745900 |
| H | 6.56800600 | 0.28008100 | 3.43249200 |
| H | 6.27809900 | 1.49501100 | 2.16834600 |
| H | 5.55095000 | 1.69521500 | 3.78558000 |
| C | 3.91942700 | -0.55720700 | 3.75917300 |
| H | 4.60895500 | -1.31522200 | 4.16600600 |
| H | 3.68169600 | 0.15229200 | 4.56925800 |
| H | 2.98937600 | -1.07046000 | 3.47066100 |
| C | -5.32823800 | 0.88059200 | 3.26538500 |
| H | -5.65341000 | 1.56485800 | 2.46693000 |
| H | -6.21680000 | 0.32630200 | 3.61157600 |
| H | -4.96207300 | 1.48939800 | 4.10887900 |
| C | -3.78107800 | -1.00776800 | 3.93737400 |
| H | -3.39100100 | -0.40333500 | 4.77299300 |
| H | -4.61912000 | -1.60921600 | 4.32669500 |
| H | -2.98859500 | -1.70344200 | 3.62130000 |
| C | -3.28992800 | -2.56721800 | -2.76867700 |
| H | -4.05523300 | -3.34410900 | -2.93746100 |
| H | -2.77833600 | -2.37603700 | -3.72509800 |
| H | -2.53863800 | -2.96236600 | -2.06967200 |
| C | -4.93484500 | -0.68741100 | -3.23789300 |
| H | -5.76988900 | -1.38989500 | -3.39996900 |
| H | -5.36413400 | 0.26347900 | -2.88375100 |
| H | -4.45426800 | -0.50314900 | -4.21259900 |



**[$^{i\text{-Pr}}$NDI]$Co_2$(allyl)Cl**
**ZPVE: -4960.608810 $E_h$**
**Charge: 0**
**Multiplicity: 3**

| | | | |
|---|---|---|---|
| Co | 1.23815900 | -0.04040700 | 0.30685100 |
| Co | -1.23564900 | -0.05017400 | 0.25549400 |
| Cl | 0.05593700 | -0.71756700 | -1.67791200 |
| N | 3.12858800 | 0.30468500 | 0.05982100 |
| N | -3.13028900 | 0.28711400 | -0.00178400 |
| N | 1.14412300 | 1.84045000 | -0.12245500 |
| N | -1.14590400 | 1.83452500 | -0.13787300 |
| C | 1.27234100 | -1.78403300 | 1.13899400 |
| C | -0.02557300 | -1.28968200 | 1.57738600 |
| C | -1.28513700 | -1.80511700 | 1.05839300 |
| C | -0.00149800 | 2.55603500 | -0.28196000 |

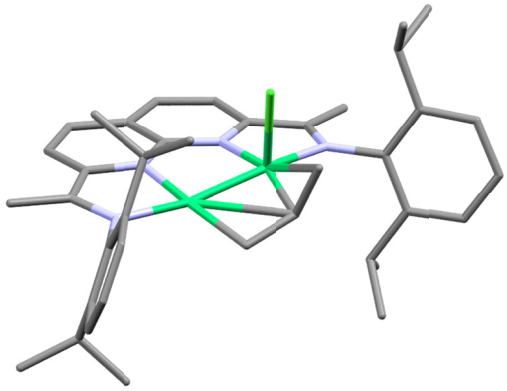
| | | | |
|---|---|---|---|
| C | 3.47527700 | 1.56827400 | -0.18925400 |
| C | -3.47738200 | 1.55792000 | -0.21620000 |
| C | 2.34985700 | 2.47401900 | -0.29172500 |
| C | 2.42255000 | 3.85722300 | -0.57697600 |
| C | 1.25891100 | 4.60075600 | -0.70638100 |
| C | -0.00312400 | 3.95903200 | -0.57356400 |
| C | -1.26712700 | 4.59926400 | -0.70069900 |
| C | -2.42880200 | 3.85313900 | -0.57191700 |
| C | -2.35384200 | 2.46643300 | -0.30292600 |
| C | 4.14959300 | -0.70736300 | 0.13874100 |
| C | 4.73313300 | -1.00899800 | 1.39875500 |
| C | 5.72429600 | -2.00361200 | 1.44687500 |
| C | 6.11765500 | -2.69338000 | 0.29679300 |
| C | 5.50626000 | -2.40456500 | -0.92548500 |
| C | 4.51351200 | -1.41556100 | -1.03448000 |
| C | -4.14850100 | -0.73033200 | 0.05080100 |
| C | -5.35669300 | -2.51812000 | -1.04966500 |
| C | -6.09042100 | -2.75044300 | 0.11732500 |
| C | -5.83553200 | -1.98365000 | 1.25613900 |
| C | -4.86622600 | -0.96474600 | 1.25350000 |
| C | 4.88336000 | 2.04558000 | -0.42381300 |
| C | -4.88707700 | 2.04655900 | -0.41300800 |
| C | -4.37149600 | -1.51934500 | -1.10785300 |
| H | -0.05926700 | -0.82826400 | 2.57469000 |
| H | 3.39788900 | 4.33167500 | -0.70069300 |
| H | 1.29902300 | 5.67109600 | -0.92356000 |
| H | -1.30964100 | 5.67071900 | -0.91172700 |
| H | -3.40530800 | 4.32783900 | -0.68546500 |
| H | 1.25032900 | -2.62243800 | 0.43138300 |
| H | 2.05847500 | -1.87152700 | 1.89860200 |
| H | 6.19222600 | -2.24562700 | 2.40488800 |
| H | 6.89059700 | -3.46421600 | 0.35638500 |
| H | 5.80259400 | -2.96006700 | -1.82003100 |
| H | -5.54725100 | -3.12779100 | -1.93716700 |
| H | -6.85200400 | -3.53438200 | 0.14172200 |
| H | -6.40058200 | -2.17679200 | 2.17266100 |
| H | -1.20407800 | -2.63536900 | 0.34550000 |
| H | -2.11477900 | -1.91605900 | 1.76715900 |
| H | 5.61265900 | 1.25427700 | -0.20960100 |
| H | 5.11768400 | 2.92117300 | 0.20389700 |
| H | 5.01543700 | 2.35529300 | -1.47526200 |
| H | -5.60240400 | 1.21531900 | -0.38212700 |
| H | -4.98799300 | 2.55577800 | -1.38618300 |
| H | -5.16739400 | 2.77631900 | 0.36572300 |
| C | 4.31666300 | -0.27298900 | 2.67361800 |
| H | 3.35092800 | 0.21716400 | 2.46058900 |
| C | 3.85068300 | -1.14680900 | -2.38495300 |
| H | 3.09128200 | -0.36266600 | -2.24022600 |
| C | -4.62301900 | -0.15887700 | 2.53219600 |
| H | -3.78684900 | 0.53301800 | 2.33859900 |
| C | -3.57894600 | -1.28538000 | -2.39199600 |
| H | -2.73085300 | -0.63006800 | -2.14082100 |
| C | 4.86859500 | -0.63946900 | -3.42966600 |
| H | 5.39596700 | 0.26284200 | -3.08061100 |
| H | 5.63083700 | -1.40487100 | -3.65243800 |
| H | 4.35702000 | -0.39231400 | -4.37431800 |
| C | 3.10491700 | -2.39493100 | -2.90336000 |
| H | 2.32822900 | -2.71158700 | -2.19229000 |
| H | 2.60429400 | -2.16705300 | -3.85817900 |
| H | 3.79536400 | -3.23872900 | -3.07154100 |
| C | 5.32946800 | 0.83076500 | 3.05464500 |
| H | 6.32065600 | 0.39410900 | 3.26310600 |
| H | 5.45237200 | 1.57043300 | 2.24983700 |
| H | 4.99738900 | 1.36582300 | 3.96002900 |
| C | 4.10163300 | -1.22175400 | 3.87133500 |
| H | 3.68364900 | -0.66349900 | 4.72506000 |
| H | 3.40752000 | -2.04007000 | 3.62523100 |
| H | 5.04853100 | -1.67353000 | 4.21006400 |
| C | -5.85981700 | 0.68339000 | 2.91980900 |
| H | -6.17333100 | 1.35194000 | 2.10395800 |
| H | -6.71667400 | 0.03332500 | 3.16362800 |
| H | -5.64578900 | 1.30227500 | 3.80711500 |
| C | -4.21191300 | -1.06226100 | 3.71619900 |
| H | -3.32133100 | -1.66377400 | 3.47912200 |
| H | -3.98525400 | -0.45018100 | 4.60497500 |
| H | -5.02220500 | -1.75801100 | 3.98928800 |
| C | -4.43774400 | -0.56697200 | -3.45607100 |
| H | -5.29435700 | -1.19078300 | -3.76399100 |
| H | -4.83935100 | 0.38684100 | -3.07798500 |
| H | -3.83545300 | -0.35020000 | -4.35363600 |
| C | -2.97719600 | -2.58678900 | -2.95732000 |
| H | -2.33002600 | -2.35553400 | -3.81809900 |
| H | -2.35674200 | -3.09476300 | -2.20417000 |
| H | -3.75618800 | -3.28945000 | -3.29926500 |



**[$^{i\text{-Pr}}$NDI]Fe$_2$(allyl)Cl**
**ZPVE: -4722.476399 E$_h$**
**Charge: 0**
**Multiplicity: 5**

| | | | |
|---|---|---|---|
| Fe | 1.14367500 | -0.04085100 | 0.27470700 |
| Fe | -1.14382200 | -0.04098600 | 0.27432200 |
| Cl | 0.00004900 | -1.12957900 | -1.52021100 |
| N | 3.11150200 | 0.28009200 | -0.00947900 |
| N | -3.11156600 | 0.28035300 | -0.00899800 |
| N | 1.14125900 | 1.82756300 | -0.29235100 |
| N | -1.14135200 | 1.82769400 | -0.29192000 |
| C | 1.27630900 | -1.33018700 | 1.76856100 |
| C | -0.00053600 | -0.73539700 | 2.08364600 |
| C | -1.27577600 | -1.33250200 | 1.76640500 |
| C | -0.00003700 | 2.54278300 | -0.50030300 |
| C | 3.46142900 | 1.51672600 | -0.41079000 |

| | | | |
|---|---|---|---|
| C | -3.46158000 | 1.51716300 | -0.40972900 |
| C | 2.35929000 | 2.42139000 | -0.55286400 |
| C | 2.43077700 | 3.78433300 | -0.95536400 |
| C | 1.27179100 | 4.51655900 | -1.13338000 |
| C | -0.00002500 | 3.89690500 | -0.93130100 |
| C | -1.27182800 | 4.51678100 | -1.13274700 |
| C | -2.43084800 | 3.78473000 | -0.95425300 |
| C | -2.35940200 | 2.42173300 | -0.55192300 |
| C | 4.12497800 | -0.72946800 | 0.14048700 |
| C | 4.84071600 | -0.84899300 | 1.36518400 |
| C | 5.81438200 | -1.85736400 | 1.47011900 |
| C | 6.07784100 | -2.73106500 | 0.41265000 |
| C | 5.35410200 | -2.61132400 | -0.77579200 |
| C | 4.36966800 | -1.62218700 | -0.93796600 |
| C | -4.12495100 | -0.72931600 | 0.14075800 |
| C | -5.35444600 | -2.61059500 | -0.77616400 |
| C | -6.07753400 | -2.73120800 | 0.41258900 |
| C | -5.81355700 | -1.85823700 | 1.47053700 |
| C | -4.84000700 | -0.84974000 | 1.36576100 |
| C | 4.86449000 | 1.93931800 | -0.76049900 |
| C | -4.86473800 | 1.93997200 | -0.75875300 |
| C | -4.37014800 | -1.62129700 | -0.93818300 |
| H | -0.00185100 | 0.05910200 | 2.83997900 |
| H | 3.40683500 | 4.24045300 | -1.13090900 |
| H | 1.31489900 | 5.56392800 | -1.44345200 |
| H | -1.31490800 | 5.56418100 | -1.44272200 |
| H | -3.40691400 | 4.24101100 | -1.12933800 |
| H | 1.26916000 | -2.35550500 | 1.37350100 |
| H | 2.11454100 | -1.11542900 | 2.43540500 |
| H | 6.37843700 | -1.95811100 | 2.40163200 |
| H | 6.84118400 | -3.50673600 | 0.51725800 |
| H | 5.55786700 | -3.29868300 | -1.60191500 |
| H | -5.55859300 | -3.29741800 | -1.60263700 |
| H | -6.84075200 | -3.50701900 | 0.51707100 |
| H | -6.37710200 | -1.95965900 | 2.40228200 |
| H | -1.26577200 | -2.35737200 | 1.37024100 |
| H | -2.11533400 | -1.12046500 | 2.43245000 |
| H | 5.58249000 | 1.13112400 | -0.57230800 |
| H | 5.17487800 | 2.82521400 | -0.18129900 |
| H | 4.93098600 | 2.21220200 | -1.82795300 |
| H | -5.58282700 | 1.13201500 | -0.56988800 |
| H | -4.93183400 | 2.21250600 | -1.82626400 |
| H | -5.17454600 | 2.82613300 | -0.17965400 |
| C | -4.60376700 | 0.09005300 | 2.55038000 |
| H | -3.67689000 | 0.65088500 | 2.34230900 |
| C | -3.61394900 | -1.51242600 | -2.26103500 |
| H | -2.80225700 | -0.78201500 | -2.12089200 |
| C | 3.61285800 | -1.51420700 | -2.26053000 |
| H | 2.80125000 | -0.78368300 | -2.12050400 |
| C | 4.60501100 | 0.09142400 | 2.54940000 |
| H | 3.67817800 | 0.65234000 | 2.34136800 |
| C | 4.53300100 | -0.99463200 | -3.38796200 |
| H | 4.98815500 | -0.02590000 | -3.12767900 |
| H | 5.35253700 | -1.70540800 | -3.58882300 |
| H | 3.96163900 | -0.86380500 | -4.32176100 |
| C | 2.95489200 | -2.84909000 | -2.66556700 |
| H | 2.28131900 | -3.21615100 | -1.87719200 |
| H | 2.35246400 | -2.71064100 | -3.57749100 |
| H | 3.70673100 | -3.62957200 | -2.87250200 |
| C | 5.75520800 | 1.11331600 | 2.70619500 |
| H | 6.70440700 | 0.59773300 | 2.92973300 |
| H | 5.90667800 | 1.70929100 | 1.79482700 |
| H | 5.54473200 | 1.80736300 | 3.53698800 |
| C | 4.41357900 | -0.66751800 | 3.88156500 |
| H | 4.12097600 | 0.03444100 | 4.67975400 |
| H | 3.63850900 | -1.44557600 | 3.80803900 |
| H | 5.34655500 | -1.15846000 | 4.20414300 |
| C | -4.41205000 | -0.66945400 | 3.88216400 |
| H | -3.63698600 | -1.44747500 | 3.80815600 |
| H | -4.11923700 | 0.03217600 | 4.68056400 |
| H | -5.34494300 | -1.16051800 | 4.20479300 |
| C | -5.75373900 | 1.11208400 | 2.70793900 |
| H | -5.90531100 | 1.70850600 | 1.79688400 |
| H | -6.70297200 | 0.59655800 | 2.93146300 |
| H | -5.54292800 | 1.80570300 | 3.53900400 |
| C | -4.53464500 | -0.99201300 | -3.38763800 |
| H | -5.35435400 | -1.70258400 | -3.58852200 |
| H | -4.98957900 | -0.02343100 | -3.12642900 |
| H | -3.96378900 | -0.86059900 | -4.32166300 |
| C | -2.95623600 | -2.84704200 | -2.66734300 |
| H | -2.35416900 | -2.70795300 | -3.57940900 |
| H | -2.28238400 | -3.21475200 | -1.87951400 |
| H | -3.70822800 | -3.62729600 | -2.87458000 |



**Transition State: [$^{i\text{-Pr}}$NDI]Ni$_2$(allyl)Cl**
**ZPVE: -5211.671515 $E_h$**
**Charge: 0**
**Multiplicity: 1**

| | | | |
|---|---|---|---|
| C | -2.30428900 | 3.98854100 | -0.18535500 |
| C | -1.14593900 | 4.73042200 | -0.38136200 |
| C | 0.11332600 | 4.06751700 | -0.45764300 |
| C | 0.09734200 | 2.64315500 | -0.33151100 |
| C | -2.24269600 | 2.57917700 | -0.06832500 |
| H | 1.45190700 | 5.76721900 | -0.72043600 |
| H | -3.27190000 | 4.49133700 | -0.12428600 |
| H | -1.18987000 | 5.81918400 | -0.46453400 |
| C | 1.38532600 | 4.68095200 | -0.62025000 |
| C | 2.44159400 | 2.49689000 | -0.48131600 |
| C | 2.53783400 | 3.89805700 | -0.62898500 |
| H | 3.51865800 | 4.36676500 | -0.73343100 |
| N | 1.22361200 | 1.88613000 | -0.37146400 |
| N | -1.04222800 | 1.92442400 | -0.15178700 |
| C | -3.35580700 | 1.67406800 | 0.17022200 |
| C | 3.53692900 | 1.53505100 | -0.40596100 |

| | | | |
|---|---|---|---|
| C | -4.75417200 | 2.20054500 | 0.35489500 |
| H | -4.78316500 | 2.98737200 | 1.12687700 |
| H | -5.13211100 | 2.64768100 | -0.58056400 |
| H | -5.44147200 | 1.39646500 | 0.64872400 |
| C | 4.96008600 | 1.94817800 | -0.66261300 |
| H | 5.35405100 | 2.54709800 | 0.17771900 |
| H | 5.60780200 | 1.06936400 | -0.78081900 |
| H | 5.03422800 | 2.56925600 | -1.56973800 |
| N | -3.00410500 | 0.39347400 | 0.23223100 |
| N | 3.14194300 | 0.30775200 | -0.08501800 |
| C | -3.96935900 | -0.62830100 | 0.49356200 |
| C | -4.78886200 | -1.13774500 | -0.55140700 |
| C | -4.02041700 | -1.18381700 | 1.80504000 |
| C | -5.65408300 | -2.20465100 | -0.25014300 |
| C | -4.90803400 | -2.24356000 | 2.04638000 |
| C | -5.72195100 | -2.75575000 | 1.03107000 |
| H | -6.29053300 | -2.60737400 | -1.04345100 |
| H | -4.96148000 | -2.67608900 | 3.04870500 |
| H | -6.40353000 | -3.58495700 | 1.23811900 |
| C | 4.08454000 | -0.76693200 | -0.00141400 |
| C | 4.11539900 | -1.71462100 | -1.06088800 |
| C | 4.88990500 | -0.92461200 | 1.15612400 |
| C | 5.00019400 | -2.79879500 | -0.95320200 |
| C | 5.75271600 | -2.03315400 | 1.21262900 |
| C | 5.82034300 | -2.95849900 | 0.16875600 |
| H | 5.04052600 | -3.53519200 | -1.75950700 |
| H | 6.37832300 | -2.17459200 | 2.09869300 |
| H | 6.50093900 | -3.81148400 | 0.23462400 |
| C | 4.78917800 | 0.02173600 | 2.35239000 |
| H | 4.16377200 | 0.87829000 | 2.05458800 |
| C | 3.21725100 | -1.53171400 | -2.28132400 |
| H | 2.32275600 | -0.97979000 | -1.93476300 |
| C | -3.16890800 | -0.60062800 | 2.93279800 |
| H | -2.30479100 | -0.10855600 | 2.45149900 |
| C | -4.76792800 | -0.57213500 | -1.97346400 |
| H | -4.00968500 | 0.22648000 | -2.01050900 |
| Ni | 1.21548800 | 0.06150700 | 0.07776300 |
| Ni | -1.06012900 | 0.05367200 | -0.01414900 |
| C | -0.57151400 | -1.79839100 | 0.49174200 |
| H | -1.30032800 | -1.94416100 | 1.30449200 |
| Cl | -0.72593300 | -1.11261400 | -2.42235600 |
| C | -1.00045100 | -2.43688100 | -0.72808300 |
| C | 0.86362100 | -1.68307200 | 0.81914600 |
| H | -0.36293400 | -3.19416900 | -1.19579800 |
| H | -2.07178600 | -2.62581000 | -0.83191700 |
| H | 1.53039200 | -2.41189200 | 0.32193500 |
| H | 1.05333300 | -1.66733800 | 1.90435400 |
| C | 2.72520000 | -2.85725700 | -2.88758400 |
| H | 1.94402800 | -2.65333900 | -3.63604500 |
| H | 3.53639000 | -3.41130900 | -3.39041200 |
| H | 2.29099500 | -3.51417400 | -2.11744800 |
| C | 3.90251500 | -0.66369000 | -3.36026400 |
| H | 4.20055300 | 0.31890700 | -2.96266200 |
| H | 4.80905100 | -1.16081700 | -3.74609200 |
| H | 3.21717300 | -0.49184400 | -4.20620000 |
| C | 4.07275300 | -0.67218400 | 3.53272700 |
| H | 4.64826800 | -1.54452300 | 3.88451100 |
| H | 3.95521700 | 0.02330900 | 4.38073200 |
| H | 3.07372200 | -1.02350900 | 3.23316000 |
| C | 6.16226400 | 0.57363400 | 2.79042100 |
| H | 6.81762800 | -0.22606100 | 3.17358100 |
| H | 6.68917500 | 1.06336100 | 1.95596800 |
| H | 6.03939200 | 1.31274500 | 3.59937900 |
| C | -4.35422500 | -1.63310800 | -3.01658900 |
| H | -5.02737200 | -2.50639600 | -2.99535300 |
| H | -4.39585500 | -1.20195300 | -4.03058200 |
| H | -3.32185000 | -1.97339000 | -2.85071200 |
| C | -6.13642000 | 0.04149800 | -2.35049500 |
| H | -6.92019100 | -0.73333100 | -2.39207200 |
| H | -6.46262700 | 0.80232200 | -1.62432900 |
| H | -6.08385600 | 0.51532500 | -3.34464200 |
| C | -3.94932800 | 0.48292800 | 3.71161000 |
| H | -4.30417700 | 1.28505600 | 3.04670600 |
| H | -4.83095800 | 0.04640100 | 4.21111200 |
| H | -3.31025600 | 0.94076600 | 4.48504200 |
| C | -2.62231300 | -1.66434500 | 3.90409200 |
| H | -1.91706400 | -1.20002200 | 4.61225700 |
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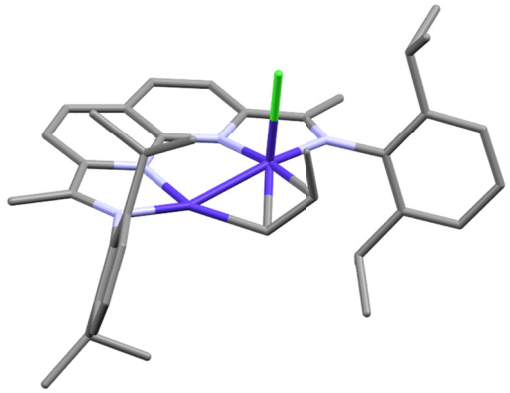
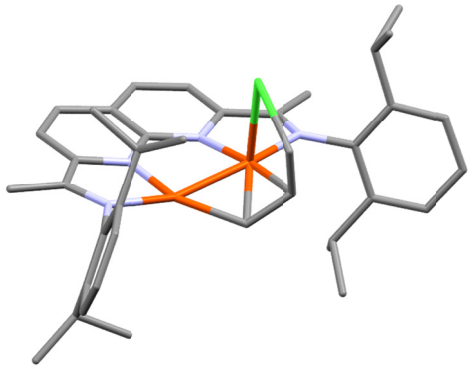
| H | -2.08941100 | -2.46725600 | 3.37076900 |



**Transition state: [$^{i\text{-Pr}}$NDI]$Co_2$(allyl)Cl**
**ZPVE: -4960.558035 $E_h$**
**Charge: 0**
**Multiplicity: 3**

| | | | |
|---|---|---|---|
| C | -2.29300000 | 3.91900000 | -0.24000000 |
| C | -1.12500000 | 4.65600000 | -0.43800000 |
| C | 0.13700000 | 4.00900000 | -0.42100000 |
| C | 0.14000000 | 2.59300000 | -0.17600000 |
| C | -2.23100000 | 2.52900000 | -0.04100000 |
| H | 1.44600000 | 5.70400000 | -0.82400000 |
| H | -3.26600000 | 4.41400000 | -0.26600000 |
| H | -1.17300000 | 5.73400000 | -0.61500000 |
| C | 1.40200000 | 4.63000000 | -0.62400000 |
| C | 2.51200000 | 2.48800000 | -0.32300000 |
| C | 2.56600000 | 3.87000000 | -0.59000000 |
| H | 3.53500000 | 4.34400000 | -0.76300000 |
| N | 1.28400000 | 1.87700000 | -0.06700000 |
| N | -1.00300000 | 1.88000000 | 0.00600000 |
| C | -3.33400000 | 1.62700000 | 0.12800000 |
| C | 3.58900000 | 1.55200000 | -0.27100000 |
| C | -4.74400000 | 2.12800000 | 0.29700000 |
| H | -4.77900000 | 2.98300000 | 0.99100000 |
| H | -5.15700000 | 2.47200000 | -0.66700000 |
| H | -5.40300000 | 1.33800000 | 0.68000000 |

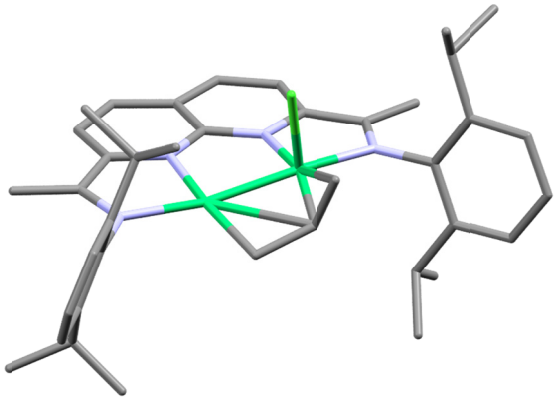
| | | | |
|---|---|---|---|
| C | 5.03200000 | 1.94900000 | -0.42200000 |
| H | 5.48900000 | 2.17800000 | 0.55800000 |
| H | 5.62000000 | 1.13600000 | -0.87000000 |
| H | 5.13400000 | 2.84500000 | -1.05100000 |
| N | -2.97900000 | 0.33300000 | 0.13800000 |
| N | 3.18500000 | 0.28300000 | -0.05800000 |
| C | -3.94800000 | -0.67700000 | 0.45900000 |
| C | -4.78700000 | -1.23100000 | -0.54400000 |
| C | -4.00900000 | -1.14400000 | 1.80300000 |
| C | -5.69900000 | -2.23300000 | -0.16700000 |
| C | -4.93900000 | -2.14700000 | 2.12300000 |
| C | -5.78500000 | -2.68800000 | 1.15000000 |
| H | -6.35700000 | -2.66400000 | -0.92800000 |
| H | -5.00200000 | -2.50800000 | 3.15300000 |
| H | -6.50400000 | -3.46700000 | 1.41800000 |
| C | 4.13700000 | -0.78200000 | 0.01900000 |
| C | 4.31300000 | -1.61500000 | -1.11900000 |
| C | 4.85600000 | -1.01800000 | 1.22300000 |
| C | 5.24600000 | -2.66200000 | -1.04000000 |
| C | 5.77100000 | -2.08300000 | 1.25000000 |
| C | 5.97700000 | -2.89400000 | 0.12900000 |
| H | 5.40000000 | -3.30900000 | -1.90800000 |
| H | 6.33600000 | -2.28000000 | 2.16400000 |
| H | 6.70000000 | -3.71200000 | 0.17100000 |
| C | 4.57700000 | -0.19000000 | 2.47800000 |
| H | 4.27800000 | 0.82000000 | 2.15100000 |
| C | 3.51100000 | -1.36700000 | -2.39400000 |
| H | 2.61500000 | -0.79400000 | -2.09600000 |
| C | -3.10900000 | -0.55000000 | 2.88500000 |
| H | -2.28400000 | -0.03700000 | 2.36100000 |
| C | -4.73300000 | -0.78000000 | -2.00400000 |
| H | -3.91800000 | -0.04400000 | -2.09900000 |
| Co | 1.29300000 | 0.05900000 | 0.28200000 |
| Co | -1.05600000 | 0.01100000 | -0.05100000 |
| C | -0.89300000 | -2.00100000 | 0.03400000 |
| H | -1.77200000 | -2.49700000 | 0.45600000 |
| Cl | -1.04100000 | -0.57800000 | -2.63100000 |
| C | -0.55900000 | -2.23300000 | -1.34200000 |
| C | 0.04700000 | -1.27900000 | 0.88200000 |
| H | 0.50100000 | -2.20000000 | -1.60300000 |
| H | -1.13400000 | -2.98000000 | -1.89300000 |
| H | 1.19900000 | -1.54200000 | 0.55700000 |
| H | -0.05000000 | -1.42500000 | 1.96800000 |
| C | 3.03700000 | -2.66800000 | -3.07000000 |
| H | 2.33000000 | -2.43400000 | -3.88200000 |
| H | 3.87400000 | -3.23100000 | -3.51700000 |
| H | 2.53100000 | -3.33600000 | -2.35500000 |
| C | 4.29800000 | -0.49300000 | -3.39700000 |
| H | 4.56800000 | 0.48000000 | -2.96000000 |
| H | 5.22800000 | -0.99600000 | -3.71000000 |
| H | 3.69200000 | -0.30000000 | -4.29800000 |
| C | 3.37000000 | -0.78500000 | 3.23700000 |
| H | 3.58300000 | -1.81400000 | 3.57100000 |
| H | 3.11900000 | -0.17600000 | 4.12200000 |
| H | 2.48500000 | -0.81200000 | 2.58000000 |
| C | 5.79400000 | -0.03700000 | 3.40900000 |
| H | 6.07400000 | -0.99200000 | 3.88300000 |
| H | 6.67600000 | 0.34300000 | 2.86800000 |
| H | 5.56000000 | 0.67000000 | 4.22100000 |
| C | -4.39800000 | -1.95500000 | -2.94700000 |
| H | -5.18900000 | -2.72300000 | -2.93100000 |
| H | -4.29600000 | -1.59500000 | -3.98400000 |
| H | -3.44700000 | -2.43000000 | -2.66600000 |
| C | -6.05200000 | -0.10700000 | -2.44300000 |
| H | -6.89300000 | -0.82000000 | -2.41200000 |
| H | -6.31600000 | 0.74400000 | -1.79600000 |
| H | -5.96800000 | 0.26500000 | -3.47800000 |
| C | -3.86400000 | 0.50500000 | 3.72400000 |
| H | -4.26800000 | 1.31100000 | 3.09300000 |
| H | -4.70900000 | 0.04500000 | 4.26400000 |
| H | -3.19200000 | 0.96200000 | 4.46900000 |
| C | -2.48300000 | -1.61900000 | 3.80200000 |
| H | -1.74800000 | -1.15400000 | 4.47900000 |
| H | -3.23900000 | -2.11500000 | 4.43400000 |
| H | -1.96800000 | -2.40100000 | 3.22100000 |



**Transition state: [$^{i\text{-Pr}}$NDI]$Fe_2$(allyl)Cl**
**ZPVE: -4722.401865 $E_h$**
**Charge: 0**
**Multiplicity: 5**

| | | | |
|---|---|---|---|
| C | -2.28096900 | 3.90976700 | -0.45594200 |
| C | -1.10868600 | 4.62769600 | -0.68596600 |
| C | 0.14734000 | 3.97214200 | -0.63661900 |
| C | 0.14733700 | 2.57133000 | -0.29792700 |
| C | -2.22992000 | 2.53624600 | -0.17055400 |
| H | 1.43991300 | 5.63964800 | -1.16741000 |
| H | -3.25082300 | 4.40652400 | -0.52807100 |
| H | -1.14711500 | 5.69254500 | -0.92858100 |
| C | 1.40463200 | 4.58017400 | -0.90265100 |
| C | 2.52252200 | 2.46001900 | -0.51075100 |
| C | 2.57053800 | 3.82148600 | -0.85487600 |
| H | 3.53446600 | 4.28316400 | -1.07946900 |
| N | 1.29660600 | 1.85874900 | -0.19209300 |
| N | -0.99945600 | 1.87601900 | -0.06180500 |
| C | -3.35270200 | 1.67239300 | 0.01673700 |
| C | 3.60520900 | 1.53848700 | -0.43903600 |
| C | -4.75981000 | 2.20442000 | 0.09977000 |
| H | -4.79726600 | 3.14343700 | 0.67230300 |
| H | -5.16365700 | 2.41397900 | -0.90608600 |
| H | -5.42702200 | 1.47410200 | 0.57788100 |
| C | 5.03613200 | 1.92950200 | -0.69340400 |
| H | 5.53318900 | 2.27636600 | 0.23045500 |
| H | 5.61670900 | 1.07553900 | -1.07087700 |
| H | 5.09833200 | 2.74596600 | -1.42781000 |

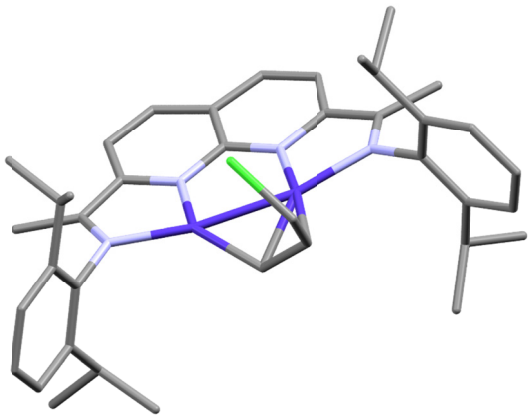
| | | | |
|---|---|---|---|
| N | -3.03644300 | 0.37025000 | 0.11411800 |
| N | 3.22131200 | 0.28544500 | -0.10580500 |
| C | -4.02828100 | -0.60236000 | 0.46733100 |
| C | -4.88203200 | -1.17309300 | -0.51421200 |
| C | -4.09655400 | -1.02421700 | 1.82651600 |
| C | -5.81108200 | -2.14565200 | -0.10172300 |
| C | -5.04324400 | -1.99738300 | 2.18294500 |
| C | -5.90110200 | -2.55520500 | 1.22995400 |
| H | -6.47972500 | -2.58927900 | -0.84538900 |
| H | -5.11221100 | -2.32306700 | 3.22455400 |
| H | -6.63362700 | -3.31127800 | 1.52492100 |
| C | 4.19463200 | -0.75345900 | 0.03978900 |
| C | 4.34203800 | -1.70411700 | -1.00602400 |
| C | 4.96927100 | -0.84432700 | 1.23011000 |
| C | 5.30239000 | -2.71851000 | -0.85484200 |
| C | 5.91319900 | -1.87891100 | 1.33044200 |
| C | 6.08977900 | -2.80368300 | 0.29611100 |
| H | 5.43441800 | -3.45511400 | -1.65155200 |
| H | 6.52220500 | -1.96552700 | 2.23343200 |
| H | 6.83500000 | -3.59780600 | 0.39326300 |
| C | 4.70783500 | 0.10068600 | 2.40333000 |
| H | 4.41585700 | 1.07971300 | 1.98752600 |
| C | 3.48141700 | -1.61360700 | -2.26443400 |
| H | 2.56359300 | -1.06710000 | -1.97949600 |
| C | -3.18593700 | -0.40408500 | 2.88648500 |
| H | -2.34538600 | 0.06943900 | 2.34598200 |
| C | -4.81929900 | -0.77650400 | -1.98927300 |
| H | -4.02302400 | -0.02345700 | -2.10048800 |
| Fe | 1.31733800 | 0.03424800 | 0.26043300 |
| Fe | -1.07371700 | -0.04359500 | 0.08851000 |
| C | -0.87922500 | -2.07321300 | 0.28836000 |
| H | -1.73457500 | -2.51643600 | 0.80891800 |
| Cl | -0.93865100 | -0.93612900 | -2.46070100 |
| C | -0.62047200 | -2.48781700 | -1.06687700 |
| C | 0.13671000 | -1.31227200 | 1.01499500 |
| H | 0.42736800 | -2.62900700 | -1.34796700 |
| H | -1.29262200 | -3.23200300 | -1.50096300 |
| H | 1.26311200 | -1.61306800 | 0.65280900 |
| H | 0.09896100 | -1.38057400 | 2.11415100 |
| C | 3.05695800 | -2.99232400 | -2.80554100 |
| H | 2.31226700 | -2.86937100 | -3.60808800 |
| H | 3.90859100 | -3.54838400 | -3.23242500 |
| H | 2.61298400 | -3.61910500 | -2.01510600 |
| C | 4.17540600 | -0.78813900 | -3.37022500 |
| H | 4.40731600 | 0.23114900 | -3.02644600 |
| H | 5.11969800 | -1.26687100 | -3.68050400 |
| H | 3.52441500 | -0.70481400 | -4.25602500 |
| C | 3.49982500 | -0.41524700 | 3.21856700 |
| H | 3.72072200 | -1.39763900 | 3.66795400 |
| H | 3.23358500 | 0.28749900 | 4.02530300 |
| H | 2.62560500 | -0.53264300 | 2.55650600 |
| C | 5.92697500 | 0.33269400 | 3.31331900 |
| H | 6.20396400 | -0.57644100 | 3.87253200 |
| H | 6.80887900 | 0.66030900 | 2.73966000 |
| H | 5.69603100 | 1.11117800 | 4.05834800 |
| C | -4.44032200 | -1.97764700 | -2.88205500 |
| H | -5.19649900 | -2.77822600 | -2.82132300 |
| H | -4.36426700 | -1.66226700 | -3.93545700 |
| H | -3.46534300 | -2.39304700 | -2.59022200 |
| C | -6.14868800 | -0.15410000 | -2.47309000 |
| H | -6.96777100 | -0.89223400 | -2.44474700 |
| H | -6.45347900 | 0.70224200 | -1.85206100 |
| H | -6.05232700 | 0.19531200 | -3.51437400 |
| C | -3.91682200 | 0.71246400 | 3.66489300 |
| H | -4.29008900 | 1.49763000 | 2.98983700 |
| H | -4.78052100 | 0.30183600 | 4.21498300 |
| H | -3.23959800 | 1.18564200 | 4.39523800 |
| C | -2.59013000 | -1.44009000 | 3.85873700 |
| H | -1.85075600 | -0.95817000 | 4.51922300 |
| H | -3.36221600 | -1.88687600 | 4.50689100 |
| H | -2.08767700 | -2.26073700 | 3.32253300 |



**Pre-OA Complex: [$^{i\text{-}Pr}$NDI]Ni$_2$(allyl)Cl**
**ZPVE: -5211.677999 $E_h$**
**Charge: 0**
**Multiplicity: 1**

| | | | |
|---|---|---|---|
| Ni | 1.15398300 | -0.00805000 | 0.16664800 |
| Ni | -1.09188900 | 0.04536300 | 0.01039300 |
| Cl | -0.13952000 | 0.07895200 | -3.19839900 |
| C | -2.39369700 | 3.85545800 | 0.87778500 |
| C | -1.23152800 | 4.61773100 | 0.95667300 |
| C | 0.03823100 | 3.98173400 | 0.86177700 |
| C | 0.03562100 | 2.56334300 | 0.67496300 |
| C | -2.31685100 | 2.45646100 | 0.69748900 |
| H | 1.37003300 | 5.69841500 | 1.05078200 |
| H | -3.37036900 | 4.34071500 | 0.93900700 |
| H | -1.28543800 | 5.70199200 | 1.08204400 |
| C | 1.31100800 | 4.61442500 | 0.92465500 |
| C | 2.38621200 | 2.45062000 | 0.64741000 |
| C | 2.47031100 | 3.85073700 | 0.81837100 |
| H | 3.44907900 | 4.33324800 | 0.86213800 |
| N | 1.17148100 | 1.82612100 | 0.58759900 |
| N | -1.10483200 | 1.82390200 | 0.62379800 |
| C | -3.42526100 | 1.51770600 | 0.57089600 |
| C | 3.49444600 | 1.51118700 | 0.50481400 |
| C | -4.81965400 | 1.91194200 | 0.97920700 |
| H | -5.14638200 | 2.82505400 | 0.45414400 |
| H | -5.53933500 | 1.11095600 | 0.76755900 |
| H | -4.85558900 | 2.13435000 | 2.05982500 |
| C | 4.92206700 | 1.96889600 | 0.63373600 |
| H | 5.05075900 | 2.60878800 | 1.52164200 |
| H | 5.60167800 | 1.11012600 | 0.71493400 |
| H | 5.23065700 | 2.56162800 | -0.24519100 |

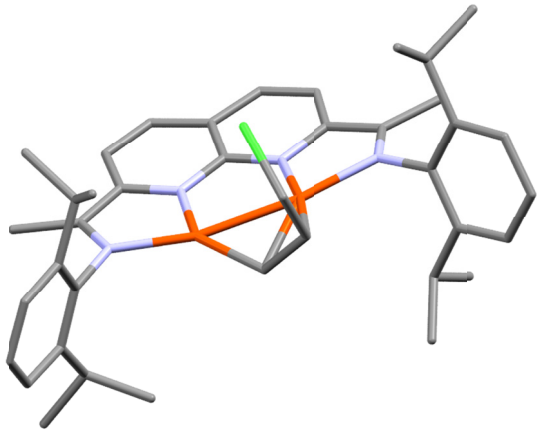
| | | | |
|---|---|---|---|
| N | -3.05525100 | 0.31218000 | 0.15082000 |
| N | 3.10908400 | 0.26475200 | 0.26157700 |
| C | -4.01422900 | -0.74945300 | 0.08346900 |
| C | -4.74190400 | -0.97350800 | -1.11796700 |
| C | -4.16403300 | -1.60815600 | 1.20438000 |
| C | -5.67027500 | -2.02817400 | -1.13887700 |
| C | -5.10149300 | -2.65087000 | 1.12471000 |
| C | -5.86419200 | -2.85479500 | -0.02801600 |
| H | -6.24748900 | -2.21006700 | -2.04916600 |
| H | -5.23192400 | -3.31519600 | 1.98393000 |
| H | -6.59348800 | -3.66804600 | -0.06921900 |
| C | 4.06138600 | -0.78764400 | 0.09592200 |
| C | 4.81580100 | -0.91587900 | -1.10017300 |
| C | 4.14979000 | -1.76080700 | 1.13029800 |
| C | 5.67953600 | -2.01990400 | -1.21770400 |
| C | 5.03518100 | -2.83486000 | 0.96391000 |
| C | 5.80246900 | -2.96632700 | -0.19883900 |
| H | 6.26354400 | -2.13911700 | -2.13476200 |
| H | 5.11936000 | -3.58546400 | 1.75368500 |
| H | 6.48470900 | -3.81264500 | -0.31453600 |
| C | 3.31041900 | -1.60069300 | 2.39418500 |
| H | 2.41520300 | -1.02411700 | 2.08831400 |
| C | 4.67159000 | 0.05188200 | -2.27541300 |
| H | 4.04387900 | 0.89629000 | -1.94940400 |
| C | -3.31678900 | -1.43011000 | 2.46416000 |
| H | -2.59897100 | -0.61687200 | 2.26441100 |
| C | -4.52621200 | -0.10429000 | -2.35900900 |
| H | -3.53483300 | 0.36987800 | -2.25126400 |
| C | -0.59201800 | -1.56136000 | -0.94845300 |
| H | -1.31062600 | -2.29773800 | -0.52922400 |
| C | -0.88129400 | -1.44813100 | -2.41949000 |
| C | 0.82334300 | -1.75431700 | -0.54858900 |
| H | -0.44417300 | -2.26401600 | -3.01839400 |
| H | -1.95226900 | -1.36123100 | -2.63123700 |
| H | 1.54492700 | -1.96326900 | -1.35843600 |
| H | 0.94481400 | -2.47418400 | 0.27991500 |
| C | -5.57631500 | 1.02485900 | -2.47150900 |
| H | -6.59253100 | 0.60368200 | -2.55531200 |
| H | -5.56108800 | 1.69382500 | -1.59944200 |
| H | -5.38701500 | 1.63651800 | -3.36923500 |
| C | -4.51657700 | -0.92539700 | -3.66597500 |
| H | -5.52394200 | -1.29232400 | -3.92433200 |
| H | -4.17200200 | -0.29729300 | -4.50277500 |
| H | -3.85003600 | -1.79911800 | -3.59882800 |
| C | -4.17656700 | -1.02127500 | 3.67923400 |
| H | -4.74410600 | -0.09847900 | 3.48077100 |
| H | -4.90344900 | -1.81039300 | 3.93538900 |
| H | -3.54157500 | -0.84873100 | 4.56404800 |
| C | -2.49102000 | -2.69601300 | 2.77590500 |
| H | -1.84540500 | -2.52594500 | 3.65323900 |
| H | -3.13975500 | -3.55921500 | 2.99961100 |
| H | -1.84659900 | -2.96748100 | 1.92559200 |
| C | 4.05660000 | -0.76783500 | 3.46028000 |
| H | 4.97204700 | -1.28701000 | 3.79135700 |
| H | 4.35185700 | 0.21816300 | 3.06889400 |
| H | 3.41769200 | -0.60352800 | 4.34415500 |
| C | 2.82700200 | -2.93622700 | 2.98536300 |
| H | 3.65758500 | -3.52995900 | 3.40358100 |
| H | 2.11676800 | -2.74848600 | 3.80688100 |
| H | 2.31780500 | -3.55086000 | 2.22681400 |
| C | 3.94027700 | -0.62495600 | -3.45641100 |
| H | 3.82069600 | 0.08239000 | -4.29377600 |
| H | 4.50852000 | -1.49586900 | -3.82378500 |
| H | 2.93734900 | -0.96647100 | -3.16029400 |
| C | 6.03043400 | 0.62572400 | -2.73307100 |
| H | 6.57760200 | 1.09854000 | -1.90183800 |
| H | 6.67977700 | -0.16017200 | -3.15318100 |
| H | 5.88097700 | 1.38277400 | -3.52052400 |



**Pre-OA Complex: [$^{i\text{-Pr}}$NDI]$Co_2$(allyl)Cl**
**ZPVE: -4960.562296 $E_h$**
**Charge: 0**
**Multiplicity: 3**

| | | | |
|---|---|---|---|
| Co | 1.26680800 | 0.16120800 | 0.16918800 |
| Co | -1.10945200 | 0.13453200 | 0.22524600 |
| Cl | -0.17016600 | -2.61075100 | -1.56164100 |
| C | -2.29405100 | 3.82221100 | -1.23780900 |
| C | -1.11801300 | 4.49609100 | -1.56473200 |
| C | 0.13736900 | 3.86675200 | -1.36593400 |
| C | 0.12253100 | 2.55266900 | -0.77556200 |
| C | -2.24486900 | 2.52652000 | -0.69775800 |
| H | 1.45080100 | 5.40299100 | -2.16983500 |
| H | -3.26223800 | 4.29438200 | -1.41655800 |
| H | -1.15381300 | 5.49624100 | -2.00357900 |
| C | 1.40229700 | 4.41074700 | -1.71472500 |
| C | 2.49842000 | 2.39534400 | -0.91946400 |
| C | 2.56437800 | 3.67236700 | -1.50139800 |
| H | 3.53530800 | 4.08434300 | -1.78458700 |
| N | 1.26684500 | 1.86704400 | -0.52365300 |
| N | -1.02108400 | 1.91490500 | -0.42508400 |
| C | -3.36020800 | 1.67947600 | -0.40219400 |
| C | 3.57239300 | 1.49931900 | -0.63320700 |
| C | -4.77953200 | 2.17800600 | -0.47835200 |
| H | -5.01148900 | 2.82839900 | 0.38313000 |
| H | -4.94255500 | 2.77575900 | -1.38868200 |
| H | -5.49602700 | 1.34601400 | -0.47439200 |
| C | 5.01823900 | 1.87166400 | -0.81118700 |
| H | 5.40320000 | 2.40649100 | 0.07505300 |
| H | 5.64427200 | 0.97958100 | -0.95368200 |
| H | 5.15007900 | 2.53625700 | -1.67827600 |
| N | -3.01643900 | 0.43443100 | -0.02916300 |
| N | 3.15702900 | 0.31091800 | -0.15264300 |

| | | | |
|---|---|---|---|
| C | -4.03097700 | -0.52246700 | 0.30663400 |
| C | -4.41603700 | -1.47947100 | -0.67528600 |
| C | -4.59238800 | -0.54708500 | 1.61067000 |
| C | -5.38488200 | -2.43539500 | -0.32912800 |
| C | -5.55276800 | -1.53170000 | 1.90488600 |
| C | -5.95563100 | -2.46453900 | 0.94781900 |
| H | -5.69432400 | -3.17356800 | -1.07269000 |
| H | -5.99281500 | -1.56312900 | 2.90609500 |
| H | -6.70724700 | -3.21855700 | 1.19648200 |
| C | 4.10552400 | -0.66620600 | 0.29074500 |
| C | 4.37200800 | -1.78581600 | -0.54513100 |
| C | 4.72979500 | -0.53211000 | 1.56034700 |
| C | 5.29658800 | -2.74338100 | -0.09924900 |
| C | 5.64104100 | -1.52443600 | 1.96036100 |
| C | 5.93449000 | -2.61512500 | 1.13887600 |
| H | 5.51527200 | -3.60881300 | -0.72925100 |
| H | 6.12647600 | -1.44092100 | 2.93699900 |
| H | 6.65103200 | -3.37275800 | 1.46751900 |
| C | 4.37739500 | 0.60367200 | 2.52065400 |
| H | 3.76704500 | 1.33520300 | 1.96737700 |
| C | 3.66811400 | -1.92903700 | -1.89269100 |
| H | 2.70123100 | -1.40391400 | -1.79245600 |
| C | -4.17619900 | 0.44549900 | 2.69777200 |
| H | -3.43208100 | 1.12967100 | 2.25878000 |
| C | -3.79838700 | -1.45225900 | -2.07385000 |
| H | -2.77095300 | -1.06408200 | -1.95454000 |
| C | -1.03252300 | -1.68813200 | 0.96412700 |
| H | -1.77919200 | -1.85105800 | 1.75666400 |
| C | -0.98690600 | -2.89719600 | 0.07049700 |
| C | 0.11976800 | -0.88930100 | 1.32190900 |
| H | -0.41255100 | -3.73079300 | 0.50553600 |
| H | -1.99988600 | -3.24453400 | -0.17168200 |
| H | 1.15936600 | -1.32938700 | 0.92638600 |
| H | 0.21469200 | -0.58573100 | 2.37643800 |
| C | 3.37110800 | -3.39150400 | -2.27075900 |
| H | 2.74205900 | -3.42462700 | -3.17441500 |
| H | 4.29247700 | -3.95634800 | -2.49354200 |
| H | 2.82936100 | -3.91397100 | -1.46785800 |
| C | 4.45991100 | -1.23184000 | -3.02202500 |
| H | 4.60487000 | -0.16052500 | -2.81723000 |
| H | 5.45441200 | -1.69360500 | -3.14549400 |
| H | 3.92162000 | -1.31992200 | -3.98033700 |
| C | 3.50724100 | 0.07438200 | 3.68272100 |
| H | 4.05809000 | -0.66770700 | 4.28430100 |
| H | 3.20367900 | 0.89838700 | 4.34980300 |
| H | 2.59608700 | -0.41090600 | 3.29968900 |
| C | 5.62254500 | 1.33883700 | 3.05896100 |
| H | 6.23931900 | 0.68331700 | 3.69612400 |
| H | 6.26379900 | 1.70517300 | 2.24140800 |
| H | 5.32141200 | 2.20419900 | 3.67189000 |
| C | -3.70527100 | -2.84001700 | -2.73559100 |
| H | -4.69954100 | -3.23446400 | -3.00634400 |
| H | -3.11654700 | -2.77070200 | -3.66360600 |
| H | -3.21181400 | -3.57847600 | -2.08511400 |
| C | -4.55393300 | -0.48348000 | -3.01285800 |
| H | -5.60542500 | -0.79589000 | -3.13148000 |
| H | -4.54556700 | 0.54777300 | -2.63270700 |
| H | -4.08564300 | -0.47540400 | -4.01110100 |
| C | -5.37100500 | 1.29128900 | 3.19091000 |
| H | -5.87537800 | 1.80685400 | 2.35911900 |
| H | -6.12375000 | 0.66403900 | 3.69694400 |
| H | -5.03287700 | 2.05316000 | 3.91279500 |
| C | -3.49771600 | -0.26578500 | 3.88941400 |
| H | -3.17426300 | 0.47036500 | 4.64387500 |
| H | -4.18843100 | -0.97057100 | 4.38164800 |
| H | -2.61098000 | -0.83291800 | 3.56687600 |



**Pre-OA Complex: [$^{i\text{-Pr}}$NDI]$Fe_2$(allyl)Cl**
**ZPVE: -4722.402312 $E_h$**
**Charge: 0**
**Multiplicity: 5**

| | | | |
|---|---|---|---|
| Fe | 1.30800000 | 0.06000000 | 0.21400000 |
| Fe | -1.10600000 | -0.00400000 | 0.21700000 |
| Cl | -0.51700000 | -1.60600000 | -2.33400000 |
| C | -2.29300000 | 3.91900000 | -0.64300000 |
| C | -1.12000000 | 4.62000000 | -0.91200000 |
| C | 0.13500000 | 3.96300000 | -0.83000000 |
| C | 0.13200000 | 2.58300000 | -0.41300000 |
| C | -2.24300000 | 2.56400000 | -0.27600000 |
| H | 1.42400000 | 5.59800000 | -1.45900000 |
| H | -3.26200000 | 4.41200000 | -0.74600000 |
| H | -1.15500000 | 5.66900000 | -1.21500000 |
| C | 1.38900000 | 4.55400000 | -1.13800000 |
| C | 2.50600000 | 2.45600000 | -0.64300000 |
| C | 2.55500000 | 3.79700000 | -1.05800000 |
| H | 3.51800000 | 4.24400000 | -1.31500000 |
| N | 1.28300000 | 1.87300000 | -0.28300000 |
| N | -1.01400000 | 1.91000000 | -0.11900000 |
| C | -3.36800000 | 1.71300000 | -0.06600000 |
| C | 3.59100000 | 1.54000000 | -0.53000000 |
| C | -4.77900000 | 2.24100000 | -0.05600000 |
| H | -4.83800000 | 3.20600000 | 0.46900000 |
| H | -5.15500000 | 2.39800000 | -1.08200000 |
| H | -5.45800000 | 1.53100000 | 0.43800000 |
| C | 5.02200000 | 1.91900000 | -0.79900000 |
| H | 5.52700000 | 2.27500000 | 0.11700000 |
| H | 5.59500000 | 1.05600000 | -1.16800000 |
| H | 5.08500000 | 2.72400000 | -1.54500000 |
| N | -3.05100000 | 0.41800000 | 0.12500000 |
| N | 3.20700000 | 0.30300000 | -0.14200000 |
| C | -4.05600000 | -0.54600000 | 0.46300000 |
| C | -4.89500000 | -1.11700000 | -0.53200000 |

| | | | |
|---|---|---|---|
| C | -4.15500000 | -0.96000000 | 1.82300000 |
| C | -5.82200000 | -2.09800000 | -0.13700000 |
| C | -5.10300000 | -1.93800000 | 2.16200000 |
| C | -5.93400000 | -2.50800000 | 1.19300000 |
| H | -6.47300000 | -2.54800000 | -0.89300000 |
| H | -5.19300000 | -2.25900000 | 3.20400000 |
| H | -6.66500000 | -3.27000000 | 1.47400000 |
| C | 4.18900000 | -0.71400000 | 0.08400000 |
| C | 4.35600000 | -1.73400000 | -0.89100000 |
| C | 4.95600000 | -0.71100000 | 1.28300000 |
| C | 5.33300000 | -2.71800000 | -0.66500000 |
| C | 5.91700000 | -1.72000000 | 1.46000000 |
| C | 6.11600000 | -2.71000000 | 0.49200000 |
| H | 5.48300000 | -3.50700000 | -1.40700000 |
| H | 6.52100000 | -1.73600000 | 2.37000000 |
| H | 6.87400000 | -3.48200000 | 0.64700000 |
| C | 4.66600000 | 0.30000000 | 2.39300000 |
| H | 4.31100000 | 1.23000000 | 1.92000000 |
| C | 3.49800000 | -1.75100000 | -2.15400000 |
| H | 2.55800000 | -1.22700000 | -1.90100000 |
| C | -3.27700000 | -0.32000000 | 2.89700000 |
| H | -2.40300000 | 0.11400000 | 2.37300000 |
| C | -4.81200000 | -0.71800000 | -2.00600000 |
| H | -4.07500000 | 0.09500000 | -2.09400000 |
| C | -0.95100000 | -1.99200000 | 0.41900000 |
| H | -1.71000000 | -2.43300000 | 1.07800000 |
| C | -0.77000000 | -2.75200000 | -0.85400000 |
| C | 0.16700000 | -1.28900000 | 1.04000000 |
| H | 0.13000000 | -3.38300000 | -0.89300000 |
| H | -1.65500000 | -3.34200000 | -1.11900000 |
| H | 1.24300000 | -1.60900000 | 0.59700000 |
| H | 0.21300000 | -1.31800000 | 2.14100000 |
| C | 3.12200000 | -3.17300000 | -2.61100000 |
| H | 2.36600000 | -3.12100000 | -3.41000000 |
| H | 3.99000000 | -3.72200000 | -3.01200000 |
| H | 2.70200000 | -3.76500000 | -1.78200000 |
| C | 4.16500000 | -0.96900000 | -3.30700000 |
| H | 4.35200000 | 0.07900000 | -3.03000000 |
| H | 5.13000000 | -1.42700000 | -3.58300000 |
| H | 3.51700000 | -0.97100000 | -4.19900000 |
| C | 3.50500000 | -0.22400000 | 3.27100000 |
| H | 3.78900000 | -1.16000000 | 3.77900000 |
| H | 3.22000000 | 0.51700000 | 4.03600000 |
| H | 2.62300000 | -0.43100000 | 2.64200000 |
| C | 5.88900000 | 0.66000000 | 3.25600000 |
| H | 6.22800000 | -0.19200000 | 3.86800000 |
| H | 6.73800000 | 0.99500000 | 2.63900000 |
| H | 5.63000000 | 1.47400000 | 3.95200000 |
| C | -4.31100000 | -1.88900000 | -2.88100000 |
| H | -4.98700000 | -2.75700000 | -2.81100000 |
| H | -4.26000000 | -1.58300000 | -3.93900000 |
| H | -3.30200000 | -2.20700000 | -2.58000000 |
| C | -6.16500000 | -0.19500000 | -2.53800000 |
| H | -6.92700000 | -0.99200000 | -2.55100000 |
| H | -6.55800000 | 0.62800000 | -1.92100000 |
| H | -6.05500000 | 0.17200000 | -3.57200000 |
| C | -4.01400000 | 0.84700000 | 3.59100000 |
| H | -4.34100000 | 1.60500000 | 2.86400000 |
| H | -4.90800000 | 0.48000000 | 4.12400000 |
| H | -3.35700000 | 1.34100000 | 4.32600000 |
| C | -2.74500000 | -1.32300000 | 3.93700000 |
| H | -2.02500000 | -0.82600000 | 4.60800000 |
| H | -3.55300000 | -1.72700000 | 4.57000000 |
| H | -2.23500000 | -2.17500000 | 3.45900000 |