Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information for:

Tuning Ligand Field Strength with Pendent Lewis Acids: Access to High Spin Iron Hydrides

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General Considerations. All air- and moisture-sensitive manipulations were performed using standard Schlenk techniques or in an inert atmosphere drybox with an atmosphere of purified nitrogen. The drybox was equipped with a cold well designed for freezing samples in liquid nitrogen as well as a −35 °C freezer for cooling samples and crystallizations. Solvents were purified using a Glass Contour solvent purification system through percolation through a Cu catalyst, molecular sieves, and alumina. Solvents were then stored over sodium and/or sieves. Benzene-d_6 was purchased from Cambridge Isotope Laboratories, dried with molecular sieves and sodium, and degassed by three freeze–pump–thaw cycles.

Ammonia (0.4 M in THF), methylamine (2.0 M in THF), potassium triethylborohydride, zinc(II) iodide, $NaN(SiMe_3)_2$, and phenylphosphine were purchased from commercial vendors and used as received. Thiophenol, phenol, and aniline were distilled from calcium hydride prior to use. Crown ethers were recrystallized from dry THF prior to use. ($^{BBN}PDP^{tBu}$), ($^{Bu}PDP^{tBu}$)$FeBr_2$, ($^{BBN}PDP^{tBu}$)$FeBr_2$,[1] $LiBDEt_3$,[2] and potassium graphite[3] were synthesized according to literature procedures.

NMR spectra were recorded on Varian Vnmrs 700 or Varian MR400 spectrometers. ^1H, ^{13}C, and ^{11}B chemical shifts are reported in parts per million (ppm) relative to tetramethylsilane and referenced internally to the residual solvent peak. ^{11}B spectra were referenced on a unified scale, where the single primary reference is the frequency of the residual solvent peak in the ^1H NMR spectrum. ^{11}B is referenced vs. $BF_3(OEt_2)$. Multiplicities are reported as follows: singlet (s), doublet (d), triplet (t), quartet (q). Infrared spectra were recorded using a Nicolet iS10 FT-IR spectrometer. Samples were diluted into dry KBr and recorded as pellets. Electronic absorption spectra were recorded in THF at ambient temperature in sealed 1 cm quartz cuvettes with a Varian Cary-50 spectrophotometer. Elemental analyses were performed by Midwest Microlab, Indianapolis, IN (USA). Many of the samples proved to be too air/moisture sensitive for satisfactory combustion analysis.

Single crystals of ($^{BBN}PDP^{tBu}$)FeH_2, [K(18-crown-6)]$_2$[($^{BBN}PDP^{tBu}$)$_2$Fe(OPh)$_4$], ($^{BBN}PDP^{tBu}$)Fe(SPh)$_2$(NH_3)$_2$, ($^{butyl}PDP^{tBu}$)Fe(SPh)$_2$, and ($^{BBN}PDP^{tBu}$)Fe(OH)$_2$ suitable for X-ray diffraction were coated with poly(isobutylene) oil and quickly transferred to the goniometer head of a Bruker AXS D8 Quest diffractometer with kappa geometry, an I-μ-S microsource X-ray tube, laterally graded multilayer (Goebel) mirror for monochromatization, a Photon2 CMOS area detector and an Oxford Cryosystems low temperature device. Examination and data collection were performed with Cu Kα radiation (λ = 1.54184 Å). Single crystals of [K(2,2,2-cryptand)][($^{BBN}PDP^{tBu}$)FeH_2], ($^{BBN}PDP^{tBu}$)Fe(SPh)$_2$, [($^{BBN}PDP^{tBu}$)Fe(NC)$_2$]$_2$, ($^{BBN}PDP^{tBu}$)Fe(PHPh)$_2$, ($^{BBN}PDP^{tBu}$)Fe(NHMe)$_2$, ($^{BBN}PDP^{tBu}$)Fe(NHPh)$_2$, and ($^{BBN}PDP^{tBu}$)ZnH_2, suitable for X-ray diffraction, were coated with poly(isobutylene) oil and quickly transferred to the goniometer head of a Bruker AXS D8 Quest diffractometer with a fixed chi angle, a sealed tube fine focus X-ray tube, single crystal curved graphite incident beam monochromator and a Photon100 CMOS area detector. Examination and data collection were performed with Mo Kα radiation (λ = 0.71073 Å). For both Quest instruments, data were collected, reflections were indexed and processed, and the data scaled and corrected for absorption using APEX3.[4] For all samples, the space groups were assigned and the structures were solved by direct methods or by isomorphous replacement using XPREP[5] and XS[6] within the SHELXTL suite of programs[5] and refined by full matrix least squares against F^2 with all reflections using Shelxl2016 or Shelxl2017[7] using the graphical interface Shelxle.[6] If not specified otherwise, H 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 C-H,

1.00, 0.99 and 0.98 Å for aliphatic C-H, CH_2, 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 CH_2, and C-H units, respectively. Additional data collection and refinement details, including description of disorder (where present) can be found with the individual structure descriptions, below.

Synthesis of (^{BBN}PDP^{tBu})FeH$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})$FeBr_2$ (0.200 g, 0.232 mmol), 6 mL THF, and stir bar and frozen. On thawing, $KBHEt_3$ (1.0 M in THF, 0.440 mL, 0.440 mmol) was added. On warming, the orange solution gradually darkened to brown-orange. After 15 min, the solution was filtered over Celite and volatiles were removed in vacuo. The solid was washed with 2 x 10 mL pentane, 2 x 10 mL benzene:pentane (4:1), and again with 2 x 10 mL pentane to afford olive-tan powder (0.114 g, 0.162 mmol, 70%) assigned as (^{BBN}PDP^{tBu})FeH_2. Single, X-ray quality crystals were obtained by layering a concentrated toluene solution of (^{BBN}PDP^{tBu})FeH_2 with *n*-pentane at -35 °C. ^{1}H NMR (THF, 24 °C) δ = -16.9 (155, 2H), -11.6 (228, 2H), -8.5 (688, 2H), -7.2 (190, 2H), 8.7 (11, 18H, C(C*H*$_3$)$_3$), 20.5 (59, 2H), 26.0 (410, 2H), 32.9 (1030, 2H), 41.5 (660, 2H), 48.7 (470, 2H), 58.3 (456, 2H), 58.7 (86, 2H), 63.6 (272, 2H). μ_{eff} = 4.6 +/- 0.2 μ_B (THF, 25 °C). MALDI-TOF of $C_{41}H_{65}N_5B_2Fe_1$: Calc. 705.48; Found 705.81. UV-Vis (THF, ambient temperature): λ_{max} = 327 nm (7,900 $M^{-1}cm^{-1}$). IR (KBr, ambient temperature): 1839 cm^{-1} (Fe-H-B, broad).

Synthesis of (^{BBN}PDP^{tBu})ZnI$_2$. A 20 mL scintillation vial was charged with zinc(II) iodide (0.282 g, 0.883 mmol), ^{BBN}PDP^{tBu} (0.571 g, 0.882 mmol), 15 mL dichloromethane and stirred for 16 hr. The solution was filtered, dried, and washed with 3 x 10 mL *n*-pentane to afford white powder (0.782 g, 0.809 mmol, 92%) assigned as (^{BBN}PDP^{tBu})ZnI_2. This sample was subjected to elemental analysis: Calc. for $C_{41}H_{63}N_5I_2B_2Zn_1$ C, 50.94; H, 6.57; N, 7.24. Found C, 49.97; H, 6.32; N, 7.01. ^{1}H NMR ($CDCl_3$, 25 °C) δ = 1.20-1.28 (m, 4H, 9-BBN-C*H*), 1.46 (s, 18H, C(C*H*$_3$)$_3$), 1.54 (t, *J* = 8.0, 4H, B-C*H*$_2$), 1.72-1.87 (m, 24H, 9-BBN-C*H*), 4.63 (t, *J* = 8.4, 4H, N-C*H*$_2$), 6.50 (s, 2H, pyrazole-C*H*), 7.61 (d, *J* = 8.0, 2H, *m*-pyridine-C*H*), 7.95 (t, *J* = 8.0, 1H, *p*-pyridine-C*H*). ^{13}C NMR ($CDCl_3$, 25 °C) δ = 23.41 (9-BBN-*C*H$_2$), 24.71 (9-BBN-*C*H), 27.04 (CH$_2$*C*H$_2$CH$_2$), 30.39 (C(*C*H$_3$)$_3$), 31.32 (B-*C*H$_2$), 32.10 (*C*(CH$_3$)$_3$), 33.34 (9-BBN-*C*H$_2$), 54.52 (N-*C*H$_2$), 101.58 (pyrazole-*C*H), 119.06 (*m*-pyridine-*C*H), 141.00 (*p*-pyridine-*C*H), 143.29 (Ar-*C*), 148.53 (Ar-*C*), 155.06 (Ar-*C*). ^{11}B NMR ($CDCl_3$, 25 °C) δ = 86.63 (9-BBN). MALDI-TOF of $C_{41}H_{63}N_5B_2I_2Zn_1$ - I: Calc. 838.360; Found 838.090.

Synthesis of (^{BBN}PDP^{tBu})ZnH$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})ZnI_2 (0.250 g, 0.259 mmol), 10 mL THF, a stir bar and frozen. On thawing, $KBHEt_3$ (1.0 M in THF, 0.505 mL, 0.505 mmol) was added. On warming, a white precipitate gradually formed. After 20 min, the solution was filtered and volatiles were removed in vacuo. The powder was washed with 2 x 10 mL pentane and dried to afford white powder (0.164 g, 0.229 mmol, 89%) assigned as (^{BBN}PDP^{tBu})ZnH_2. Single, X-ray quality crystals were obtained by slow diffusion of *n*-pentane into a toluene solution of (^{BBN}PDP^{tBu})ZnH_2 at room temperature. ^{1}H NMR (THF-d_8, 25 °C) δ = 0.05-0.22 (m, 4H), 0.56 (t, *J* = 7.2, 2H), 0.65 (s, 2H, Zn-*H*), 0.69-0.79 (m, 4H), 0.87-1.02 (m, 4H), 1.27-1.42 (m, 8H), 1.48 (s, 18H, C*H*$_3$), 1.75-2.05 (m, 14H), 4.55-4.71 (m, 4H, N-C*H*$_2$ x 2), 6.78 (s, 2H, pyrazole-C*H*), 7.76 (d, *J* = 7.6, 2H, *m*-pyr-C*H*), 8.07 (t, *J* = 7.6, 1H, *p*-pyr-C*H*). ^{13}C NMR (THF-d_8, 25 °C) δ = 18.62 (broad), 25.80, 26.24 (broad), 26.37, 26.94 (broad), 28.93, 30.37 (C(*C*H$_3$)$_3$), 30.86, 32.91, 34.00-36.00 (broad, 3 resonances), 54.03 (N-*C*H$_2$), 102.74 (pyrazole-*C*H), 119.80 (*m*-pyr-*C*H), 143.07 (Ar-*C*), 143.81 (Ar-*C*), 148.40 (Ar-*C*), 157.21 (Ar-*C*). ^{11}B NMR (THF-d_8, 25 °C) δ = 5.43 (*B*-H). MALDI-TOF of $C_{41}H_{65}N_5B_2Zn_1$: Calc. 713.472; Found 713.855. IR (KBr, ambient temperature): 1775 cm^{-1} (Zn-H-B, broad).

Synthesis of [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$]. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.053 g, 0.075 mmol), 2,2,2-cryptand (0.028 g, 0.074 mmol), and 5 mL THF and frozen. On thawing, potassium graphite (0.010 g, 0.074 mmol) was added resulting in an immediate color change to dark green. Upon reaching room temperature, the solution was filtered and volatiles were removed in vacuo. The material was washed with 10 mL *n*-pentane and 10 mL diethyl ether to afford dark green powder (0.068 g, 0.061 mmol, 81%) assigned as [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$]. Single, X-ray quality crystals were obtained by layering a THF solution of [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$] with *n*-pentane at -35 °C. ^{1}H NMR (THF, 24 °C) δ = -70.6 (409, 2H), -61.6 (349, 2H), -26.9 (40, 2H), 20.1 (57, 2H), -8.0 (39, 2H), -6.7 (39, 2H), -1.3 (51, 2H), -1.0 (53, 2H), 7.1 (14, 2H), 10.7 (12, 18H, C(C*H*$_3$)$_3$), 13.7 (265), 18.2 (23, 2H), 18.6 (127), 28.1 (44, 2H), 30.1 (680), 36.4 (400), 39.2 (35, 2H), 60.4 (71, 2H), 95.0 (25, 2H). UV-Vis (THF, ambient temperature): λ_{max} = 344 nm (7,200 M^{-1}cm^{-1}), 475 nm (3,500 M^{-1}cm^{-1}), 646 nm (1700 M^{-1}cm^{-1}). IR (KBr, ambient temperature): 1866 cm^{-1} (Fe-H-B, broad). This reduction protocol can be performed without crown ethers or with crown ethers other than 2,2,2-cryptand.

Synthesis of (^{BBN}PDP^{tBu})Fe(NH$_2$)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.076 g, 0.108 mmol) and 6 mL THF and frozen. On thawing, ammonia (0.4 M in THF, 0.324 mmol) was added and the reaction stirred for 30 min. Volatiles were removed in vacuo and the resulting solid washed with 10 mL *n*-pentane to afford salmon powder (0.060 g, 0.082 mmol, 76%) identified as (^{BBN}PDP^{tBu})Fe(NH$_2$)$_2$ by ^{1}H NMR spectroscopy.[1]

Synthesis of (^{BBN}PDP^{tBu})Fe(NHMe)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.085 g, 0.120 mmol) and 6 mL THF and frozen. On thawing, methylamine (2.0 M in THF, 0.300 mmol) was added and the reaction stirred for 25 min. Volatiles were removed in vacuo and the resulting solid washed with 10 mL *n*-pentane to afford tan powder (0.040 g, 0.052 mmol, 43%) assigned as (^{BBN}PDP^{tBu})Fe(NHMe)$_2$. Single, X-ray quality crystals were obtained by layering a DCM solution of (^{BBN}PDP^{tBu})Fe(NHMe)$_2$ with hexamethyldisiloxane at room temperature. ^{1}H NMR (THF, 24 °C) δ = -23.1 (35, 1H, *p*-pyridine-C*H*), -21.2 (390, 2H), -2.3 (55, 2H), -0.8 (29, 2H), -0.5 (23, 2H), -0.3 (50, 2H), 0.4 (54, 2H x 2), 4.2 (38, 2H), 4.5 (11, 18H, C(C*H*$_3$)$_3$), 5.9 (25, 2H), 11.0 (164, 2H), 12.3 (65, 2H), 12.4 (29, 2H), 13.8 (163, 2H), 30.5 (86, 2H), 31.8 (67, 2H), 33.7 (40, 2H), 46.9 (55, 2H). μ_{eff} = 5.2 +/- 0.1 μ_B (THF, 25 °C). MALDI-TOF of $C_{43}H_{71}N_7B_2Fe_1$: Calc. 763.53; Found 763.36. UV-Vis (THF, ambient temperature): λ_{max} = 339 nm (10,000 M^{-1}cm^{-1}). IR (KBr, ambient temperature): 3321, 3288, 3220, 3144 cm^{-1} (NH).

Synthesis of (^{BBN}PDP^{tBu})Fe(NHPh)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.050 g, 0.071 mmol) and 4 mL THF and frozen. A separate vial was charged with aniline (0.0133 mL, 0.146 mmol) and 1 mL THF. Upon thawing the vial containing (^{BBN}PDP^{tBu})FeH$_2$, the solution of aniline was added and stirred for 30 min. Volatiles were removed in vacuo and the solid was washed with 10 mL *n*-pentane and 10 mL diethyl ether to afford light yellow powder (0.045 g, 0.051 mmol, 73%) assigned as (^{BBN}PDP^{tBu})Fe(NHPh)$_2$. Single, X-ray quality crystals were obtained by layering a THF solution of (^{BBN}PDP^{tBu})Fe(NHPh)$_2$ with 2,2,4-trimethylpentane at room temperature. ^{1}H NMR (THF, 25 °C) δ = -48.1 (23, 2H), -43.8 (288, 2H), -22.6 (207, 2H), -19.7 (240, 2H), -17.3 (23, 1H, *p*-pyridine-C*H*), -7.7 (43, 2H), -3.5 (45, 2H), -1.7 (27, 2H), -1.5 (40, 2H), -1.0 (47, 2H), 0.5 (31, 2H), 0.6 (49, 2H), 1.1 (35, 2H), 8.2 (14, 18H, C(C*H*$_3$)$_3$), 17.2 (31, 2H), 19.0 (127, 2H), 23.8 (31, 2H), 26.5 (158, 2H), 28.6 (58, 2H), 41.6 (39, 2H), 48.0 (77, 2H), 50.8 (35, 2H). μ_{eff} = 4.5 +/- 0.1 μ_B (THF, 25 °C). UV-Vis (THF, ambient temperature): λ_{max} = 330 nm (8,600 M^{-1}cm^{-1}). IR (KBr, ambient temperature): 3372, 3293, 3135, 3067 cm^{-1} (NH).

Synthesis of (^{BBN}PDP^{tBu})Fe(OH)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.083 g, 0.118 mmol) and 6 mL THF and frozen. On thawing, a stock solution of water in THF (0.111 M, 2.100 mL, 0.233 mmol) was added and the reaction stirred for 20 min. Volatiles were removed in vacuo and the solid was washed with 10 mL *n*-pentane and dried to afford yellow powder (0.076 g, 0.103 mmol, 88%) assigned as (^{BBN}PDP^{tBu})Fe(OH)$_2$. This sample was subjected to elemental analysis: Calc. for $C_{41}H_{65}N_5O_2B_2Fe_1$ C, 66.78; H, 8.88; N, 9.50. Found C, 65.98; H, 8.73; N, 9.08. Single, X-ray quality crystals were obtained by diffusion *n*-pentane into a dichloromethane solution of (^{BBN}PDP^{tBu})Fe(OH)$_2$ at room temperature. ^{1}H NMR ($CDCl_3$, 24 °C) δ = -28.9 (29, 1H, *p*-pyridine-C*H*), -23.0 (316, 2H), -6.3 (201, 2H), -3.9 (179, 2H), -3.4 (51, 2H), -0.2 (32, 2H), 0.6 (54, 2H), 0.8 (33, 2H), 3.3 (36, 2H), 5.3 (19, 18H, C(CH_3)$_3$), 6.2 (61, 2H), 7.4 (53, 2H), 9.6 (117, 2H), 13.0 (38, 2H), 15.7 (310, 2H), 16.3 (24, 2H), 18.7 (334, 2H), 35.8 (71, 2H), 48.7 (70, 2H). μ_{eff} = 5.3 +/- 0.1 μ_B (THF, 25 °C). MALDI-TOF of $C_{41}H_{65}N_5O_2B_2Fe_1$: Calc. 737.47; Found 737.53. UV-Vis (THF, ambient temperature): λ_{max} = 333 nm (10,200 $M^{-1}cm^{-1}$). IR (KBr, ambient temperature): 3630 cm^{-1} (OH).

Synthesis of (^{BBN}PDP^{tBu})Fe(PHPh)$_2$. Caution! This compound is extremely malodorous even in trace quantities! A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.044 g, 0.062 mmol) and 4 mL THF and frozen. On thawing, a stock solution of phenylphosphine (0.433 M in THF, 0.128 mmol) was added and the mixture was stirred for 30 min. Volatiles were removed in vacuo and the resulting solid was washed with 10 mL *n*-pentane and 10 mL diethyl ether to afford orange powder (0.041 g, 0.044 mmol, 72%) assigned as (^{BBN}PDP^{tBu})Fe(PHPh)$_2$. Single, X-ray quality crystals were obtained by slow diffusion of *n*-pentane into a THF solution of (^{BBN}PDP^{tBu})Fe(PHPh)$_2$ at -35 °C. ^{1}H NMR ($CDCl_3$, 24 °C) δ = -29.5 (45, 1H, *p*-pyridine-C*H*), -29.2 (36, 2H), -23.1 (226, 2H), -18.1 (493, 2H), -15.6 (296, 2H), -14.5 (286, 2H), -6.1 (308, 2H), -3.6 (392, 2H), -0.7 (318, 2H), 3.0 (18, 2H), 4.4 (21, 2H), 8.6 (15, 18H, C(CH_3)$_3$), 15.1 (227, 2H), 17.3 (24, 2H), 36.2 (212, 2H), 45.7 (41, 2H), 62.0 (117, 2H), 71.7 (36, 2H), 73.5 (86, 2H), 139.8 (130, 2H, P-*H*). μ_{eff} = 5.2 +/- 0.1 μ_B (THF, 25 °C). UV-Vis (THF, ambient temperature): λ_{max} = 336 nm (11,500 $M^{-1}cm^{-1}$), 405 nm (3,800 $M^{-1}cm^{-1}$). IR (KBr, ambient temperature): 2340 cm^{-1} (PH).

Synthesis of (^{BBN}PDP^{tBu})Fe(SPh)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.094 g, 0.133 mmol) and 6 mL THF and frozen. On thawing, thiophenol (0.027 mL, 0.264 mmol) was added and stirred for 45 min resulting in a slight color change to brown. Volatiles were removed in vacuo and 20 mL *n*-pentane were added to the solid resulting in a rapid color change to orange. The solution was decanted and the solid dried to afford light orange powder (0.088 g, 0.095 mmol, 72%) assigned as (^{BBN}PDP^{tBu})Fe(SPh)$_2$. This sample was subjected to elemental analysis: Calc. for $C_{53}H_{73}N_5S_2B_2Fe_1$ C, 69.09; H, 7.98; N, 7.60. Found C, 68.88; H, 8.08; N, 7.49. Single, X-ray quality crystals were obtained by slow diffusion of *n*-pentane into a benzene solution of (^{BBN}PDP^{tBu})Fe(SPh)$_2$ at room temperature. ^{1}H NMR (C_6D_6, 24 °C) δ = -32.1 (214, 4H), -28.7 (21, 2H, *p*-phenyl-C*H*), -18.8 (39, 1H, *p*-pyridine-C*H*), -0.3 (44, 4H), 1.8 (58, 16H (3 overlapping resonances: 4H, 4H, 8H), BBN-CH_2 (for 8H)), 4.0 (18, 8H, BBN-CH_2), 7.0 (12, 18H, C(CH_3)$_3$), 18.2 (26, 4H), 25.2 (172, 4H), 29.4 (760, 4H), 31.9 (285, 4H), 45.5 (43, 2H, IM-C*H* or *m*-pyridine-C*H*), 57.5 (46, 2H, IM-C*H* or *m*-pyridine-C*H*). μ_{eff} = 5.5 +/- 0.1 μ_B (THF, 25 °C). MALDI-TOF of $C_{53}H_{73}N_5B_2S_2Fe_1$ - SPh: Calc. 812.47; Found 812.55. UV-Vis (THF, ambient temperature): λ_{max} = 330 nm (5,200 $M^{-1}cm^{-1}$).

Alternative synthesis of (^{BBN}PDP^{tBu})Fe(SPh)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.055 g, 0.078 mmol) and 6 mL THF and frozen. On thawing, diphenyldisulfide (0.017 g, 0.078 mmol) was added resulting in an immediate color charge to bright green which gradually dissipates to brown-orange. After 30 min, volatiles were removed in vacuo and the solid washed with 10 mL *n*-pentane to afford light orange powder (0.064 g, 0.069 mmol, 90%) identified as (^{BBN}PDP^{tBu})Fe(SPh)$_2$. Repeating the reaction in a sealed J-Young NMR tube revealed the formation of H_2 by ^{1}H NMR spectroscopy.

Synthesis of (^{BBN}PDP^{tBu})Zn(SPh)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})ZnH$_2$ (0.080 g, 0.112mmol) and 4 mL THF and frozen. A separate vial was charged with diphenyldisulfide (0.025 g, 0.114 mmol) and 2 mL THF and frozen. On thawing, the solution of diphenyldisulfide was added to the solution of (^{BBN}PDP^{tBu})ZnH$_2$ and stirred for 30 min. Volatiles were removed in vacuo and the solid washed with 20 mL *n*-pentane to afford white powder (0.079 g, 0.085 mmol, 76%) assigned as (^{BBN}PDP^{tBu})Zn(SPh)$_2$. Single, X-ray quality crystals were obtained by diffusing *n*-pentane into a C_6H_6 solution of (^{BBN}PDP^{tBu})Zn(SPh)$_2$ at room temperature. Repeating the reaction in a sealed J-Young NMR tube revealed the formation of H_2. ^{1}H NMR (C_6D_6, 23 °C) δ = 1.13 (s, 18H, C(C*H*$_3$)$_3$), 1.40 (t, *J* = 8.4, 4H, B-C*H*$_2$), 1.58-1.66 (m, 4H, BBN-C*H*), 1.76 (s, 4H, BBN-C*H*), 1.97-2.06 (m, 8H, BBN-C*H*), 2.07-2.23 (m, 12H (4H and 8H), BBN-C*H*), 2.74 (p, *J* = 7.6, 4H, CH$_2$C*H*$_2$CH$_2$), 4.27 (t, *J* = 7.2, 4H, N-C*H*$_2$), 6.08 (s, 2H, IM-C*H*), 6.60-6.66 (m, 8H, *m*-pyridine-C*H* and phenyl-C*H*), 6.85 (t, *J* = 8.0, 1H, *p*-pyridine-C*H*), 7.22-7.27 (m, 4H, phenyl-C*H*). ^{13}C NMR (C_6D_6, 23 °C) δ = 22.38 (B-*C*H$_2$), 24.79 (9-BBN-*C*H), 26.40 (CH$_2$*C*H$_2$CH$_2$), 29.01 (9-BBN-*C*H), 29.89 (C(*C*H$_3$)$_3$), 31.63 (*C*(CH$_3$)$_3$), 33.54 (9-BBN-*C*H$_2$), 54.51 (N-*C*H$_2$), 100.84 (pyrazole-*C*H), 118.35 (*m*-pyridine-*C*H), 123.23, 127.27 (SPh-*C*H), 134.17 (SPh-*C*H), 139.49, 141.72 (*p*-pyridine-*C*H), 143.99, 148.63, 155.03. The ^{11}B resonance was not observed. MALDI-TOF of $C_{53}H_{73}N_5B_2S_2Zn_1$ - SPh: Calc. 820.467; Found 820.454.

Synthesis of (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})Fe(SPh)$_2$ (0.079 g, 0.086 mmol) and 2 mL THF. While stirring, a stock solution of ammonia (0.4 M in THF, 0.43 mmol) was added. After 15 min, volatiles were removed in vacuo and the solid washed with 10 mL *n*-pentane to afford dark orange powder (0.071 g, 0.074 mmol, 87%) assigned as (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$. This sample was subjected to elemental analysis: Calc. for $C_{53}H_{79}N_7S_2B_2Fe_1$ C, 66.60; H, 8.33; N, 10.26. Found C, 65.11; H, 8.41; N, 9.17. Single, X-ray quality crystals were obtained by diffusing pentane into a toluene solution of (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$ at room temperature. ^{1}H NMR (CH_2Cl_2, 23 °C) δ = -30.8 (317, 4H), -28.6 (72, 1H, *p*-pyr-C*H*), -26.8 (57, 2H), -8.2 (96, 6H, N*H*$_3$), -0.9 (56, 4H, BBN-C*H*), -0.7 (58, 4H, BBN-C*H*), 0.3 (56, 2H, BBN-C*H*), 0.6 (55, 2H, BBN-C*H*), 1.2 (65, 2H, BBN-C*H*), 1.6 (53, 4H, BBN-C*H*), 1.9 (55, 2H, BBN-C*H*), 2.4 (55, 4H, BBN-C*H*), 3.2 (78, 4H, BBN-C*H*), 7.7 (34, 18H, C(C*H*$_3$)$_3$), 7.8 (31, 4H), 9.8 (326, 4H, CH$_2$C*H*$_2$CH$_2$), 22.1 (58, 4H), 27.2 (424, 4H, N-C*H*$_2$), 44.8 (72, 2H, IM-C*H* or *m*-pyridine-C*H*), 57.1 (72, 2H, IM-C*H* or *m*-pyridine-C*H*). μ_{eff} = 5.16 +/- 0.05 μ_B (THF, 25 °C). MALDI-TOF of $C_{53}H_{73}N_5B_2S_2Fe_1$ – (SPh + 2(NH$_3$)): Calc. 812.473; Found 812.667. UV-Vis (THF, ambient temperature): λ_{max} = 336 nm (10,500 M^{-1}cm^{-1}). IR (KBr, ambient temperature): 3353, 3306, 3135, 3062 cm^{-1} (N-*H*).

Synthesis of [(^{BBN}PDP^{tBu})Fe(NC)$_2$]$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.058 g, 0.082 mmol) and 6 mL THF and frozen. A separate 20 mL scintillation vial was charged with trimethylsilyl cyanide (0.020 mL, 0.160 mmol) and 2 mL THF and frozen. On thawing, the solution of Me_3SiCN was added to the solution containing (^{BBN}PDP^{tBu})FeH$_2$ and stirred for 30 min. Volatiles were removed in vacuo and the resulting solid washed with 10 mL *n*-pentane to afford light yellow powder (0.052 g, 0.034 mmol, 84%) assigned as [(^{BBN}PDP^{tBu})Fe(NC)$_2$]$_2$. Single, X-ray quality crystals were obtained by diffusing *n*-pentane into a dichloromethane solution of [(^{BBN}PDP^{tBu})Fe(NC)$_2$]$_2$ at room temperature (note: crystals rapidly desolvate when removed from mother liquor). ^{1}H NMR ($CDCl_3$, 23 °C) δ = -35.0 (25, 1H, *p*-pyridine-C*H*), -8.8 (69, 4H), -6.7 (265, 4H), -3.8 (40, 2H), -0.6 (52, 4H, BBN-C*H*), -0.4 (28, 2H, BBN-C*H*), 0.3 (36, 4H, BBN-C*H*), 1.4 (22, 4H, BBN-C*H*), 2.8 (33, 4H), 7.8 (264, 2H), 10.0 (13, 18H, C(CH_3)$_3$), 13.1 (67, 4H, $CH_2CH_2CH_2$), 13.3 (280, 2H), 25.4 (339, 4H, N-CH_2), 44.7 (53, 2H, IM-C*H* or *m*-pyridine-C*H*), 53.1 (39, 2H, IM-C*H* or *m*-pyridine-C*H*). MALDI-TOF of $C_{86}H_{126}N_{14}B_4Fe_2$: Calc. 1510.94; Found 1511.59. UV-Vis (THF, ambient temperature): λ_{max} = 330 nm (7,600 $M^{-1}cm^{-1}$). IR (KBr, ambient temperature): 2170 cm^{-1} (CN).

Synthesis of [K(2,2,2-cryptand)]$_2$[(^{BBN}PDP^{tBu})$_2$Fe(OPh)$_4$]. A 20 mL scintillation vial was charged with [K(2,2,2-crypt)][(^{BBN}PDP^{tBu})FeH$_2$] (0.051 g, 0.045 mmol) and 6 mL THF and frozen. Upon thawing, phenol (0.217 M stock solution in THF, 0.044 mmol) was added and the solution stirred for 16 hr resulting in a color change from deep green to dark brown. The reaction was filtered and volatiles were removed in vacuo. The resulting solid was washed with 10 mL diethyl ether to afford light brown powder (0.040 g) assigned as [K(2,2,2-cryptand)]$_2$[(^{BBN}PDP^{tBu})$_2$Fe(OPh)$_4$]. This species is unstable and attempts at purification resulted in further degradation of the compound. A representative ^{1}H NMR spectrum of the species obtained from the above synthetic procedure is given below. Single, X-ray quality crystals were obtained by diffusing *n*-pentane into a THF solution of the 18-crown-6 analogue at room temperature.

Reaction between (^{BBN}PDP^{tBu})FeH$_2$ and 2,4,6-tri-*tert*-butylphenylisocyanide. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeH$_2$ (0.054 g, 0.077 mmol) and 2 mL THF. While stirring, a solution of 2,4,6-tri-*tert*-butylphenylisocyanide (0.041 g, 0.151 mmol) in 1 mL THF was added resulting in an immediate color change to deep brown. After 5 min, volatiles were removed in vacuo. The resulting material was triturated with pentane and dried to afford brown/black powder assigned as (^{BBN}PDP^{tBu})Fe(CNAr)$_2$. The complex is highly soluble and readily dissolves in non-polar solvents such as *n*-pentane, isooctane, and hexamethyldisiloxane and was unable to be purified further. Impurities are evident by infrared spectroscopy (see below). The assignment as (^{BBN}PDP^{tBu})Fe(CNAr)$_2$ is made on the basis of ^{1}H NMR and infrared spectroscopies, MALDI-TOF mass spectrometry, and the production of H_2 (see details below). Characterization associated with complex: ^{1}H NMR (tol-d_8, 25 °C) δ = 1.09 (s, broad, C(CH_3)$_3$), 1.13 (s, broad), 1.22 (s, broad, C(CH_3)$_3$), further broad resonances spanning 1.25-1.80, 4.77 (broad, N-CH_2), 6.65 (s, 2H, pyrazole-C*H*), 7.26 (t, *J* = 7.5, 1H, *p*-pyridine-C*H*), 7.30 (s, 4H, ArNC-C*H*), 7.73 (d, *J* = 7.0, 2H, *m*-pyr-C*H*). MALDI-TOF of $C_{79}H_{121}N_7B_2Fe_1$ – (CNAr): Calc. 974.692; Found 974.715. IR (KBr, ambient temperature): 2002, 1895 cm^{-1} (CNAr), other CNAr impurities at 2191 and 2071 cm^{-1}.

Attempts to synthesize analogues to 2-E with ^{butyl}PDP^{tBu} ligand, (^{butyl}PDP^{tBu})Fe(E)$_2$ (E = H, NH$_2$, OH, PHPh, NHPh, SPh).

A) Reaction between (^{Bu}PDP^{tBu})FeBr$_2$ and KBHEt$_3$. A 20 mL scintillation vial was charged with (^{Bu}PDP^{tBu})FeBr$_2$ (0.020 g, 0.031 mmol) and 2 mL THF and the yellow slurry frozen. On thawing, KBHEt$_3$ (1.0 M in THF, 0.061 mmol) was added resulting in an immediate color change to deep green which slowly dissipated over 2 min, becoming brown/green. In situ NMR (THF) was attempted, however, the sample could not be shimmed. In both THF and C_6D_6, insoluble black material gradually precipitates. After 20 min of reaction time, volatiles were removed in vacuo. Addition of C_6D_6 (0.8 mL) resulted in a rapid color change to deep red/brown. The solution was filtered into a J. Young NMR tube and a poorly resolved ^{1}H NMR spectrum was obtained (see below).

B) Reaction between (^{Bu}PDP^{tBu})FeBr$_2$ and NaOH/NaNH$_2$. These reactions provided analogous results. A 20 mL scintillation vial was charged with (^{Bu}PDP^{tBu})FeBr$_2$ (0.020 g, 0.031 mmol) and 6 mL THF. While stirring, NaOH or NaNH$_2$ (0.310 mmol) was added. No immediate color change was noted. After 45 min, the solution color began to change from yellow to dark brown/green. An aliquot of each reaction was filtered into a J-Young NMR tube and a ^{1}H NMR (the precipitate was black and the filtrate was faint yellow). ^{1}H NMR spectroscopy revealed only starting material ((^{Bu}PDP^{tBu})FeBr$_2$) and uncoordinated (^{Bu}PDP^{tBu}). No other paramagnetic resonances were observed. The reaction was allowed to stir an addition 14 hr at room temperature. Filtration of the black precipitate afforded a colorless solution which was identified to only contain uncoordinated (^{Bu}PDP^{tBu}) by ^{1}H NMR spectroscopy.

C) Reaction between (^{Bu}PDP^{tBu})FeBr$_2$ and LiPHPh/LiNHPh. These reactions provided analogous results. A 20 mL scintillation vial was charged with (^{Bu}PDP^{tBu})FeBr$_2$ (0.030 g, 0.046 mmol), 8 mL THF, and either aniline or phenylphosphine (0.092 mmol). The vial was frozen. A separate 20 mL scintillation vial was charged lithium bis(trimethylsilyl)amide (0.015 g, 0.090 mmol) and 2 mL THF and frozen. Upon thawing, the solution of lithium bis(trimethylsilyl)amide was added to the iron containing vial resulting in a rapid color change from yellow to dark orange and gradually to dark brown. After stirring to room temperature for 20 min, volatiles were removed in vacuo. ^{1}H NMR spectroscopy of each (THF) revealed primarily uncoordinated (^{Bu}PDP^{tBu}) ligand as well a trace paramagnetic species that is identical between the two reactions.

D) Synthesis of (^{Bu}PDP^{tBu})Fe(SPh)$_2$. A 20 mL scintillation vial was charged with (^{Bu}PDP^{tBu})FeBr$_2$ (0.156 g, 0.240 mmol), 10 mL THF, and thiophenol (0.049 mL, 0.479 mmol). The vial was frozen. A separate 20 mL scintillation vial was charged sodium bis(trimethylsilyl)amide (0.087 g, 0.474 mmol) and 3 mL THF and frozen. Upon thawing, the solution of sodium bis(trimethylsilyl)amide was added to the iron containing vial resulting in a rapid color change from yellow to dark black, to dark yellow, and finally to olive green over 20 min. Volatiles were removed in vacuo to afford a light orange solid. The material was extracted into 10 mL dichloromethane, filtered, and dried. The resulting solid was washed with 10 mL *n*-pentane to afford light orange powder (0.161 g, 0.227 mmol, 95%) assigned as (^{Bu}PDP^{tBu})Fe(SPh)$_2$. Single, X-ray quality crystals were obtained by slow diffusion on *n*-pentane into a DCM solution at room temperature. MALDI-TOF of $C_{39}H_{51}N_5S_2Fe_1$ – SPh: Calc. 600.282; Found 600.511. ^{1}H NMR (THF, 23 °C) δ = -33.7 (236, 4H, SPh-C*H*), -31.3 (20, 2H, *p*-SPh-C*H*), -24.3 (27, 1H, *p*-pyr-C*H*), 0.5 (24, 6H, CH_3), 3.3 (55, 4H, CH_2), 6.1 (10, 18H, C(CH_3)$_3$), 7.6 (214, 4H, CH_2), 22.1 (19, 4H, SPh-C*H*), 22.7 (284, 4H, N-CH_2), 44.0 (42, 2H, pyridine or pyrazole-C*H*), 57.0 (45, 2H, pyridine or pyrazole-C*H*). μ_{eff} = 5.30 +/- 0.09 μ_B (THF, 25 °C). UV-Vis (THF, ambient temperature): λ_{max} = 330 nm (13,600 M^{-1}cm^{-1}).

E) Validation of salt metathesis route for attempts to form (^{butyl}PDP^{tBu})Fe(E)$_2$ variants

The compounds (^{Bu}PDP^{tBu})Fe(PHPh)$_2$ and (^{Bu}PDP^{tBu})Fe(OH)$_2$ were inaccessible through salt metathesis. The boron containing variants, **2-PHPh** and **2-OH**, were confirmed to be accessible through this method. Below are the synthetic protocol.

1) Alternate synthesis of (^{BBN}PDP^{tBu})Fe(PHPh)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeBr$_2$ (0.196 g, 0.227 mmol), 8 mL THF, and phenylphosphine (0.455 mmol from THF stock solution) and the solution frozen. A separate vial was charged with potassium bis(trimethylsilyl)amide (0.091 g, 0.456 mmol) and 4 mL THF and frozen. Upon thawing, the solution containing KN(SiMe$_3$)$_2$ was added to the vial containing (^{BBN}PDP^{tBu})FeBr$_2$. The solution was stirred to room temperature for 20 min then filtered over Celite. Volatiles were removed in vacuo. The resulting orange solid was washed with 3 x 10 mL *n*-pentane and dried to afford light orange powder (0.171 g, 0.185 mmol, 82%) identified as (^{BBN}PDP^{tBu})Fe(PHPh)$_2$. The spectroscopic data and purity by this method were analogous to the protonation method.

2) Alternate synthesis of (^{BBN}PDP^{tBu})Fe(OH)$_2$. A 20 mL scintillation vial was charged with (^{BBN}PDP^{tBu})FeBr$_2$ (0.057 g, 0.066 mmol), 4 mL THF, and water (0.132 mmol from THF stock solution) and the solution frozen. A separate vial was charged with potassium bis(trimethylsilyl)amide (0.026 g, 0.130 mmol) and 4 mL THF and frozen. Upon thawing, the solution containing KN(SiMe$_3$)$_2$ was added to the vial containing (^{BBN}PDP^{tBu})FeBr$_2$ and stirred to room temperature for 20 min. Volatiles were then removed in vacuo. The resulting orange solid was extracted into 8 mL dichloromethane, filtered, dried, and washed with 3 x 6 mL *n*-pentane to afford light orange powder (0.021 g, 0.028 mmol, 43%) identified as (^{BBN}PDP^{tBu})Fe(OH)$_2$. The spectroscopic data and purity by this method were analogous to the protonation method.

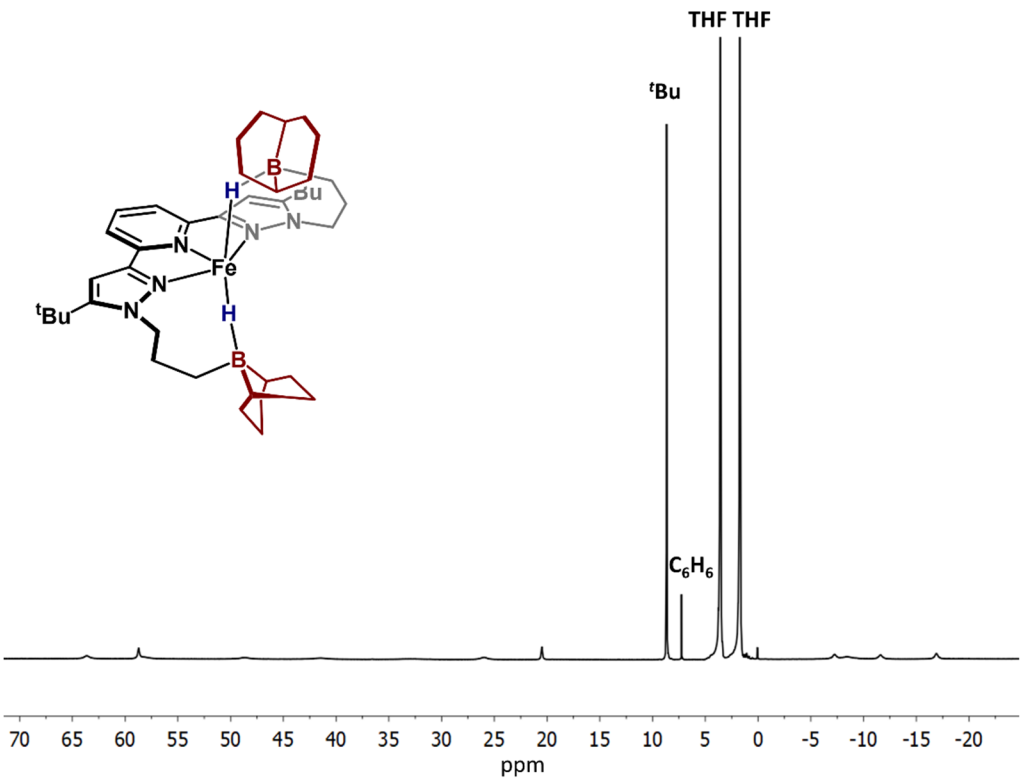


Figure S1. ^{1}H NMR spectrum (THF, 24 °C) of (^{BBN}PDP^{tBu})FeH$_2$.

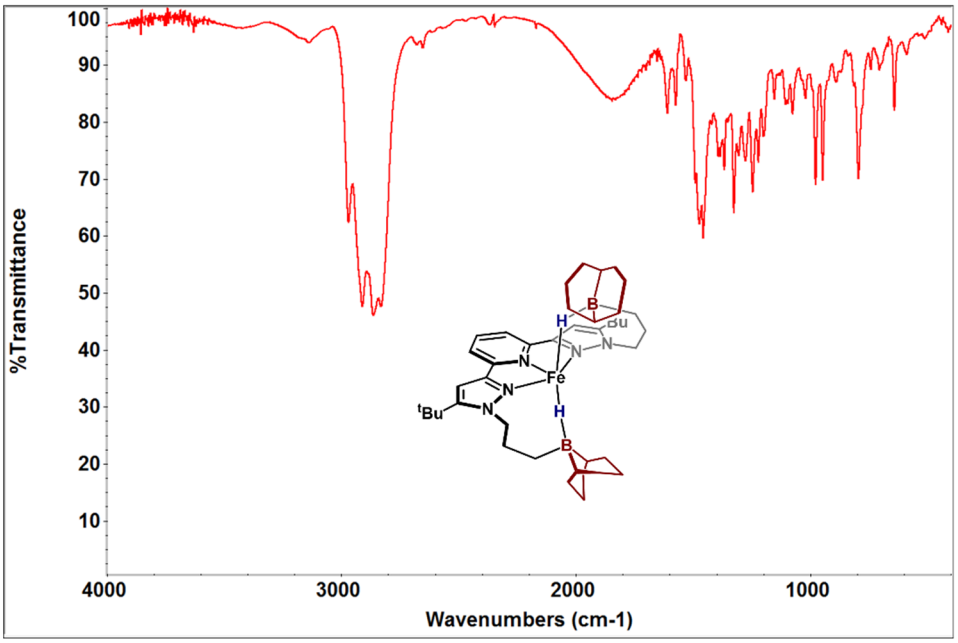


Figure S2. Infrared spectrum (KBr) of (^{BBN}PDP^{tBu})FeH$_2$.

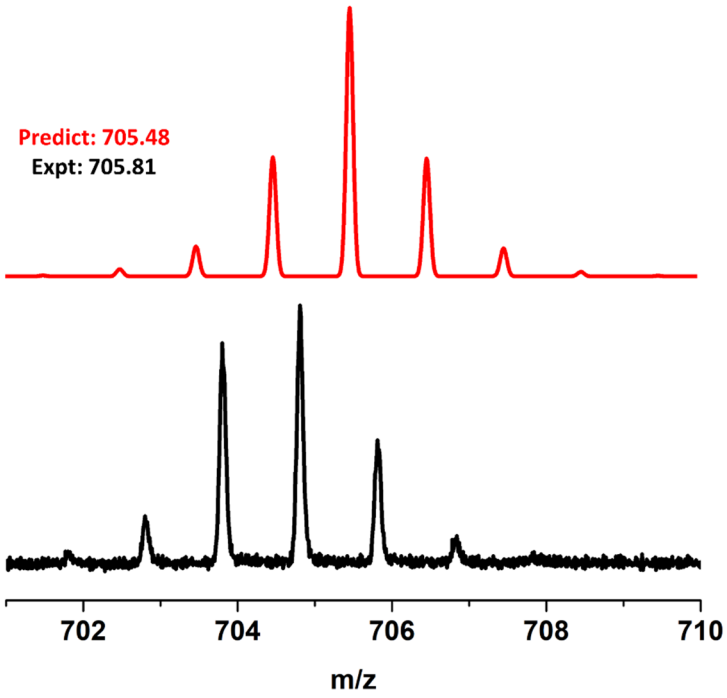


Figure S3. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})FeH$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{41}H_{65}N_5B_2Fe_1$.

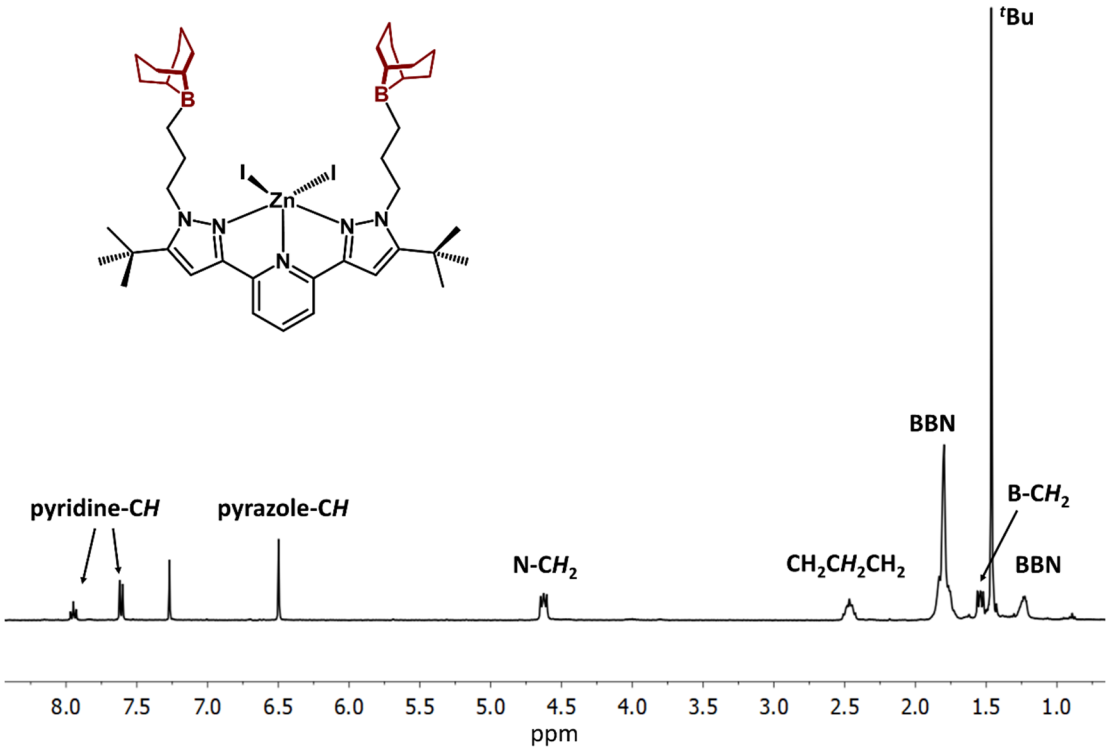


Figure S4. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of (^{BBN}PDP^{tBu})ZnI$_2$.

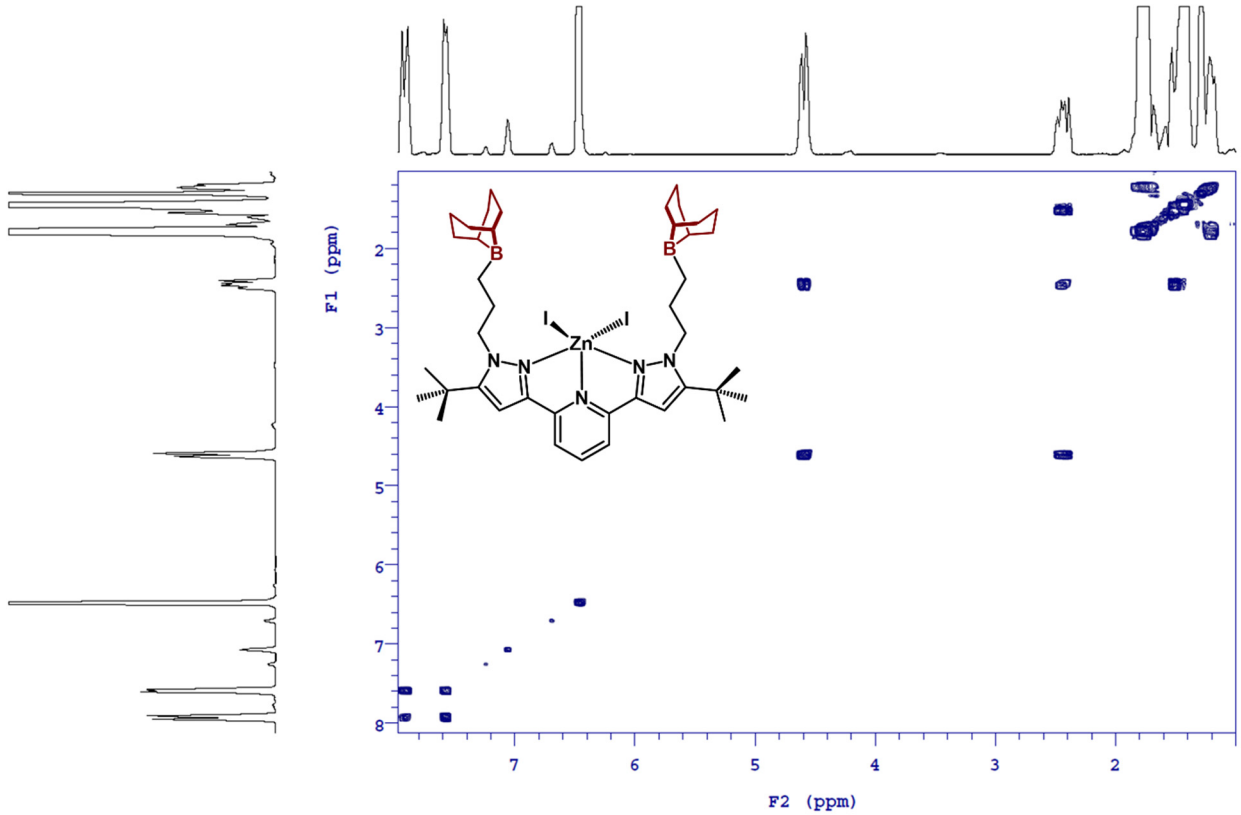


Figure S5. ^{1}H-^{1}H COSY spectrum ($CDCl_3$, 25 °C) of ($^{BBN}PDP^{tBu}$)ZnI_2.

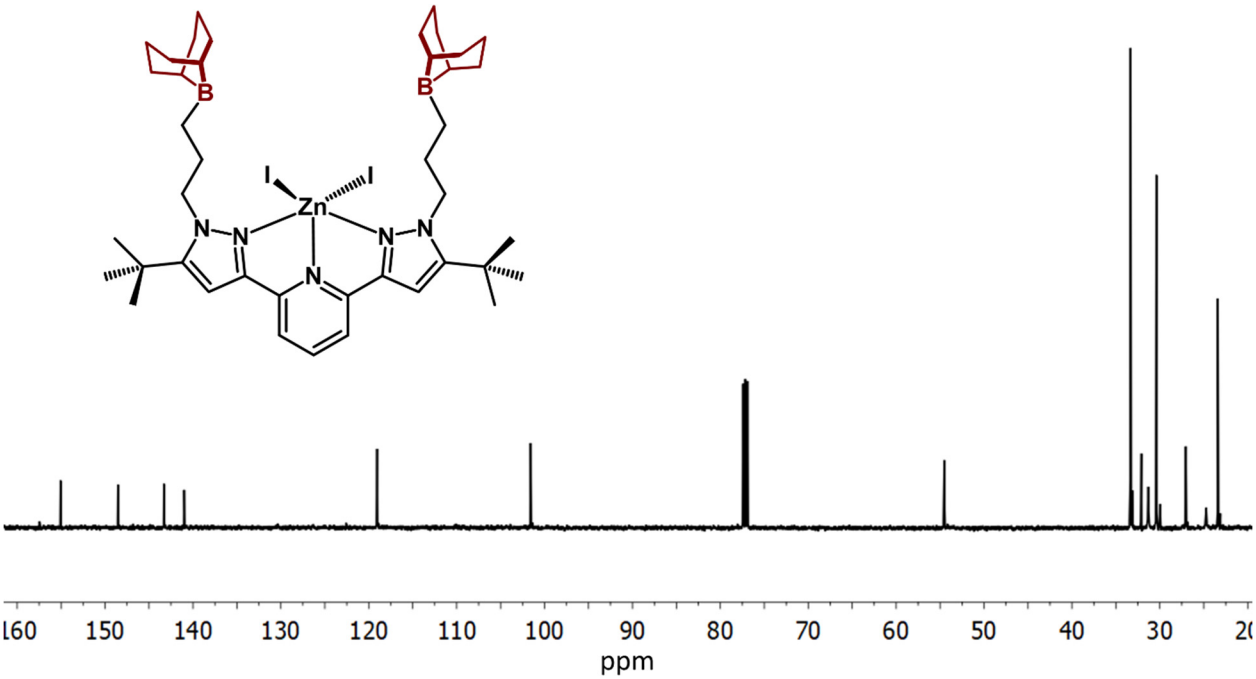


Figure S6. ^{13}C NMR spectrum ($CDCl_3$, 25 °C) of ($^{BBN}PDP^{tBu}$)ZnI_2.

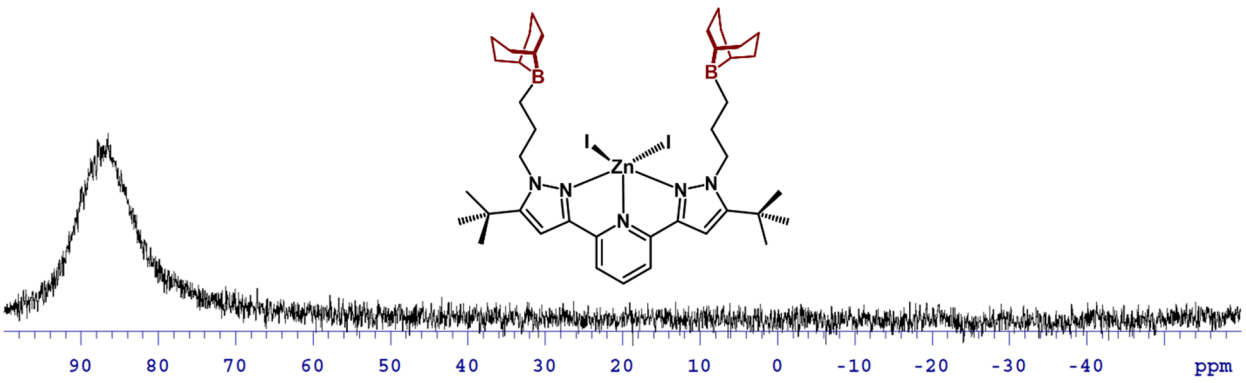


Figure S7. ^{11}B NMR spectrum ($CDCl_3$, 25 °C) of ($^{BBN}PDP^{tBu}$)ZnI_2.

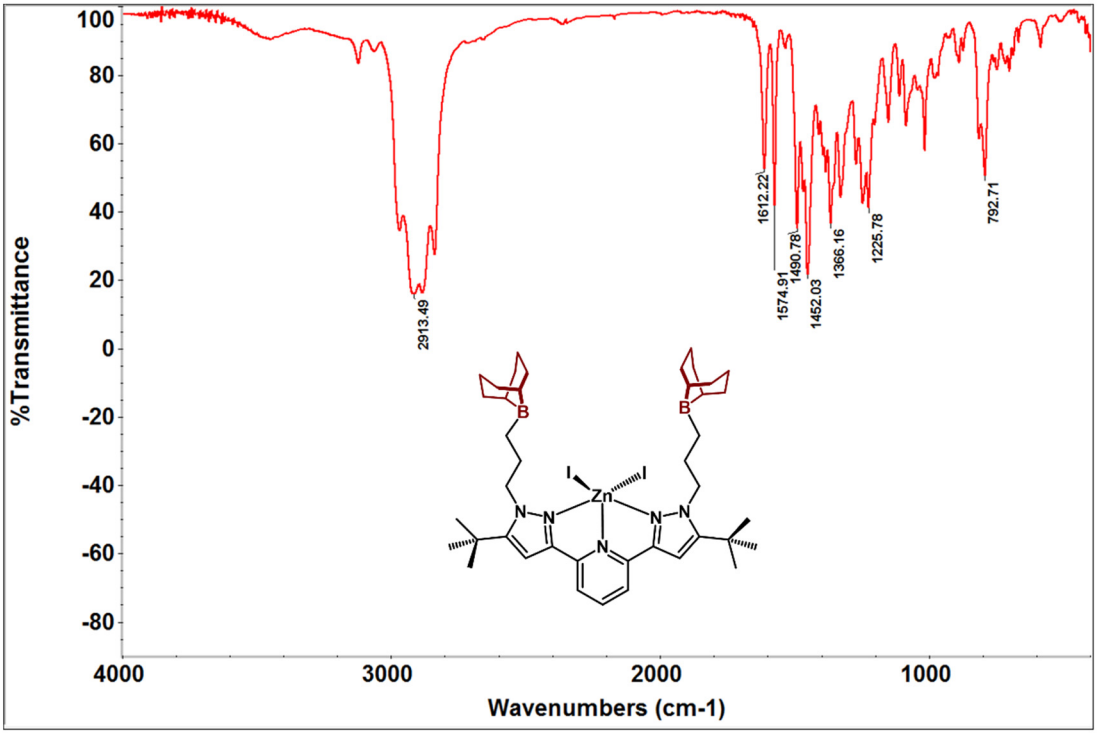


Figure S8. Infrared spectrum (KBr) of ($^{BBN}PDP^{tBu}$)ZnI_2.

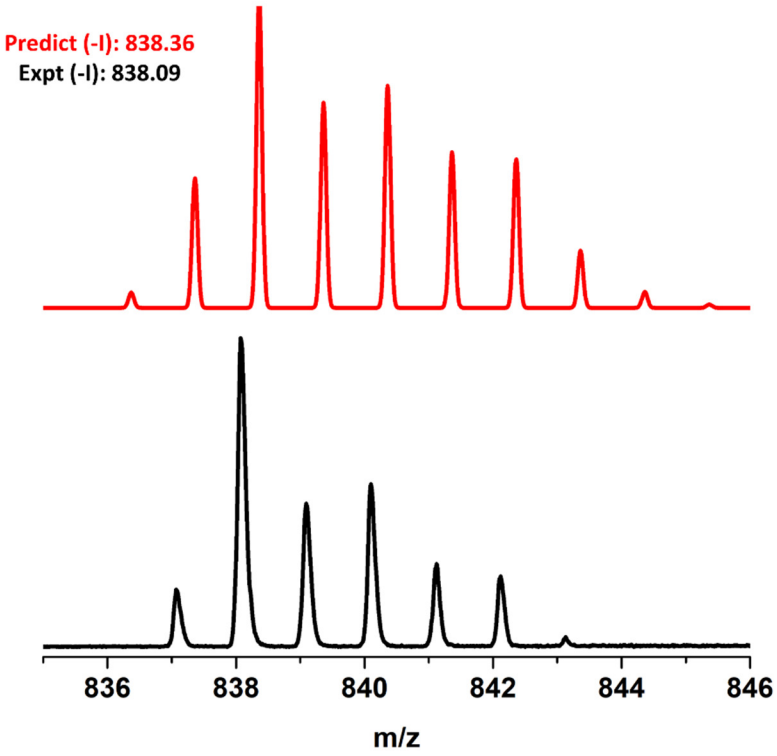


Figure S9. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})ZnI$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{41}H_{63}N_5B_2I_2Zn_1$ – I.

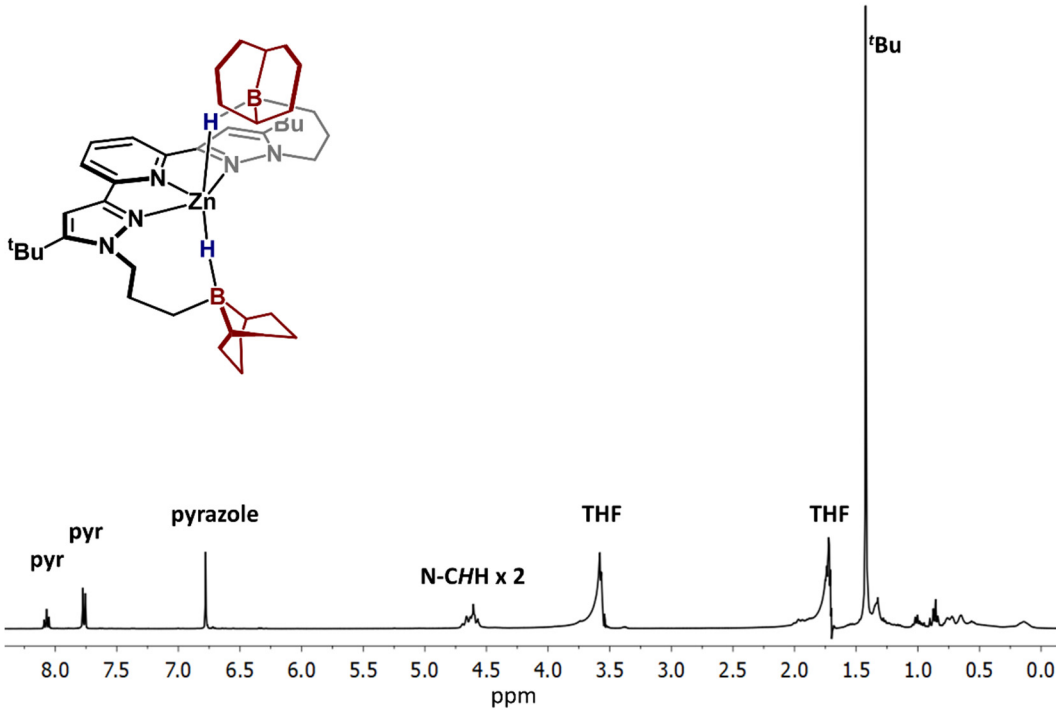


Figure S10. ^{1}H NMR spectrum (THF, 25 °C) of (^{BBN}PDP^{tBu})ZnH$_2$.

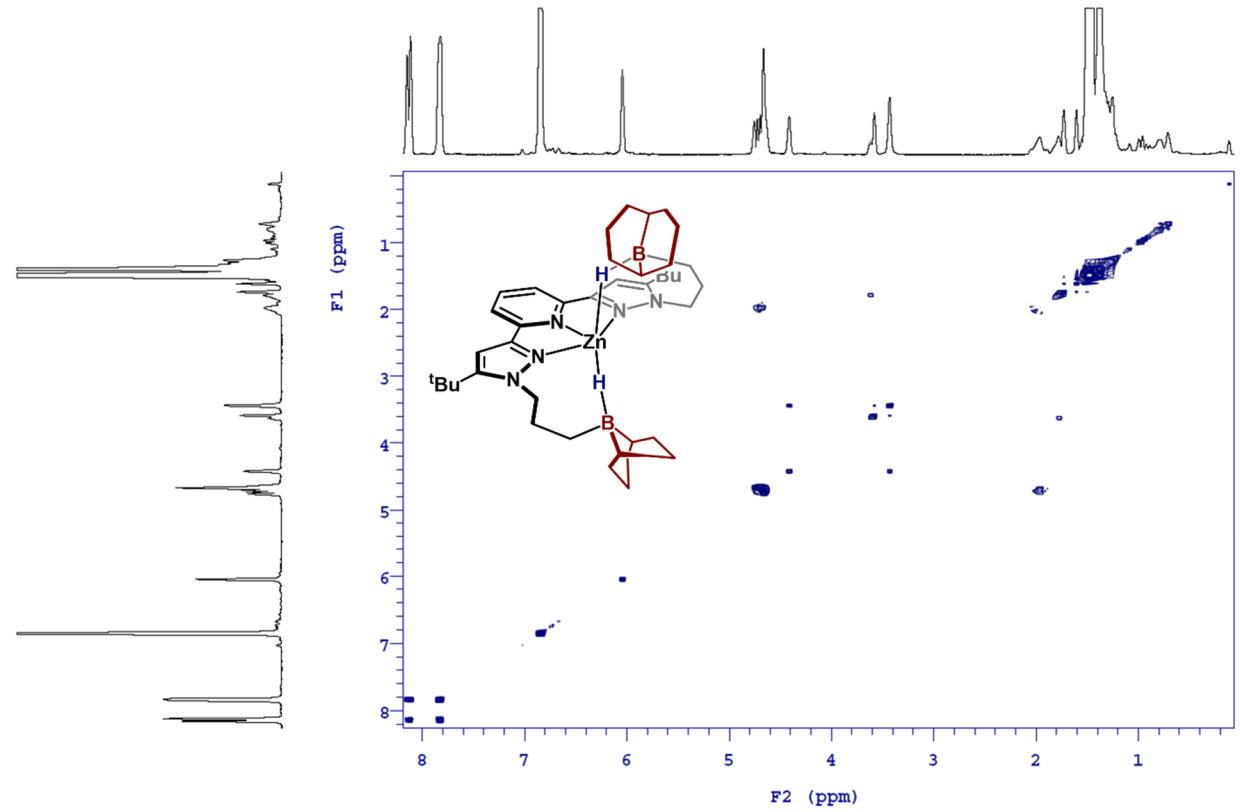


Figure S11. ^{1}H-^{1}H COSY spectrum (THF-d_8, 25 °C) of (^{BBN}PDP^{tBu})ZnH$_2$.

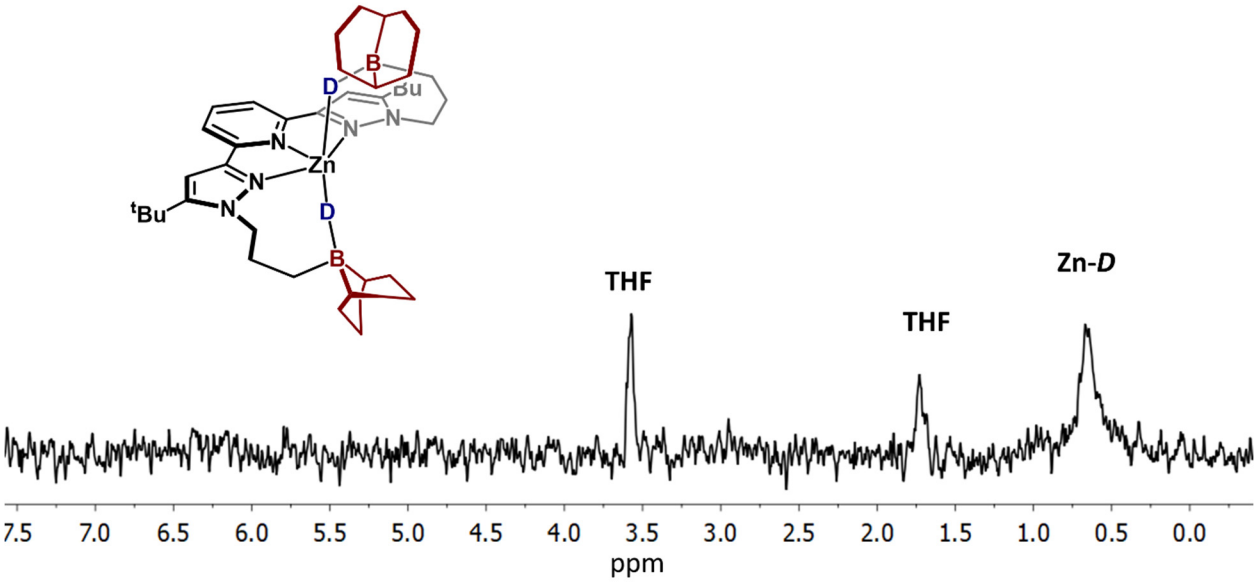


Figure S12. ^{2}H NMR spectrum (THF, 25 °C) of (^{BBN}PDP^{tBu})ZnD$_2$.

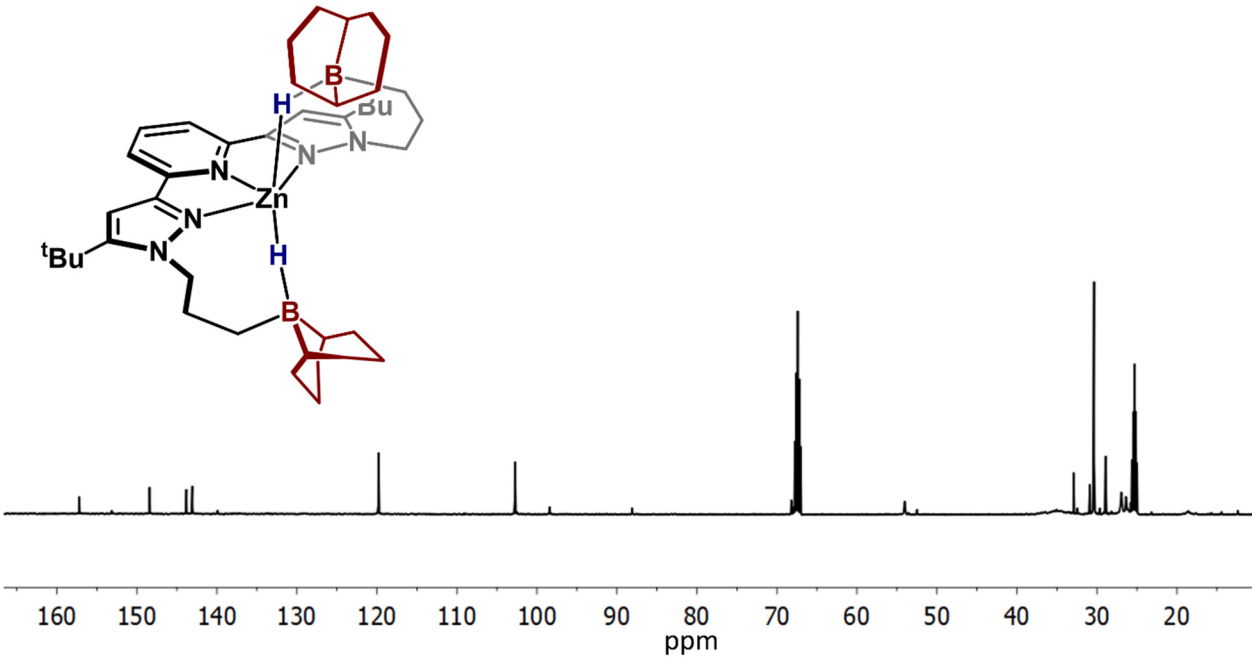


Figure S13. ^{13}C NMR spectrum (THF, 25 °C) of ($^{BBN}PDP^{tBu}$)ZnH_2.

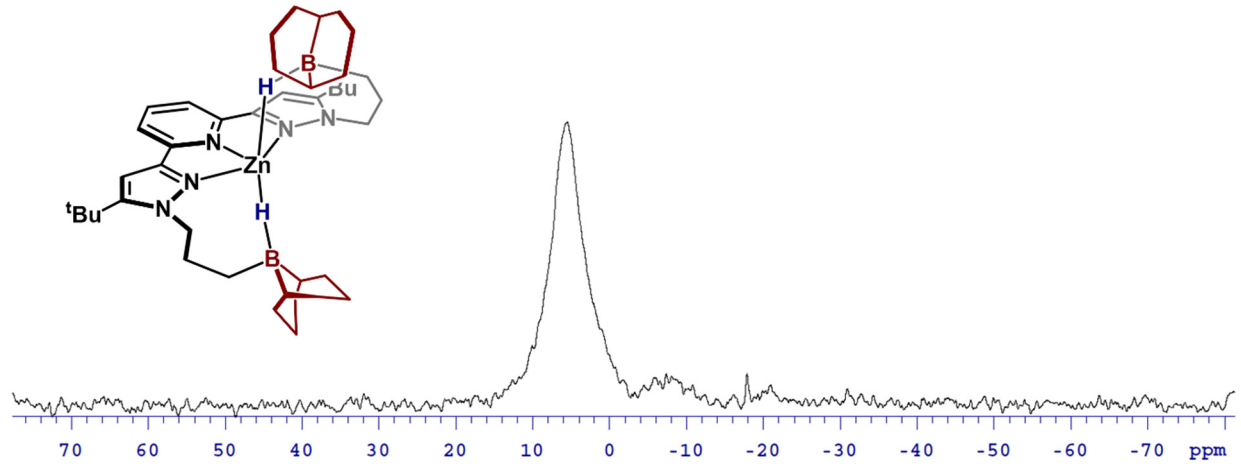


Figure S14. ^{11}B NMR spectrum (THF, 25 °C) of ($^{BBN}PDP^{tBu}$)ZnH_2.

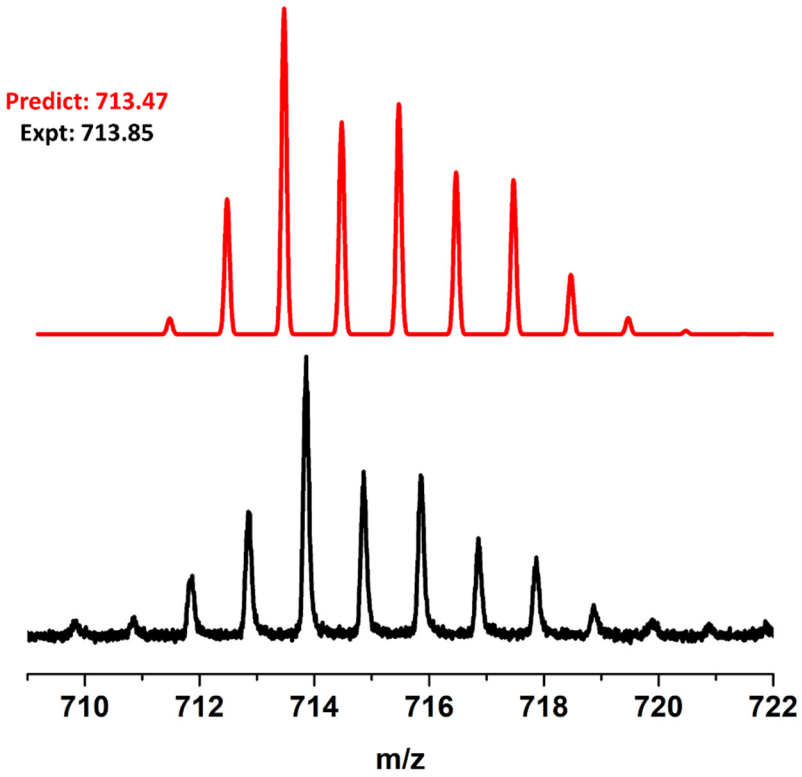


Figure S15. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})ZnH$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{41}H_{65}N_5B_2Zn_1$.

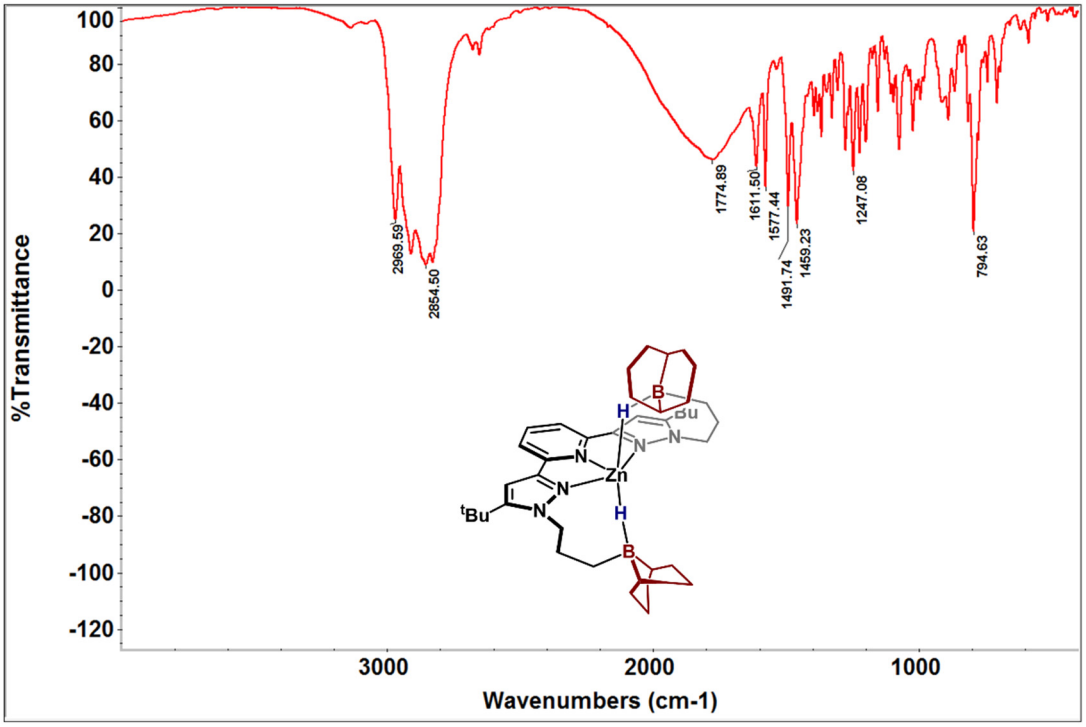


Figure S16. Infrared spectrum (KBr) of (^{BBN}PDP^{tBu})ZnH$_2$.

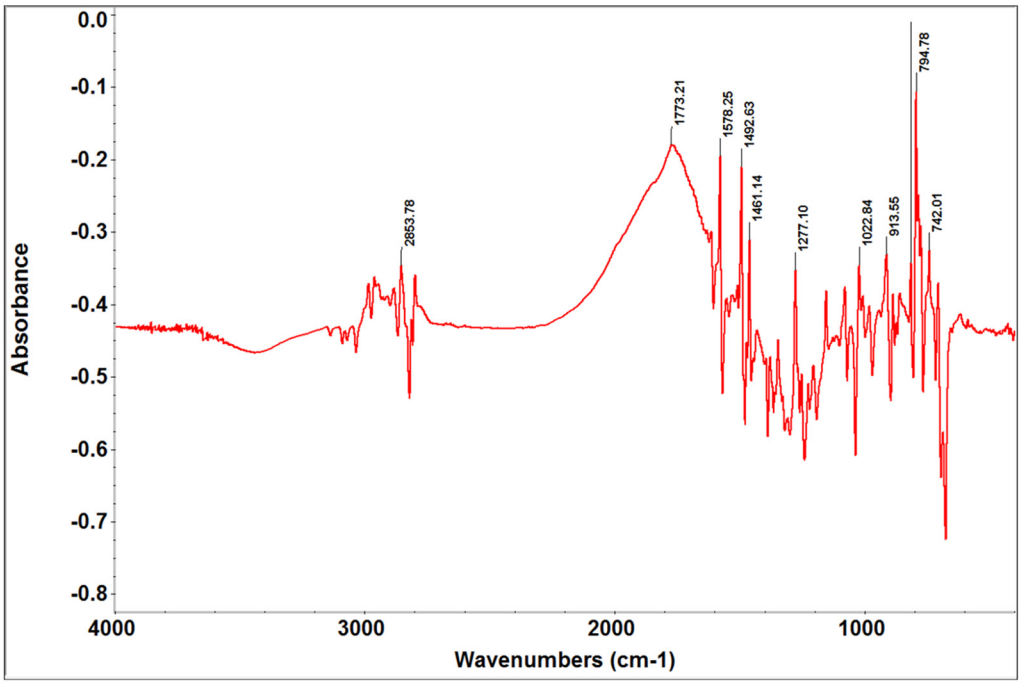


Figure S17. Difference infrared spectrum (KBr) of (^{BBN}PDP^{tBu})ZnH$_2$ minus (^{BBN}PDP^{tBu})ZnD$_2$.

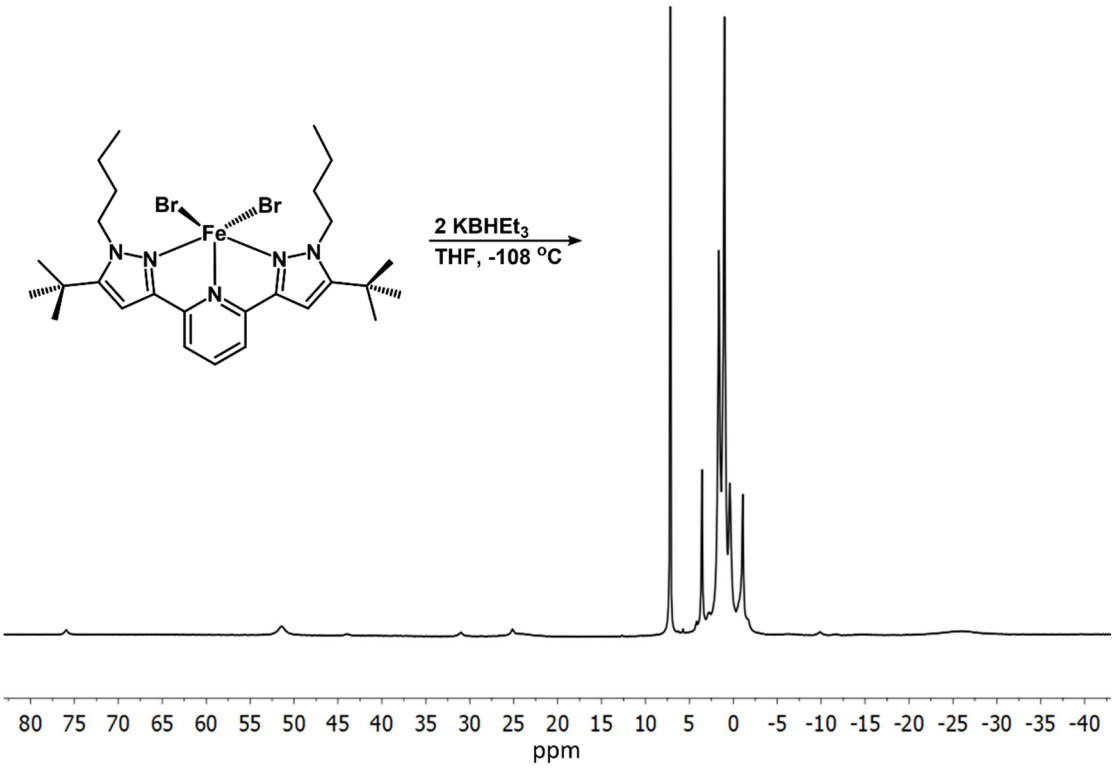


Figure S18. ^{1}H NMR spectrum (C_6D_6, 25 °C) of reaction between (^{Bu}PDP^{tBu})FeBr$_2$ and two equiv. KBHEt$_3$.

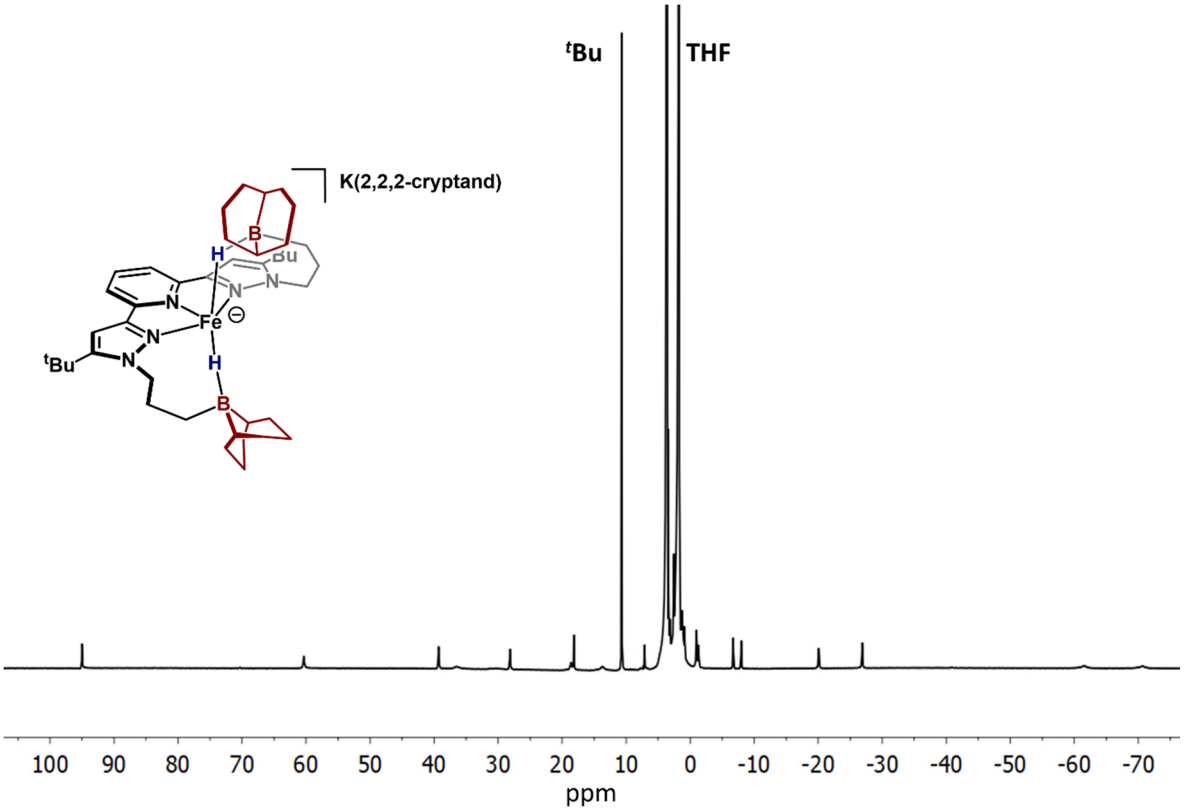


Figure S19. ^{1}H NMR spectrum (THF, 25 °C) of [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$].

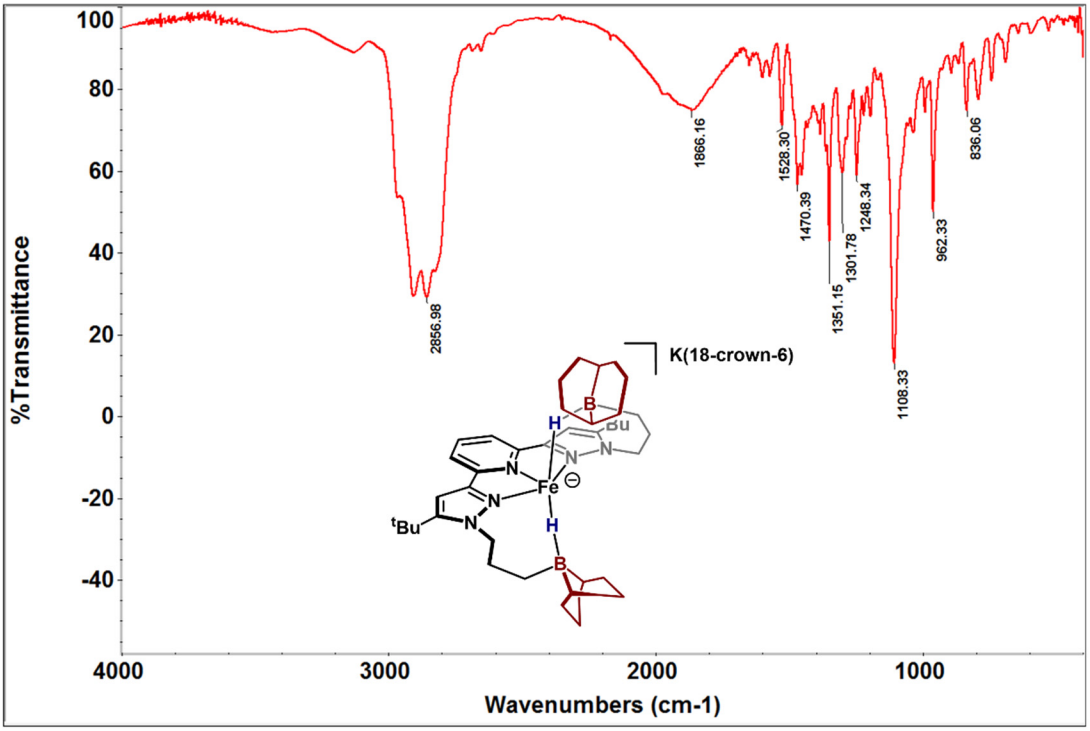


Figure S20. Infrared spectrum (KBr) of [K(18-crown-6)][(^{BBN}PDP^{tBu})FeH$_2$].

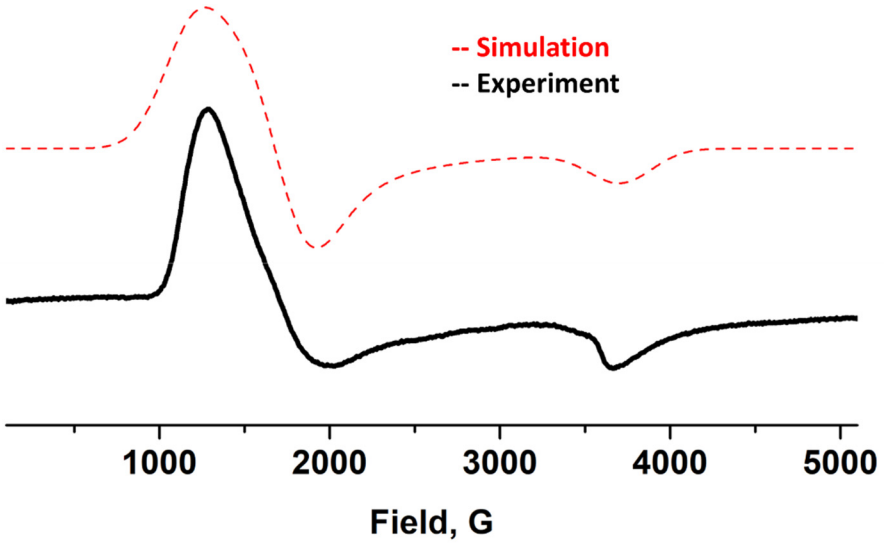


Figure S21. X-band EPR spectrum (black) of [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$] (0.92 mM) recorded in frozen THF/toluene (1:1) at 10 K. Power: 0.502 mW. Modulation: 0.20 mT/100 kHz. Simulated spectrum (red, dotted) for g_x = 5.628, g_y = 3.979, g_z = 1.825, linewidth = 43 G.

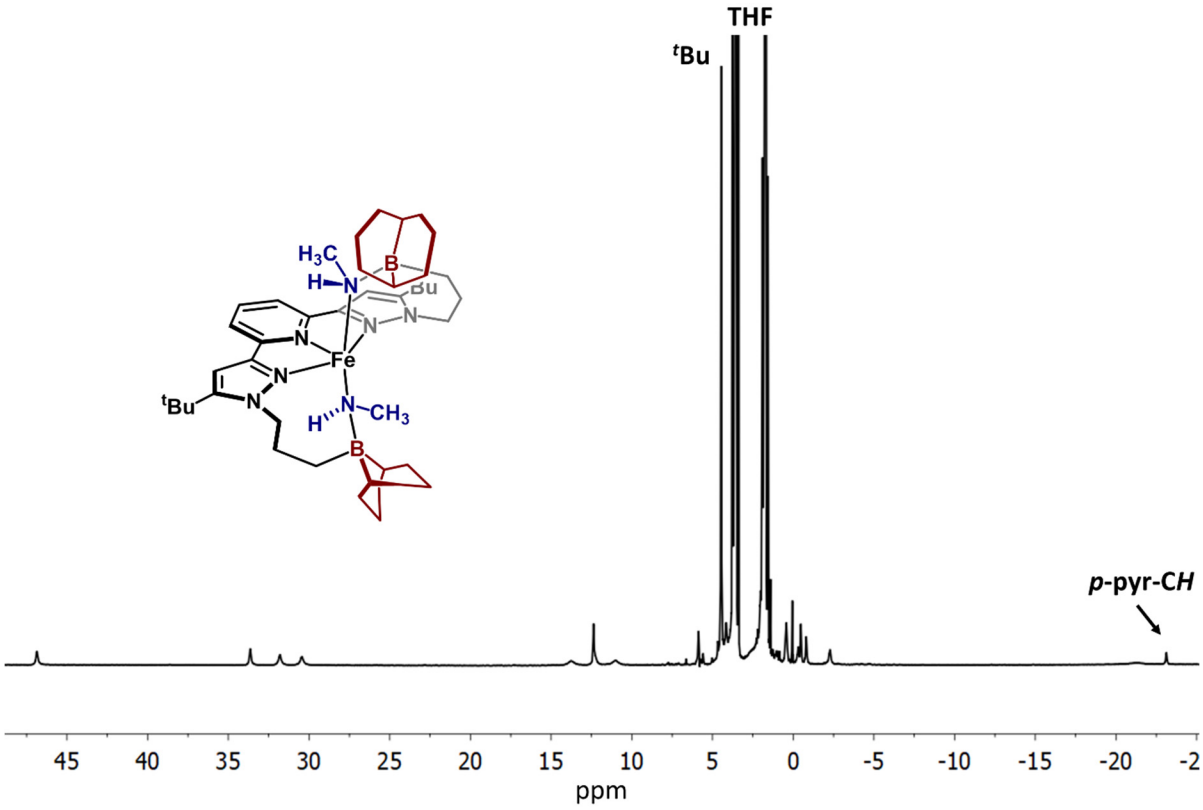


Figure S22. ^{1}H NMR spectrum (THF, 25 °C) of (^{BBN}PDP^{tBu})Fe(NHMe)$_2$.

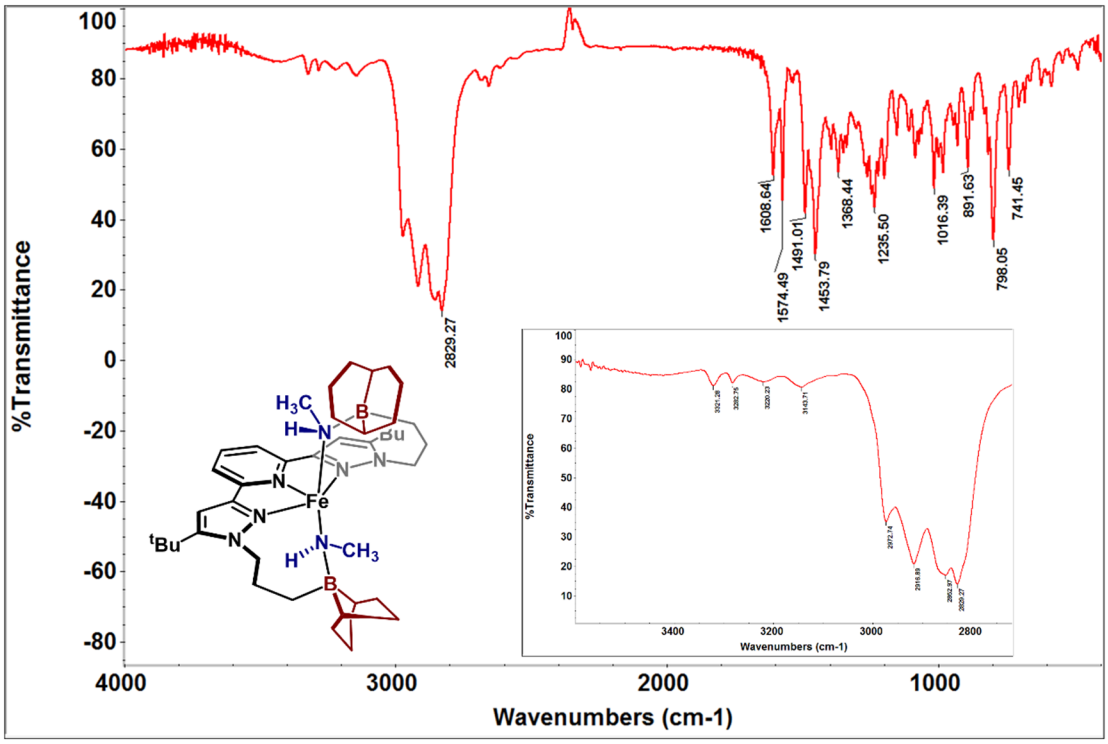


Figure S23. Infrared spectrum (KBr) of (^{BBN}PDP^{tBu})Fe(NHMe)$_2$. Inset highlights N-H region.

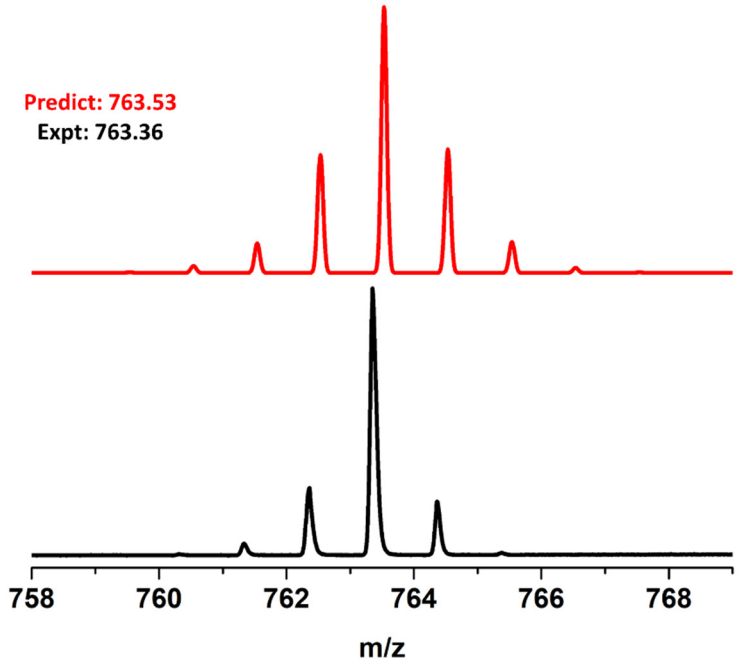


Figure S24. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})Fe(NHMe)$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{43}H_{71}N_7B_2Fe_1$.

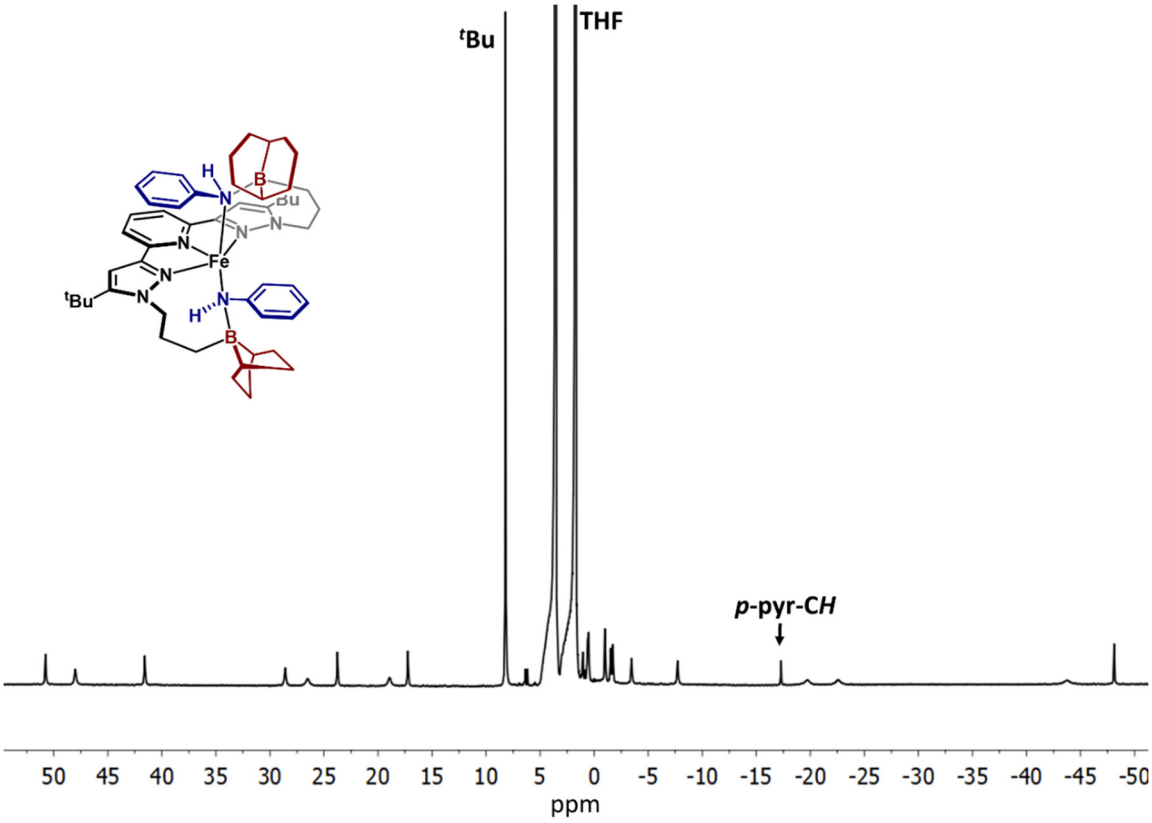


Figure S25. ^{1}H NMR spectrum (THF, 25 °C) of (^{BBN}PDP^{tBu})Fe(NHPh)$_2$.

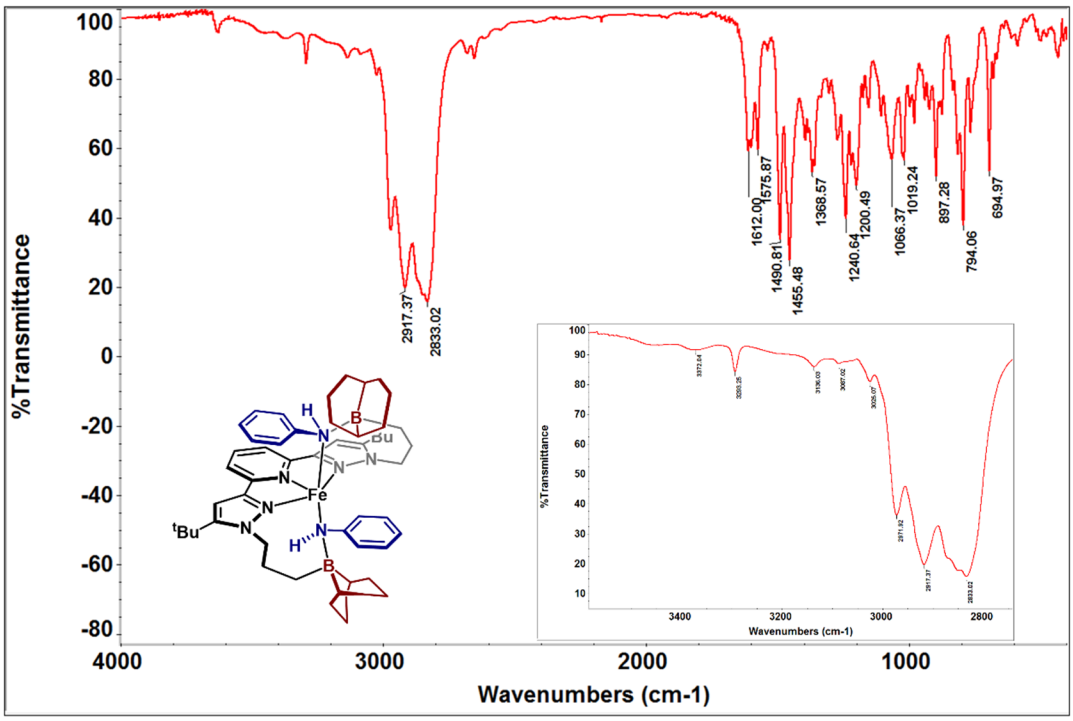


Figure S26. Infrared spectrum (KBr) of (^{BBN}PDP^{tBu})Fe(NHPh)$_2$. Inset highlights N-H region.

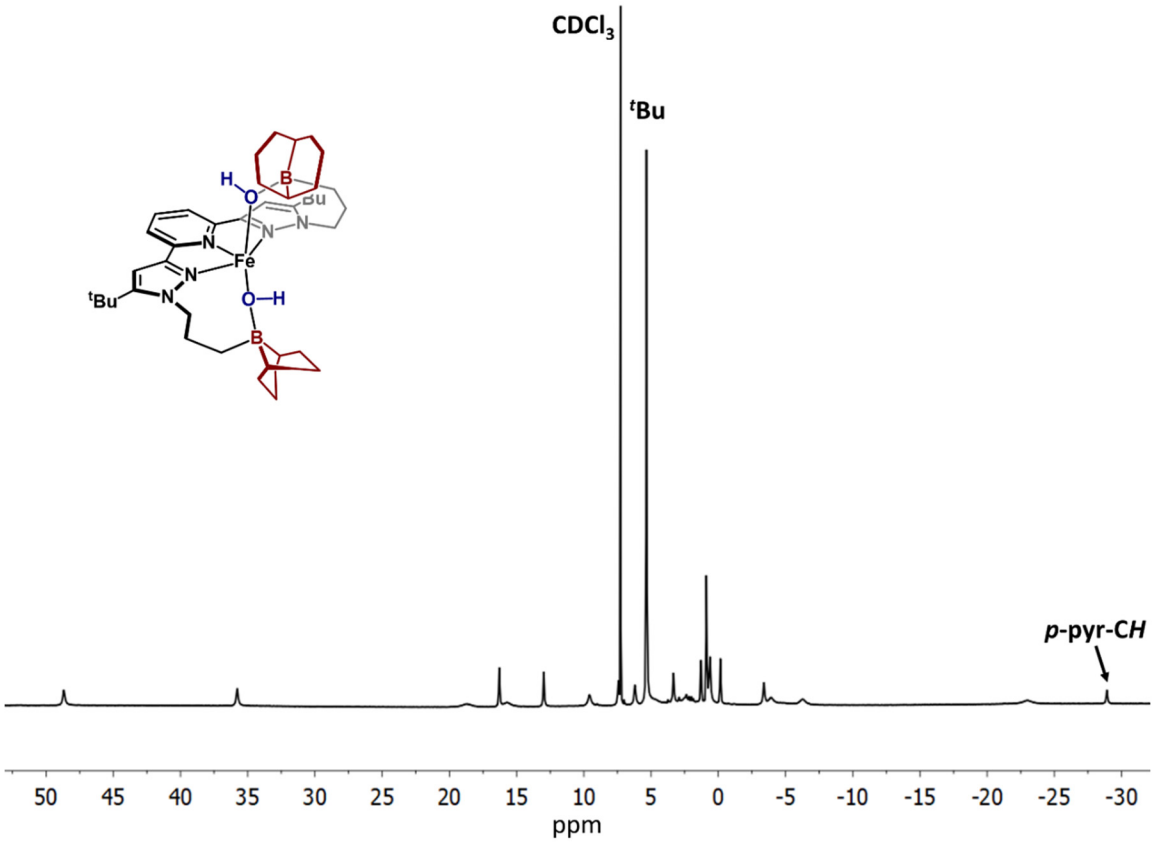


Figure S27. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of ($^{BBN}PDP^{tBu}$)$Fe(OH)_2$.

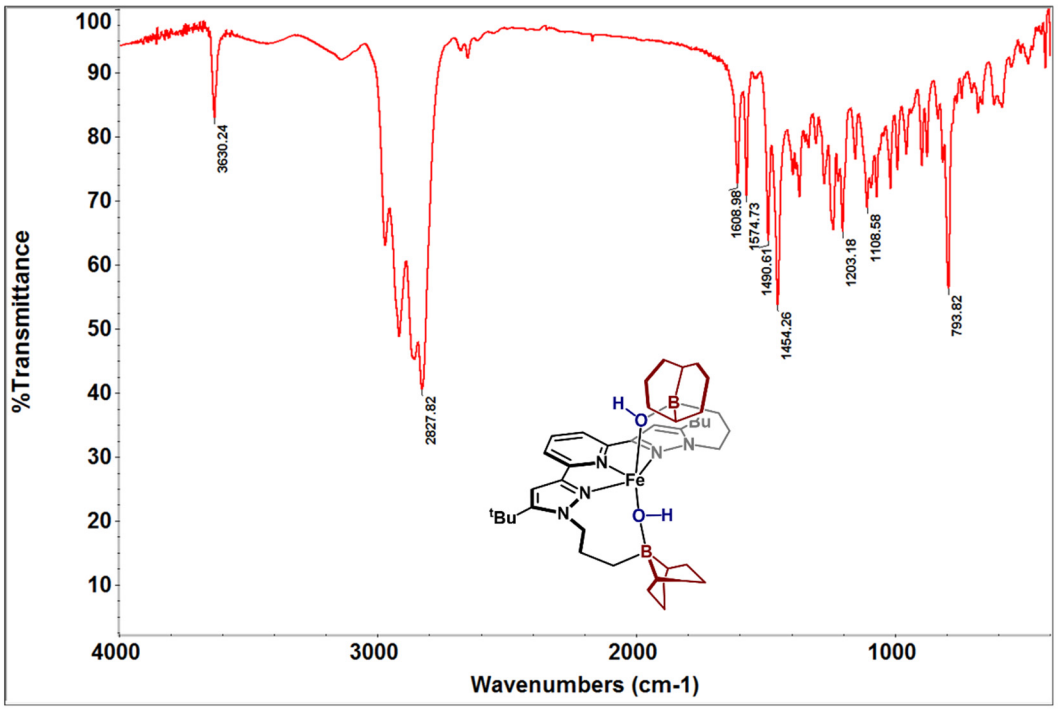


Figure S28. Infrared spectrum (KBr) of ($^{BBN}PDP^{tBu}$)$Fe(OH)_2$.

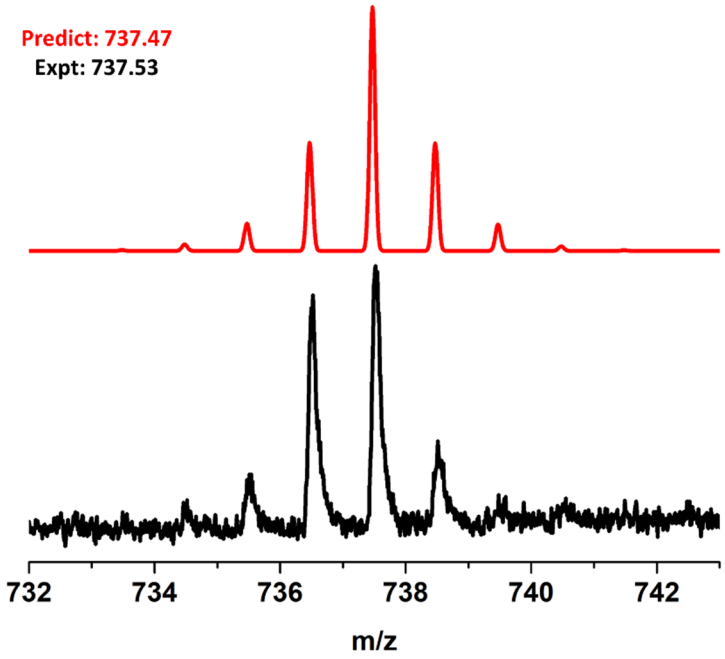


Figure S29. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})Fe(OH)$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{41}H_{65}N_5O_2B_2Fe_1$.

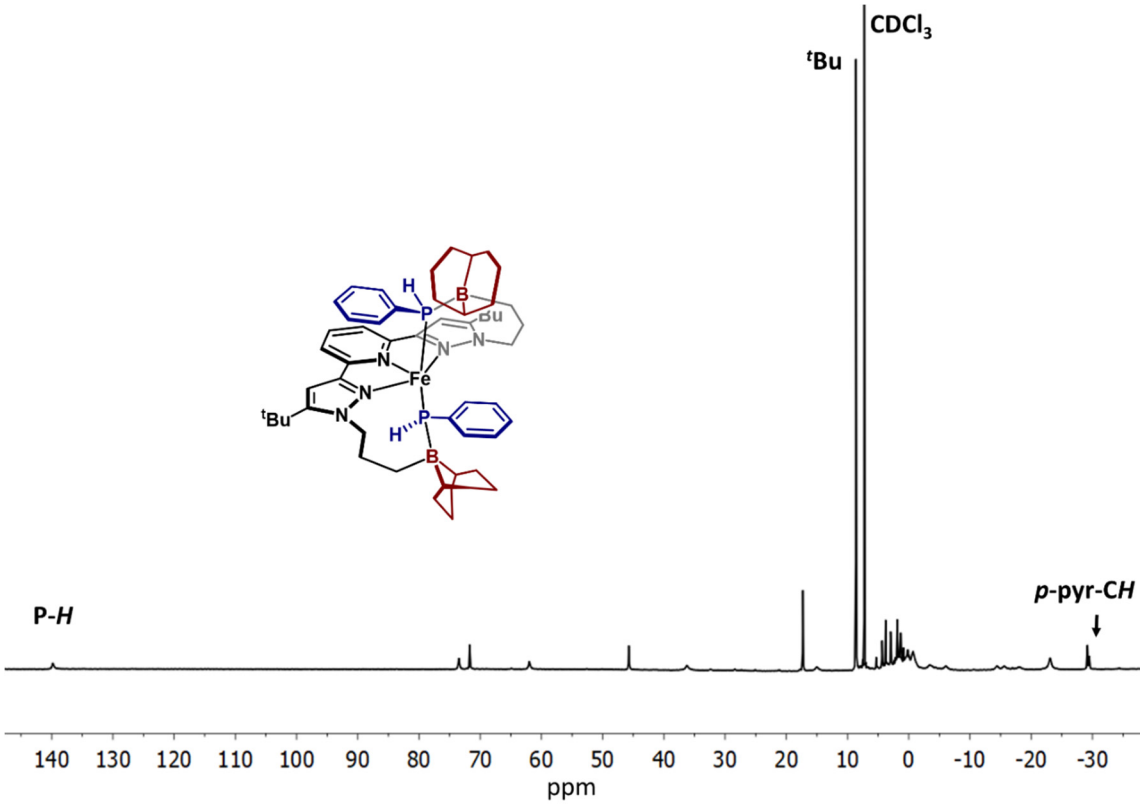


Figure S30. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of (^{BBN}PDP^{tBu})Fe(PHPh)$_2$.

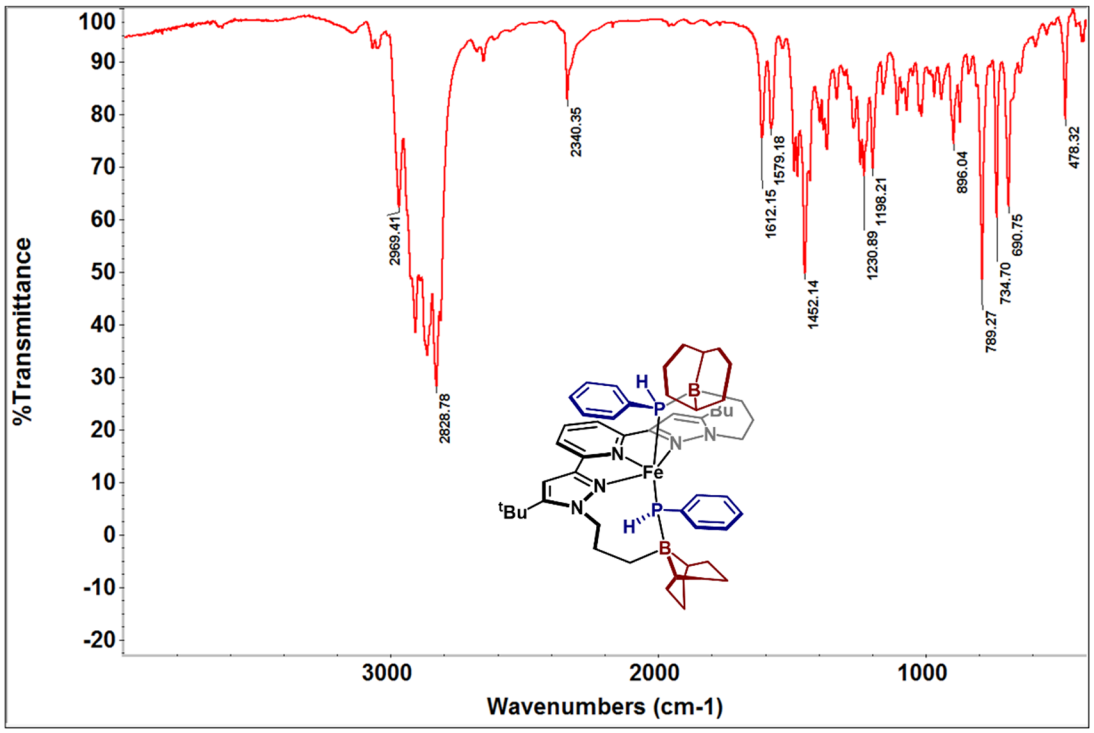


Figure S31. Infrared spectrum (KBr) of (^{BBN}PDP^{tBu})Fe(PHPh)$_2$.

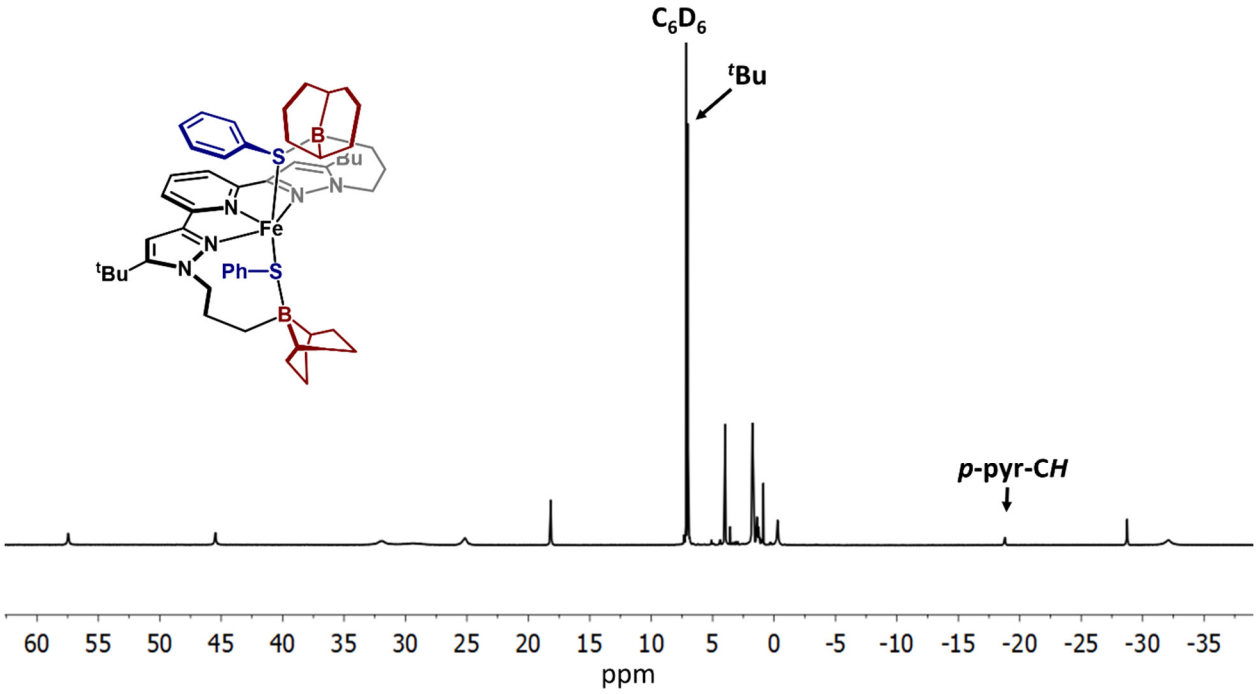


Figure S32. ^{1}H NMR spectrum (C_6D_6, 25 °C) of (^{BBN}PDP^{tBu})Fe(SPh)$_2$.

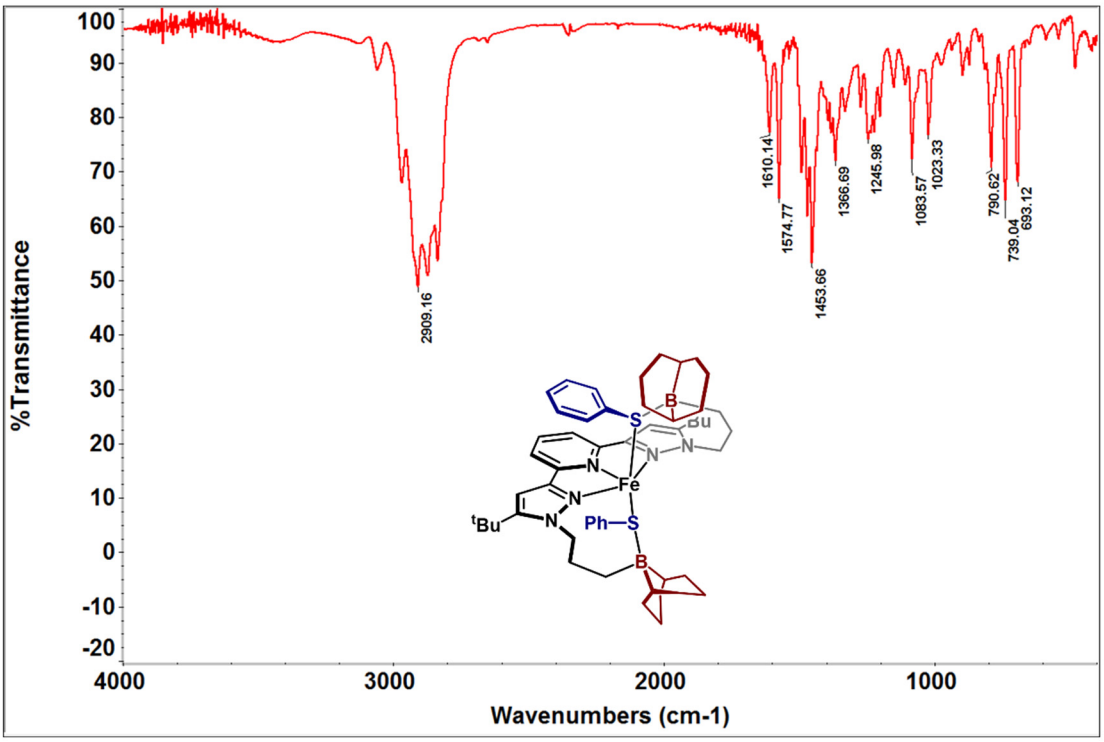


Figure S33. Infrared spectrum (KBr) of (^{BBN}PDP^{tBu})Fe(SPh)$_2$.

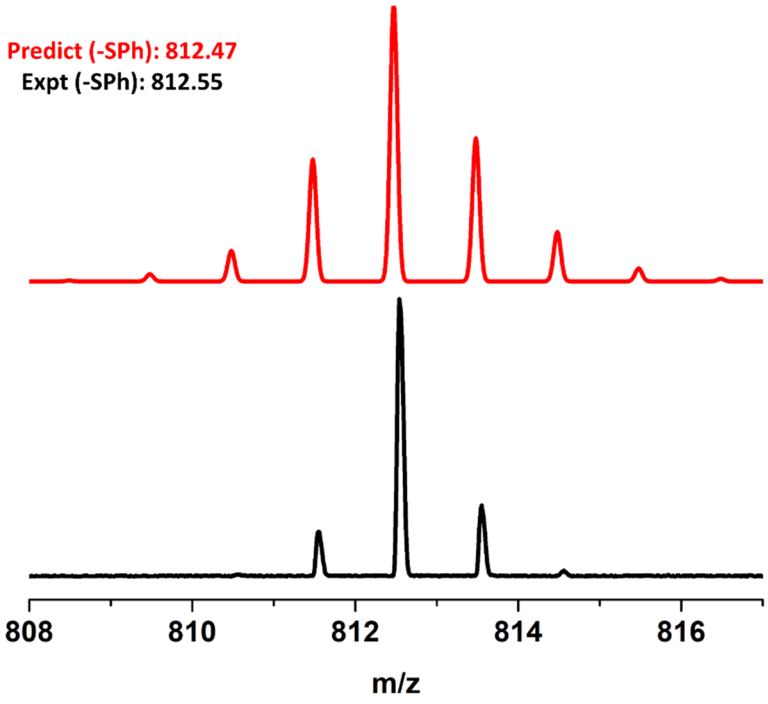


Figure S34. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})Fe(SPh)$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{53}H_{73}N_5B_2S_2Fe_1$ - SPh.

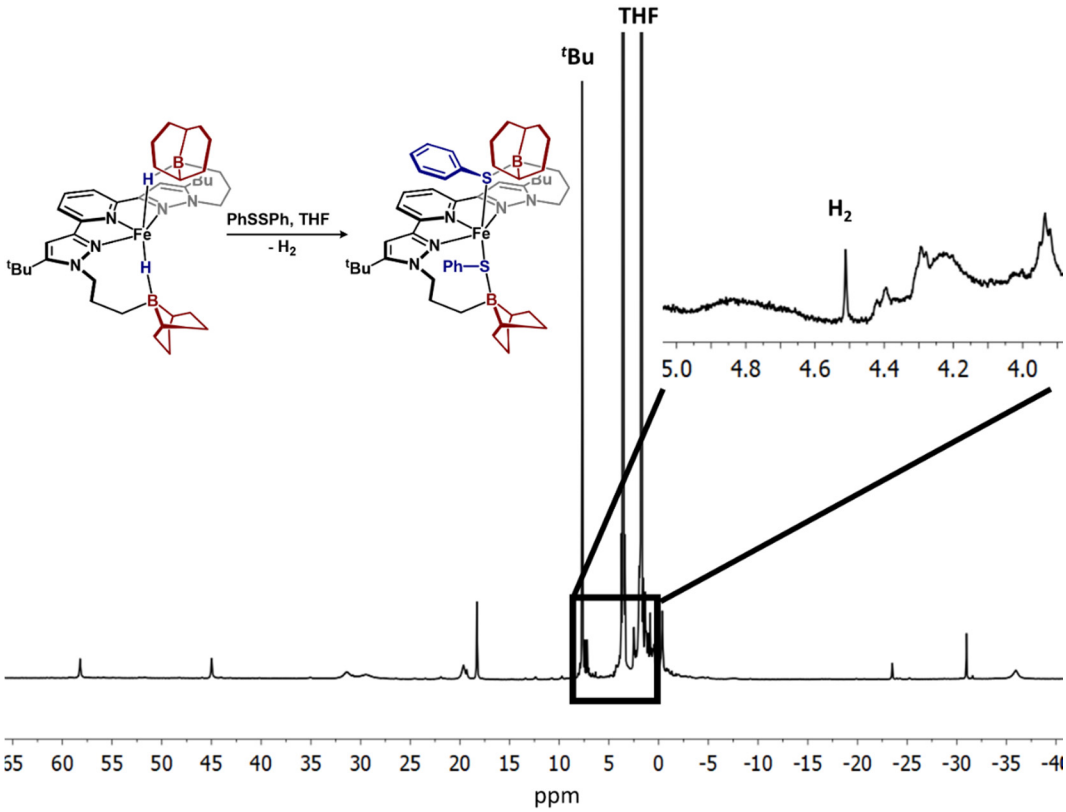


Figure S35. Crude ^{1}H NMR spectrum (THF, 25 °C) of the reaction between (^{BBN}PDP^{tBu})FeH$_2$ and PhSSPh to produce (^{BBN}PDP^{tBu})Fe(SPh)$_2$ and H$_2$ in a sealed J-Young NMR tube.

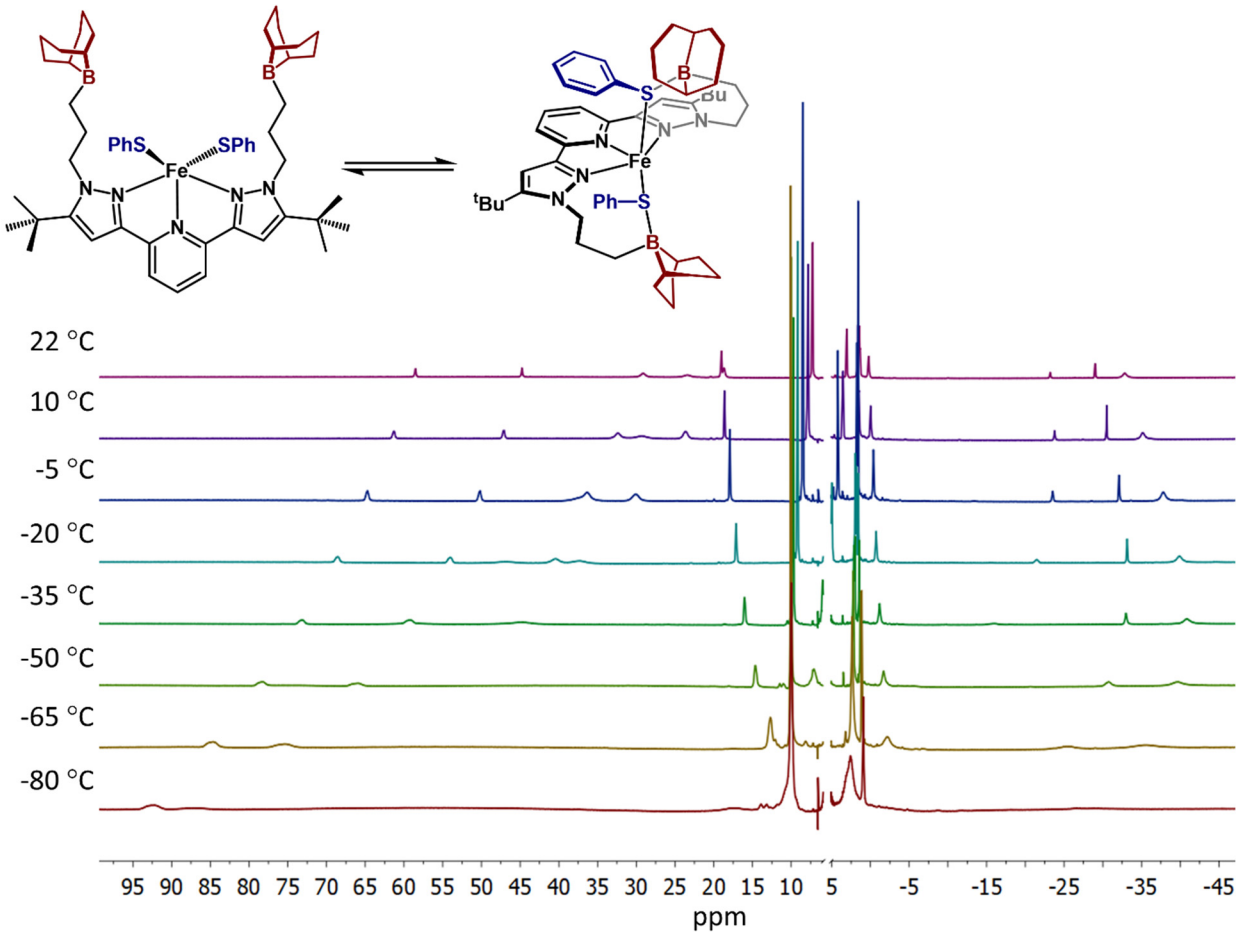


Figure S36. Variable temperature ^{1}H NMR spectra (CH_2Cl_2) of ($^{BBN}PDP^{tBu}$)Fe(SPh)$_2$. The residual CH_2Cl_2 resonance is omitted to increase clarity.

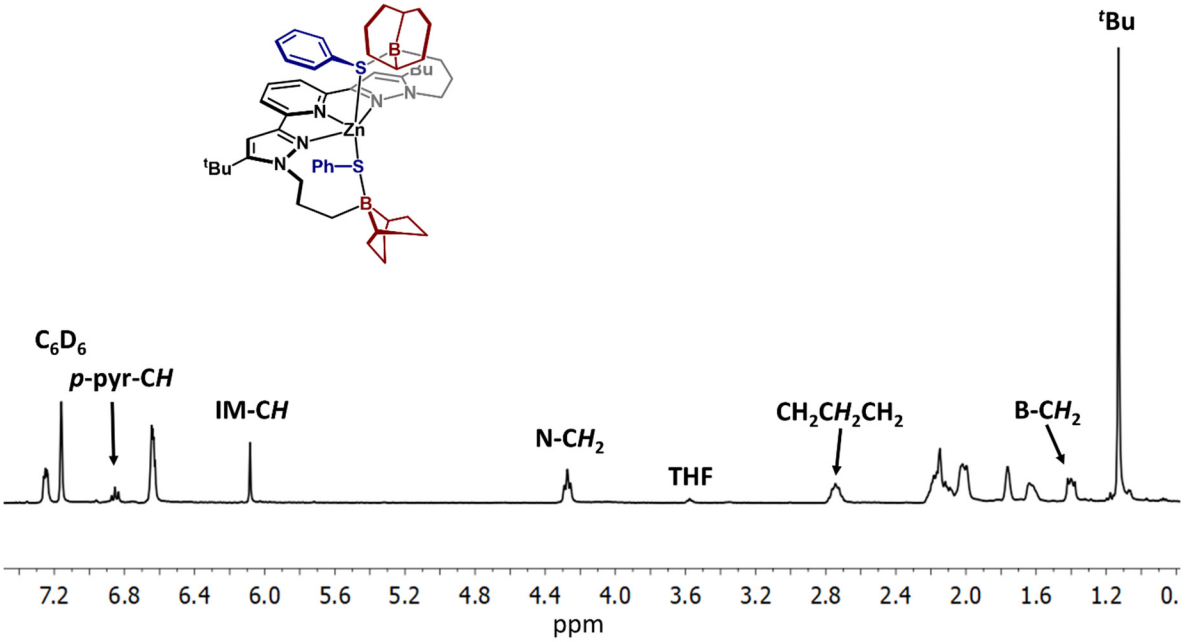


Figure S37. ^{1}H NMR spectrum (C_6D_6, 25 °C) of (^{BBN}PDP^{tBu})Zn(SPh)$_2$.

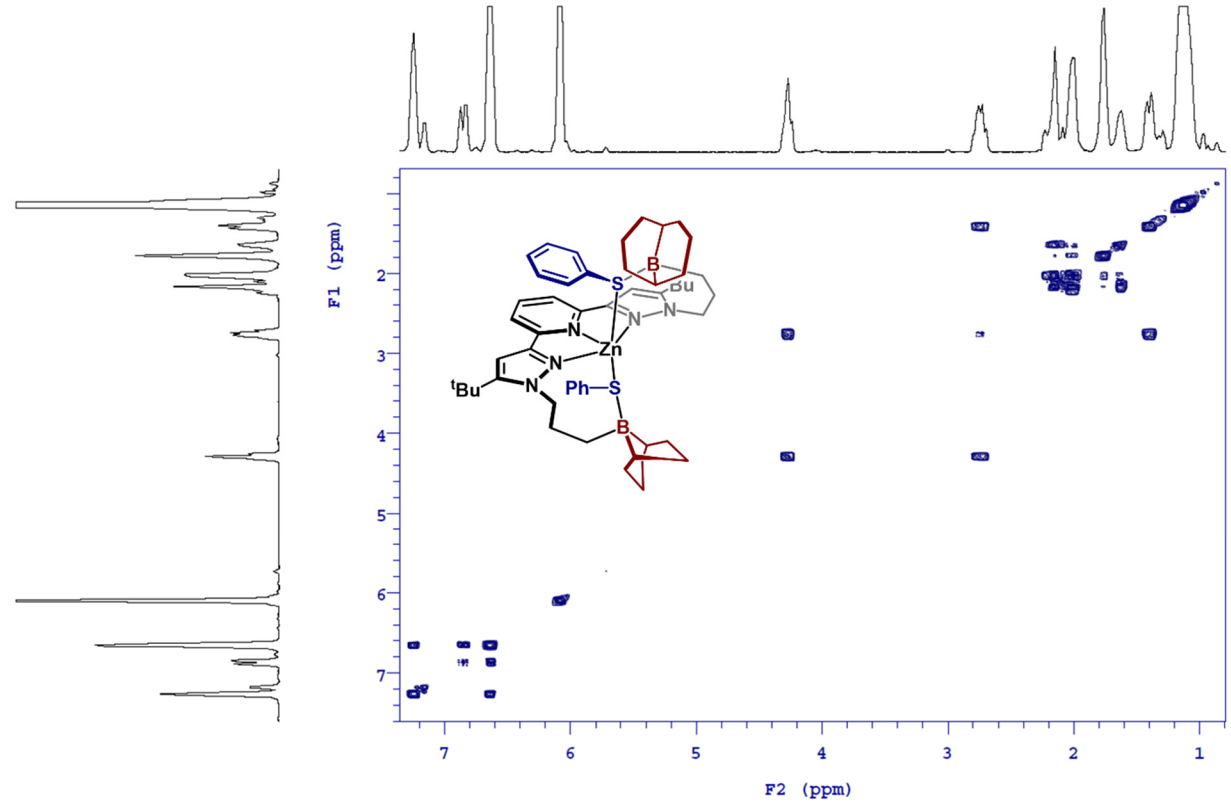


Figure S38. ^{1}H-^{1}H COSY spectrum (C_6D_6, 25 °C) of (^{BBN}PDP^{tBu})Zn(SPh)$_2$.

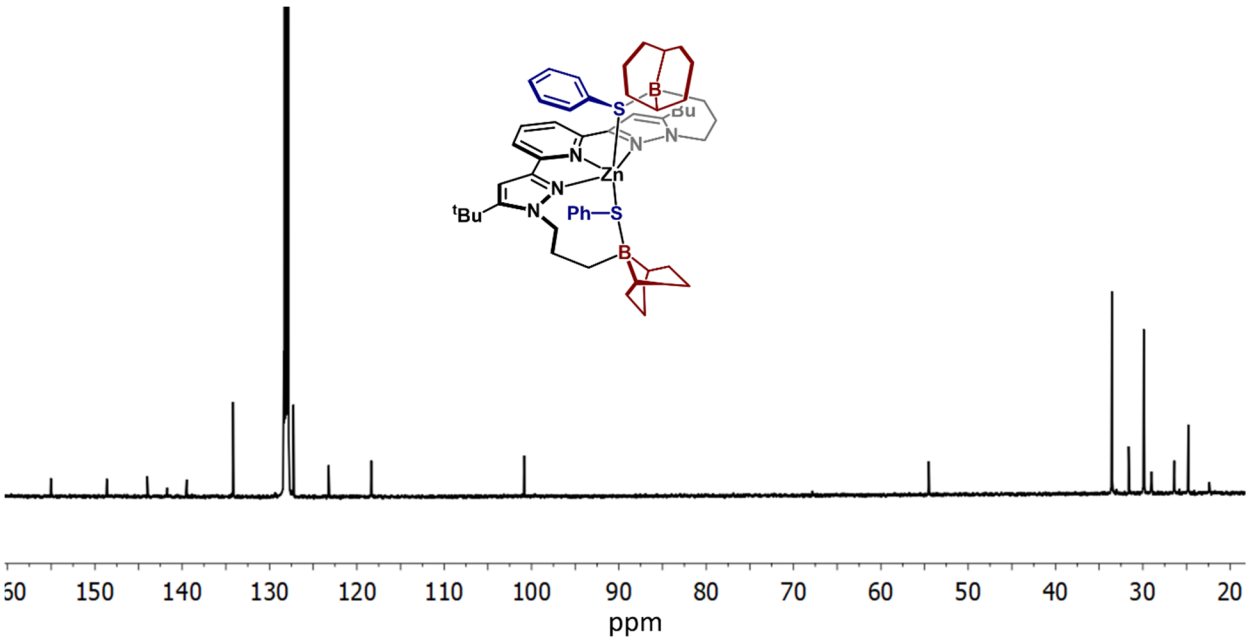


Figure S39. ^{13}C NMR spectrum (C_6D_6, 25 °C) of ($^{BBN}PDP^{tBu}$)Zn(SPh)$_2$.

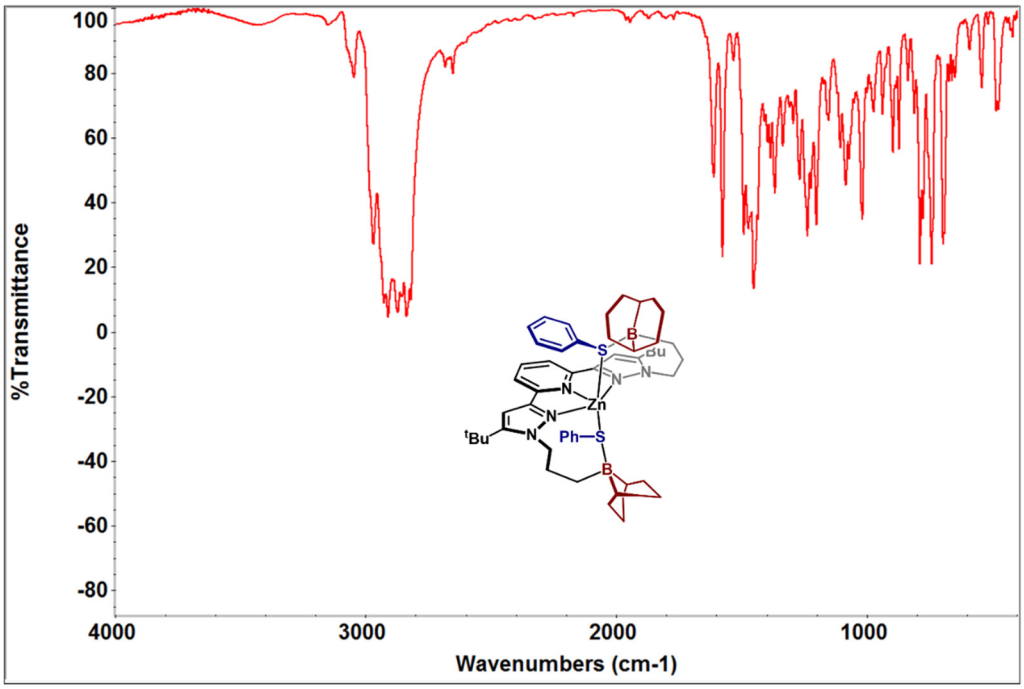


Figure S40. Infrared spectrum (KBr) of ($^{BBN}PDP^{tBu}$)Zn(SPh)$_2$.

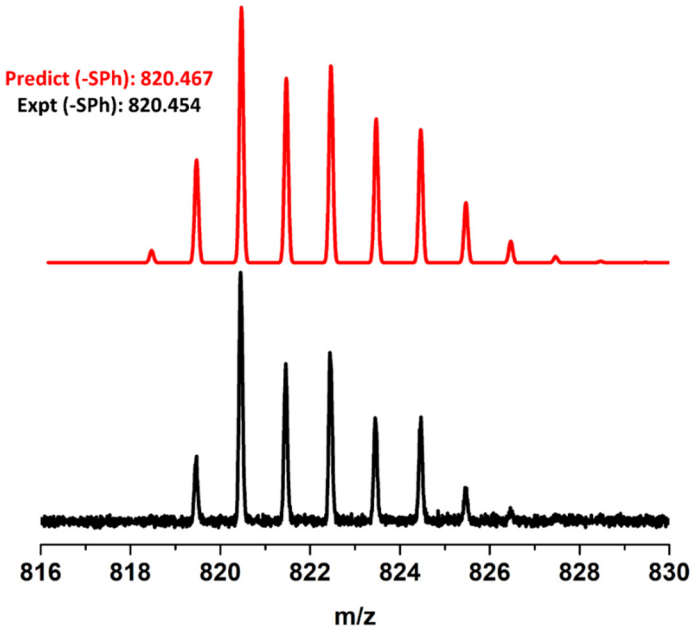


Figure S41. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})Zn(SPh)$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{53}H_{73}N_5B_2S_2Zn_1$ - SPh.

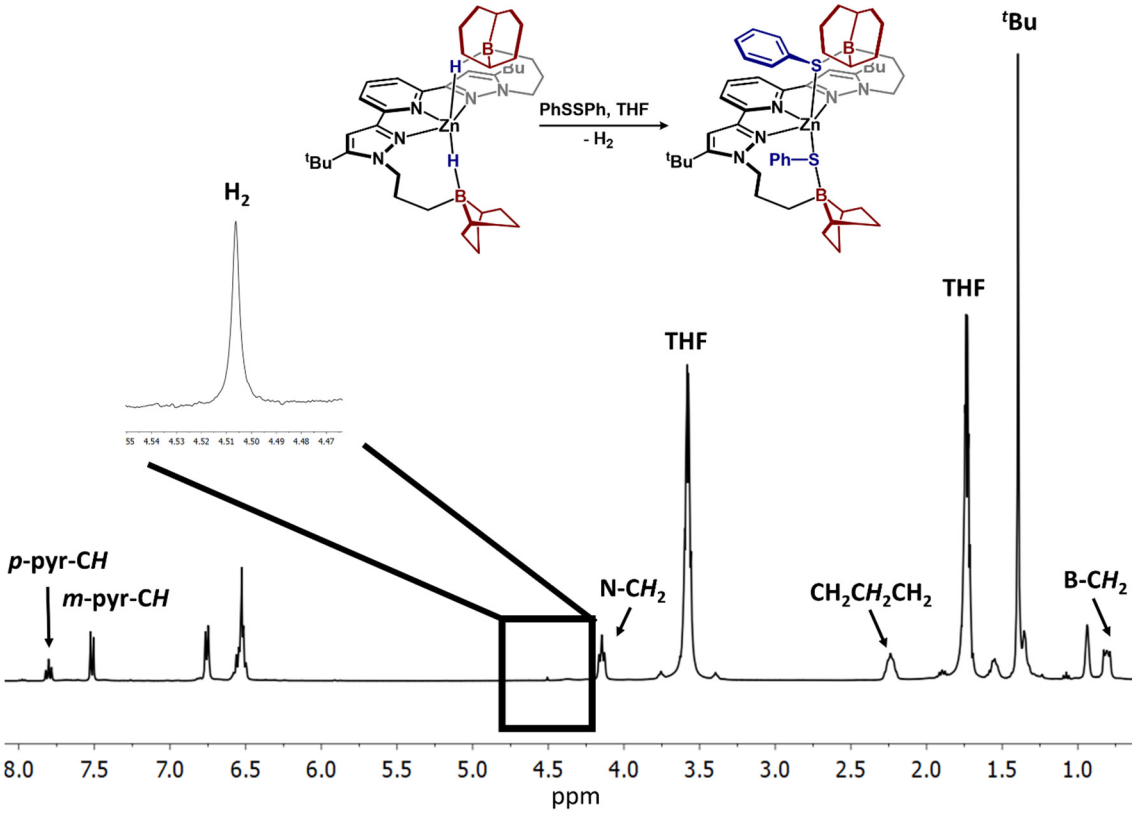


Figure S42. Crude ^{1}H NMR spectrum (THF, 25 °C) of the reaction between (^{BBN}PDP^{tBu})ZnH$_2$ and PhSSPh to produce (^{BBN}PDP^{tBu})Zn(SPh)$_2$ and H$_2$ in a sealed J-Young NMR tube.

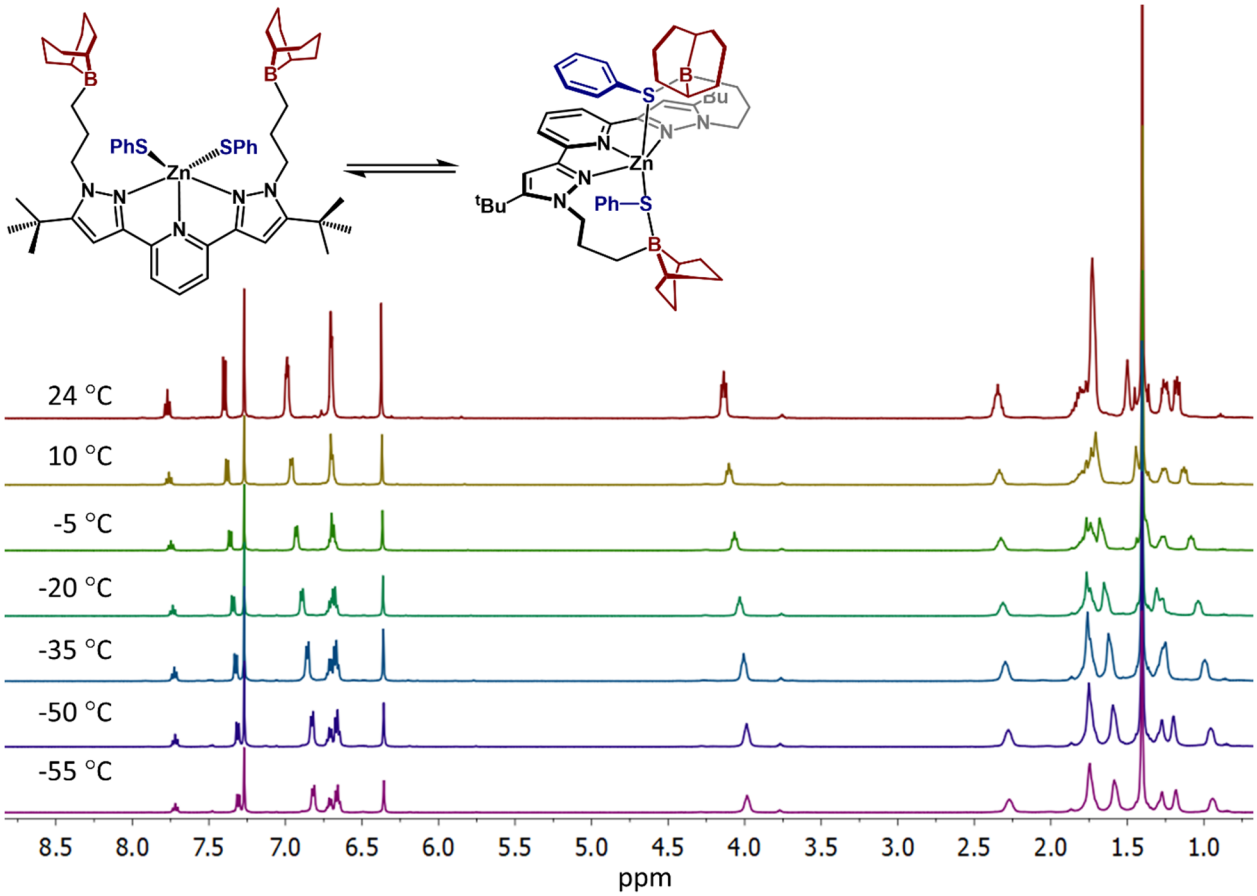


Figure S43. Variable temperature ^{1}H NMR spectra ($CDCl_3$) of ($^{BBN}PDP^{tBu}$)Zn(SPh)$_2$.

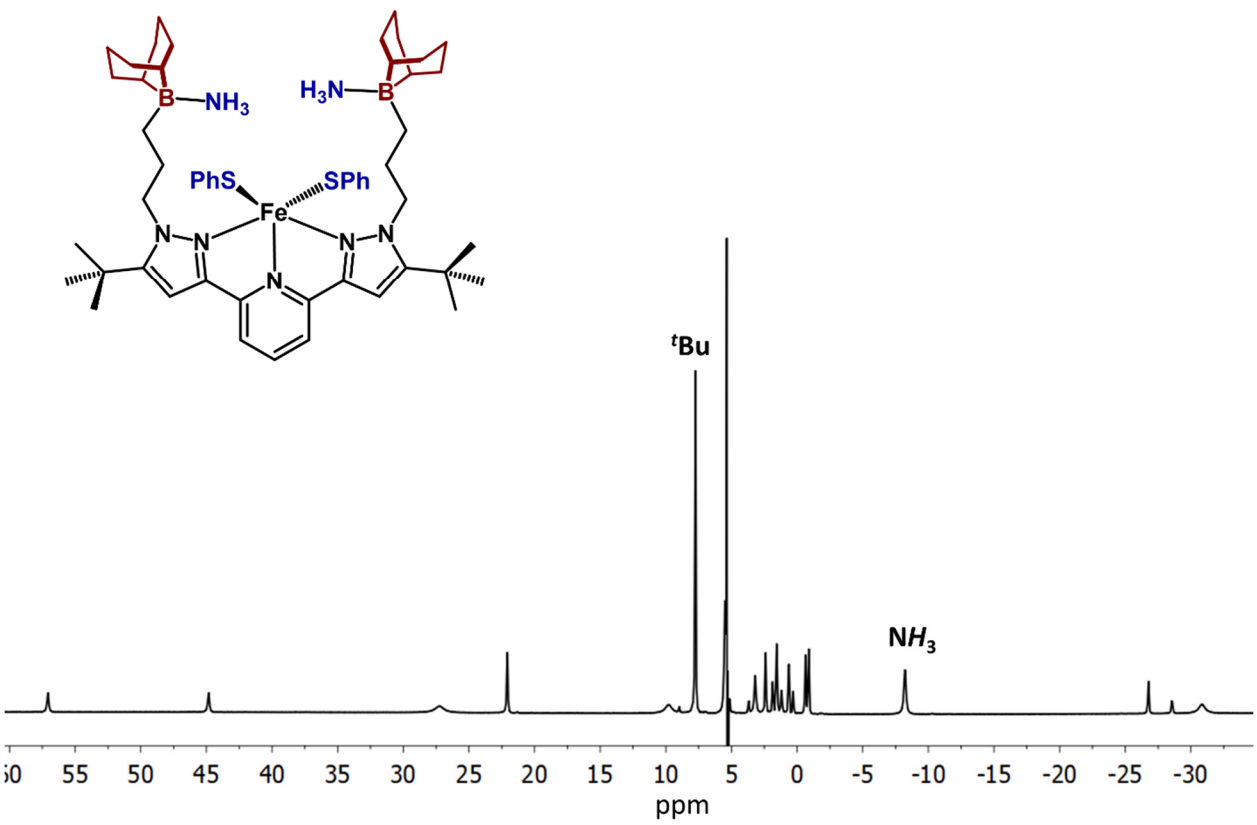


Figure S44. ^{1}H NMR spectrum (CH_2Cl_2, 25 °C) of ($^{BBN}PDP^{tBu}$)Fe(SPh)$_2$(NH_3)$_2$.

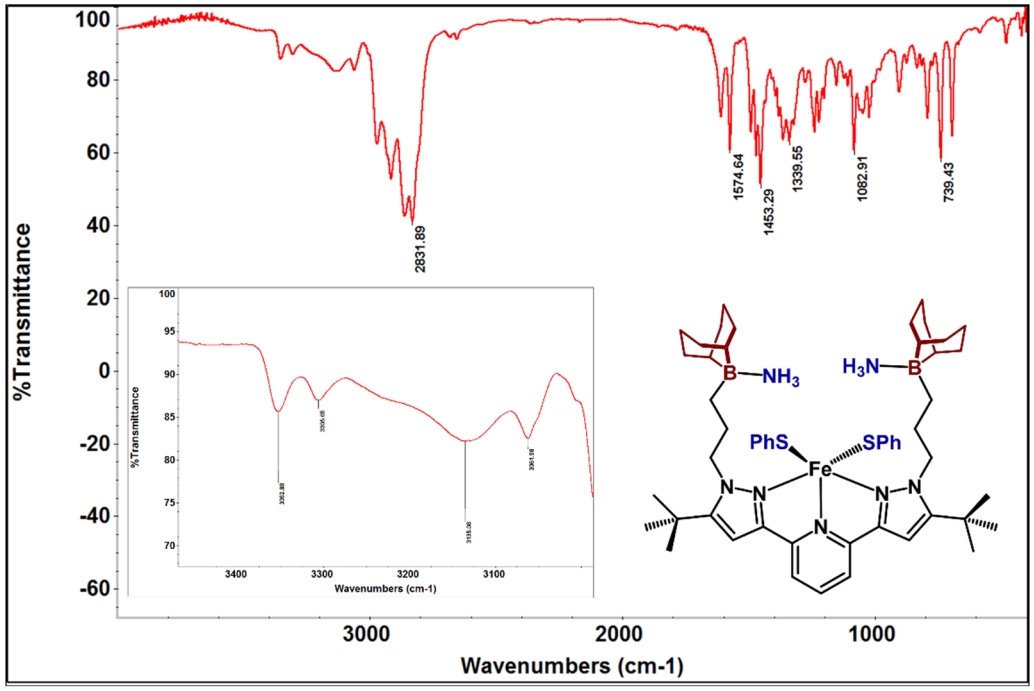


Figure S45. Infrared spectrum (KBr) of ($^{BBN}PDP^{tBu}$)Fe(SPh)$_2$(NH_3)$_2$.

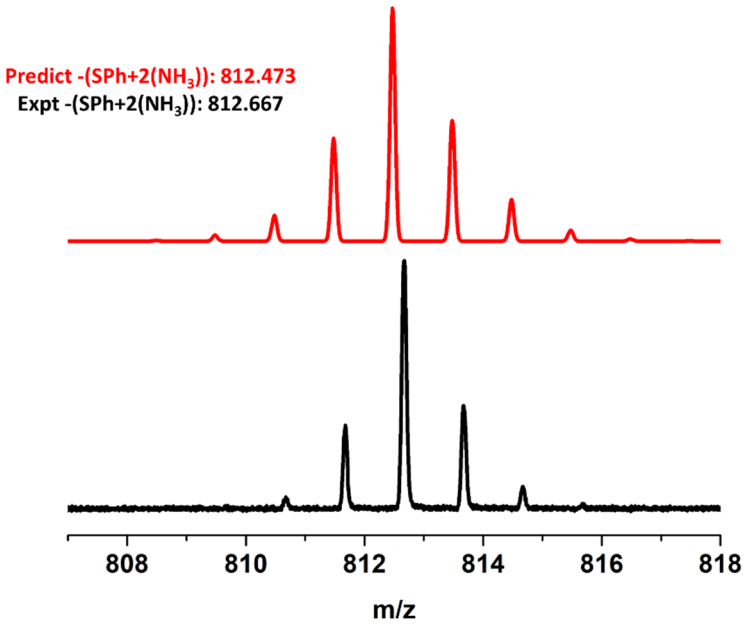


Figure S46. MALDI-TOF spectrum of (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{53}H_{73}N_5B_2S_2Fe_1$ – (SPh + 2(NH$_3$)).

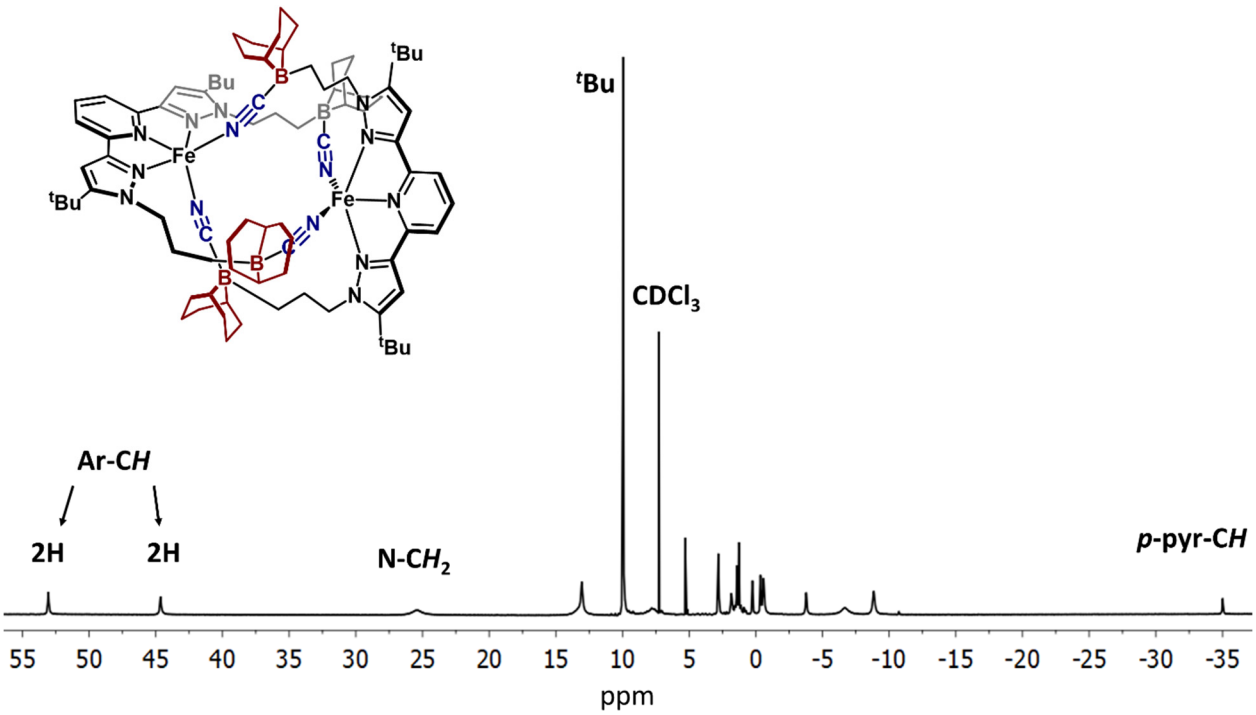


Figure S47. ^{1}H NMR spectrum ($CDCl_3$, 25 °C) of [(^{BBN}PDP^{tBu})Fe(NC)$_2$]$_2$.

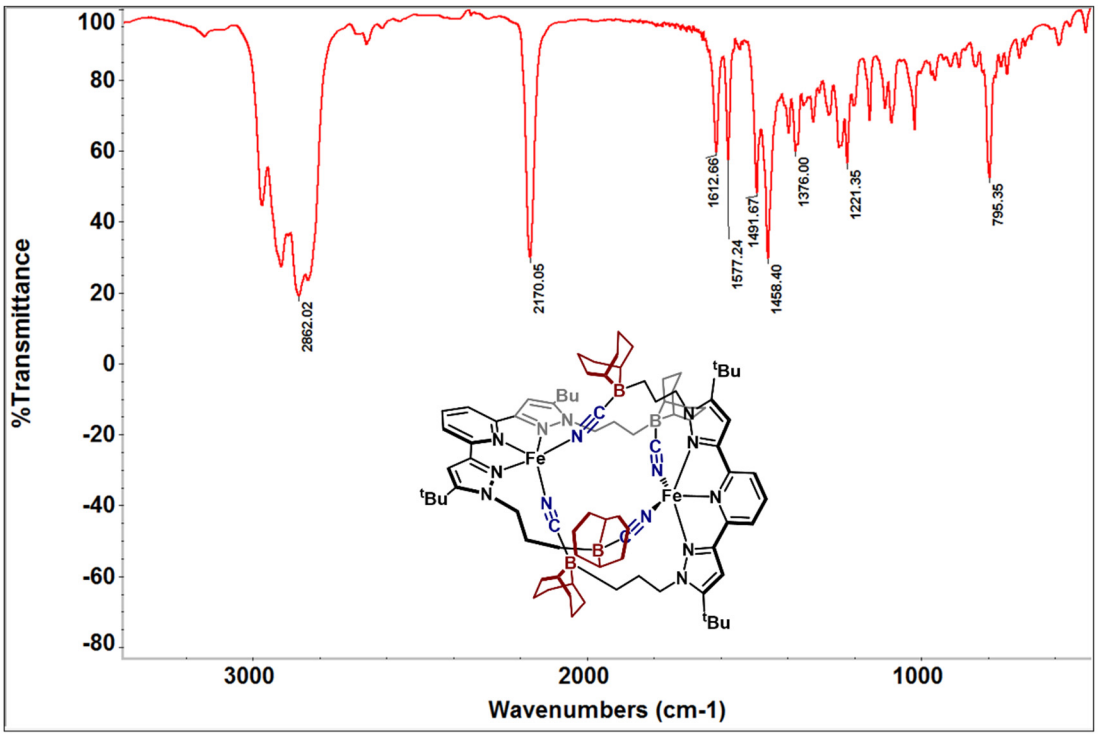


Figure S48. Infrared spectrum (KBr) of $[(^{BBN}PDP^{tBu})Fe(NC)_2]_2$.

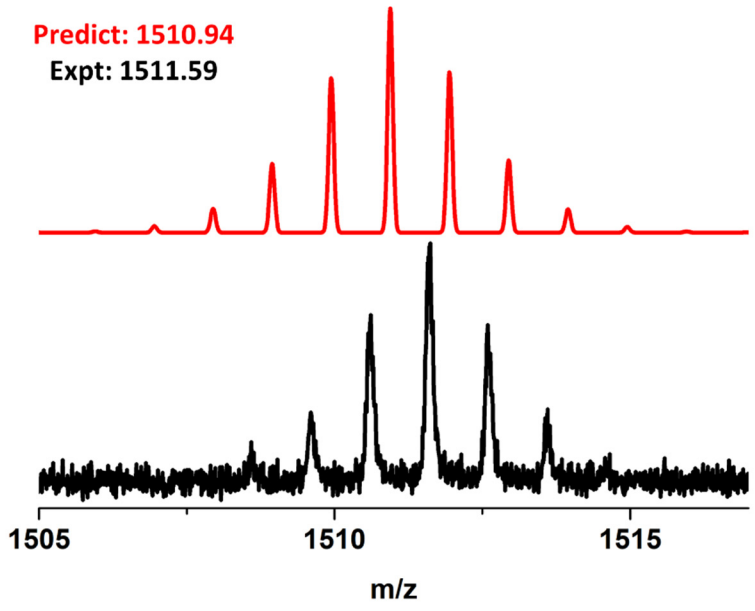


Figure S49. MALDI-TOF spectrum of $[(^{BBN}PDP^{tBu})Fe(NC)_2]_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{86}H_{126}N_{14}B_4Fe_2$.

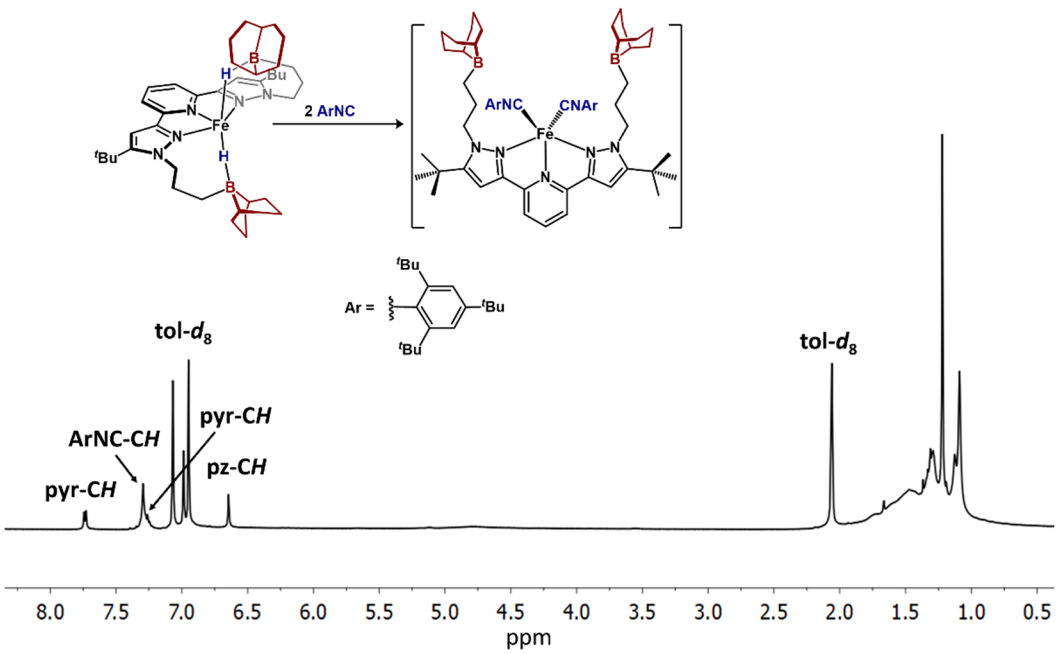


Figure S50. ^{1}H NMR spectrum (tol-d_8, 25 °C) of the reaction between (^{BBN}PDP^{tBu})FeH$_2$ and two equivalents of ArNC (Ar = 2,4,6-tri-*tert*-butylphenyl).

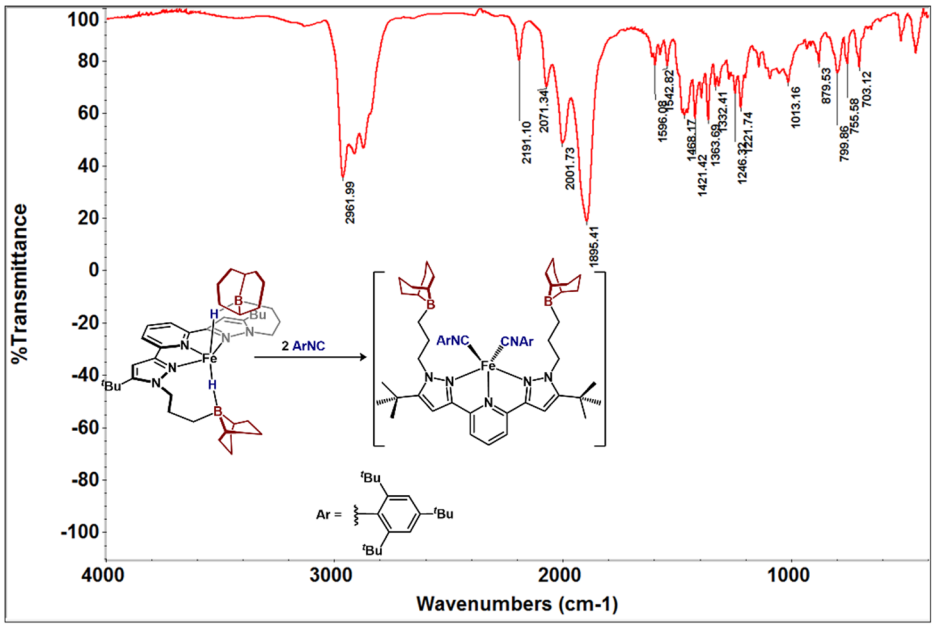


Figure S51. Infrared spectrum (KBr) of the reaction between (^{BBN}PDP^{tBu})FeH$_2$ and two equivalents of ArNC (Ar = 2,4,6-tri-*tert*-butylphenyl).

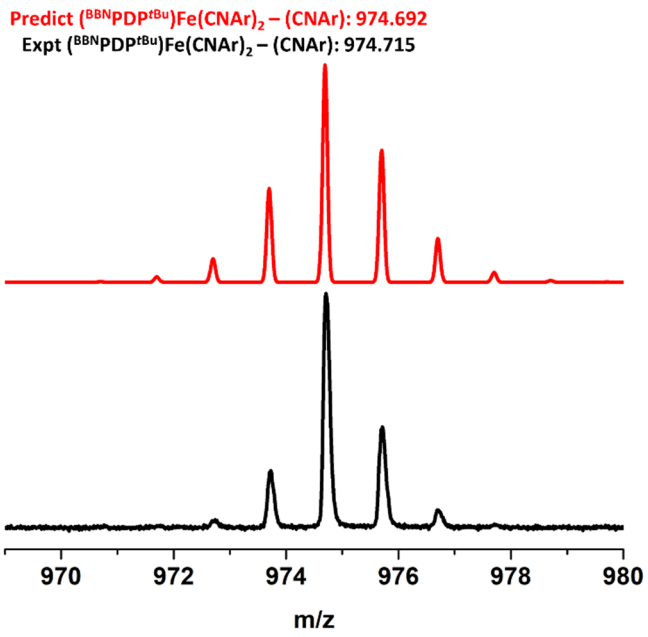


Figure S52. MALDI-TOF spectrum of reaction between (^{BBN}PDP^{tBu})FeH$_2$ and 2 equiv. ArNC (Ar = 2,4,6-tri-*tert*-butylphenyl) (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). The calculated isotopic pattern corresponds to loss of CNAr from (^{BBN}PDP^{tBu})Fe(CNAr)$_2$. Monoisotopic mass calculated for $C_{60}H_{92}N_6B_2Fe_1$.

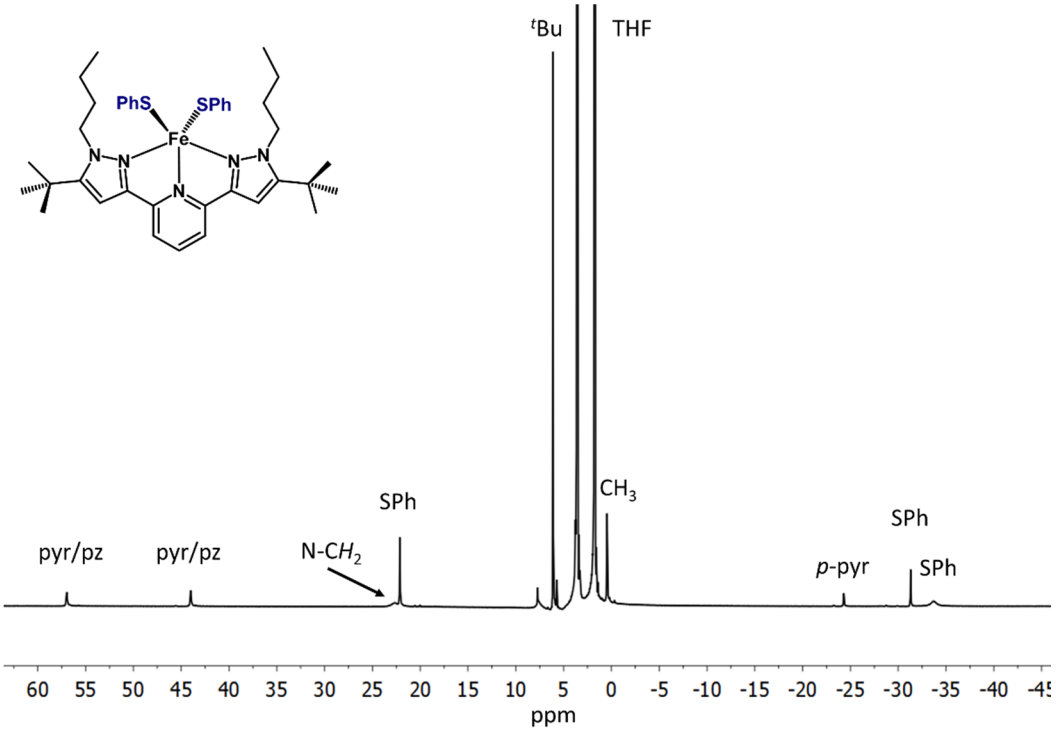


Figure S53. ^{1}H NMR spectrum (THF, 25 °C) of (^{butyl}PDP^{tBu})Fe(SPh)$_2$.

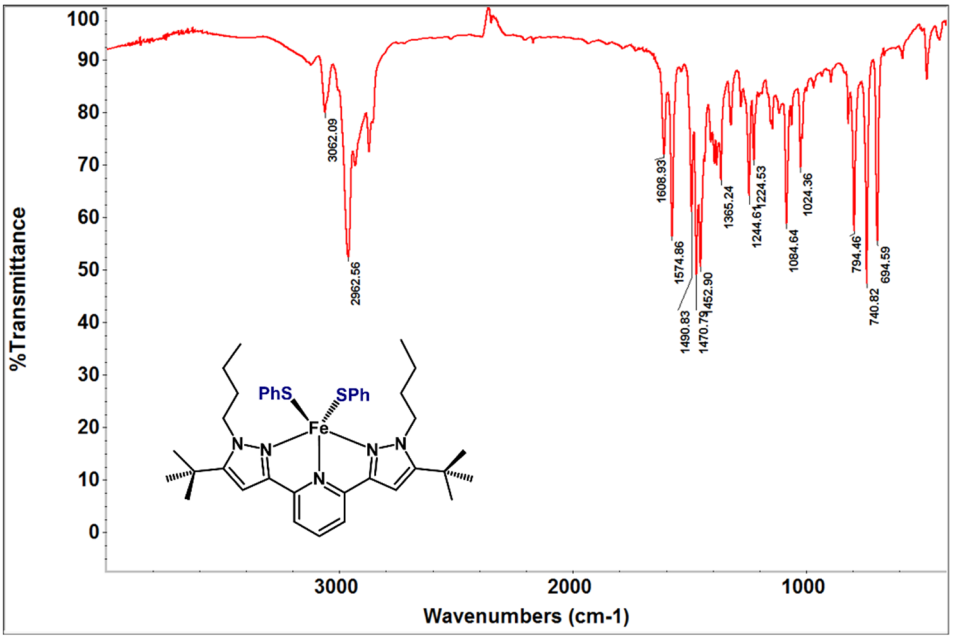


Figure S54. Infrared spectrum (KBr) of (^{butyl}PDP^{tBu})Fe(SPh)$_2$.

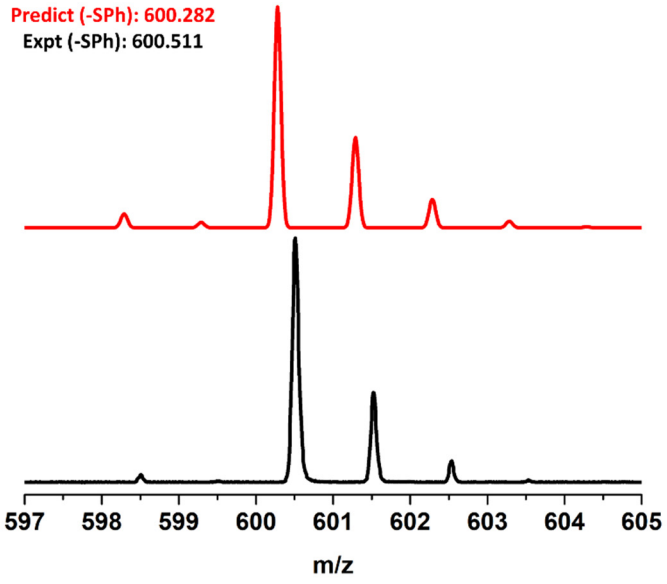


Figure S55. MALDI-TOF spectrum of (^{butyl}PDP^{tBu})Fe(SPh)$_2$ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for $C_{39}H_{51}N_5S_2Fe_1$ - SPh.

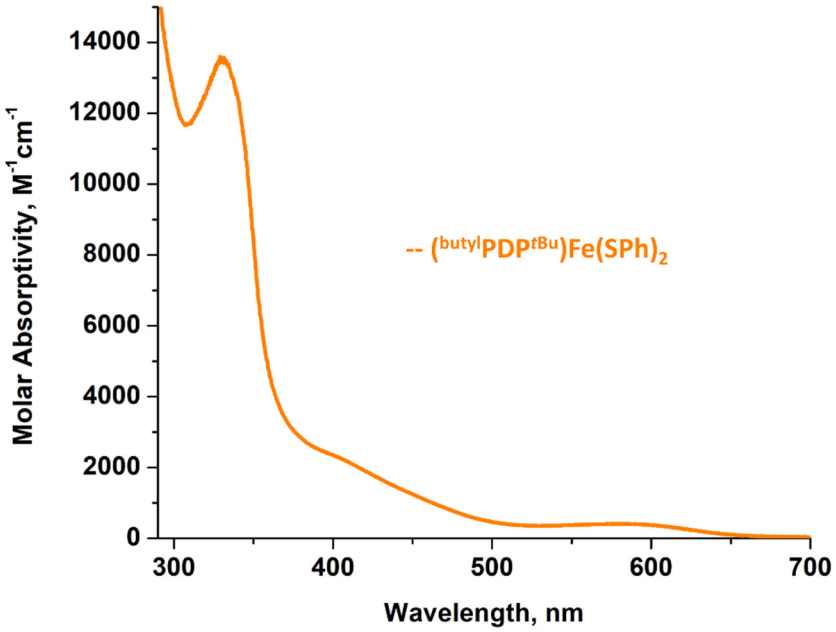


Figure S56. Electronic absorption spectrum of (^{butyl}PDP^{tBu})Fe(SPh)$_2$ recorded in THF at ambient temperature.

Quantification of H_2 produced by addition of 2,4,6-tri-*tert*-butylphenylisocyanide

Four samples for each (^{BBN}PDP^{tBu})FeH$_2$ and (^{BBN}PDP^{tBu})ZnH$_2$ were set up under analogous conditions:

A C_6H_6 slurry (approx. 1.0 mL) of a known quantity of (^{BBN}PDP^{tBu})MH$_2$ was transferred to a J-Young NMR tube. Additional C_6H_6 (approx. 1.0 mL) was used to ensure all (^{BBN}PDP^{tBu})MH$_2$ was transferred. The tube was then carefully layered with additional C_6H_6 until completely full. Approx. 1.0 mL benzene from the top of the tube was removed and used to dissolve 2,4,6-tri-*tert*-butylphenylisocyanide (2 equiv.) in a separate vial. To this, one equiv. of (trimethyl)phenylsilane was added and the solution was subsequently layered back on top of the NMR tube. The tube was sealed so that no headspace remained. The tube was subjected to sonication for 5 min to aid in dissolution of (^{BBN}PDP^{tBu})MH$_2$. The tube was then slowly inverted repeatedly for 30 min and an ^{1}H NMR spectrum was obtained. The Fe complexes gradually become dark brown in color while the Zn species gradually become light pink. The tables and figures below illustrate the H_2 production.

Table S1. Quantification of H_2 from reaction between ($^{BBN}PDP^{tBu}$)FeH_2 and 2,4,6-tri-*tert*-butylphenylisocyanide.

	($^{BBN}PDP^{tBu}$)FeH_2 (mass, mg)	**ArNC (mass, mg)**	**Percent H_2**
Sample A	9.6	7.4	89.9
Sample B	9.7	7.5	91.5
Sample C	9.8	7.6	87.3
Sample D	11.0	8.5	92.2
			Average: 90.2 +/- 2.2 %

Table S2. Quantification of H_2 from reaction between ($^{BBN}PDP^{tBu}$)ZnH_2 and 2,4,6-tri-*tert*-butylphenylisocyanide.

	($^{BBN}PDP^{tBu}$)ZnH_2 (mass, mg)	**ArNC (mass, mg)**	**Percent H_2**
Sample A	8.7	6.6	10.6
Sample B	8.9	6.8	6.1
Sample C	9.4	7.2	6.1
Sample D	10.9	8.3	4.9
			Average: 6.9 +/- 2.5 %

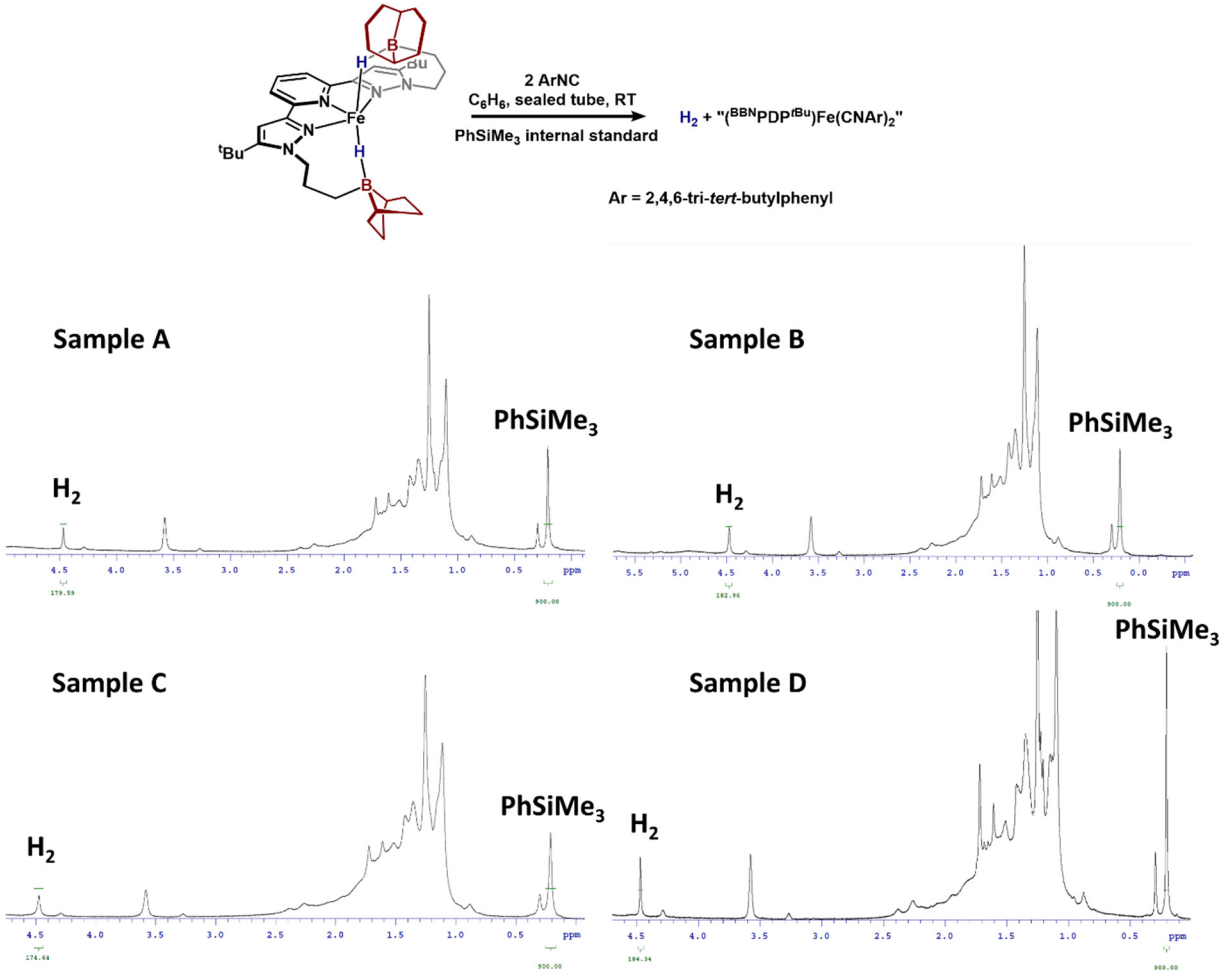


Figure S57. ^{1}H NMR spectra (C_6H_6, 25 °C) of reaction between ($^{BBN}PDP^{tBu}$)FeH_2 and two equivalents 2,4,6-tri-*tert*-butylphenylisocyanide in a sealed J-Young NMR tube. Details for sample preparation are described above.

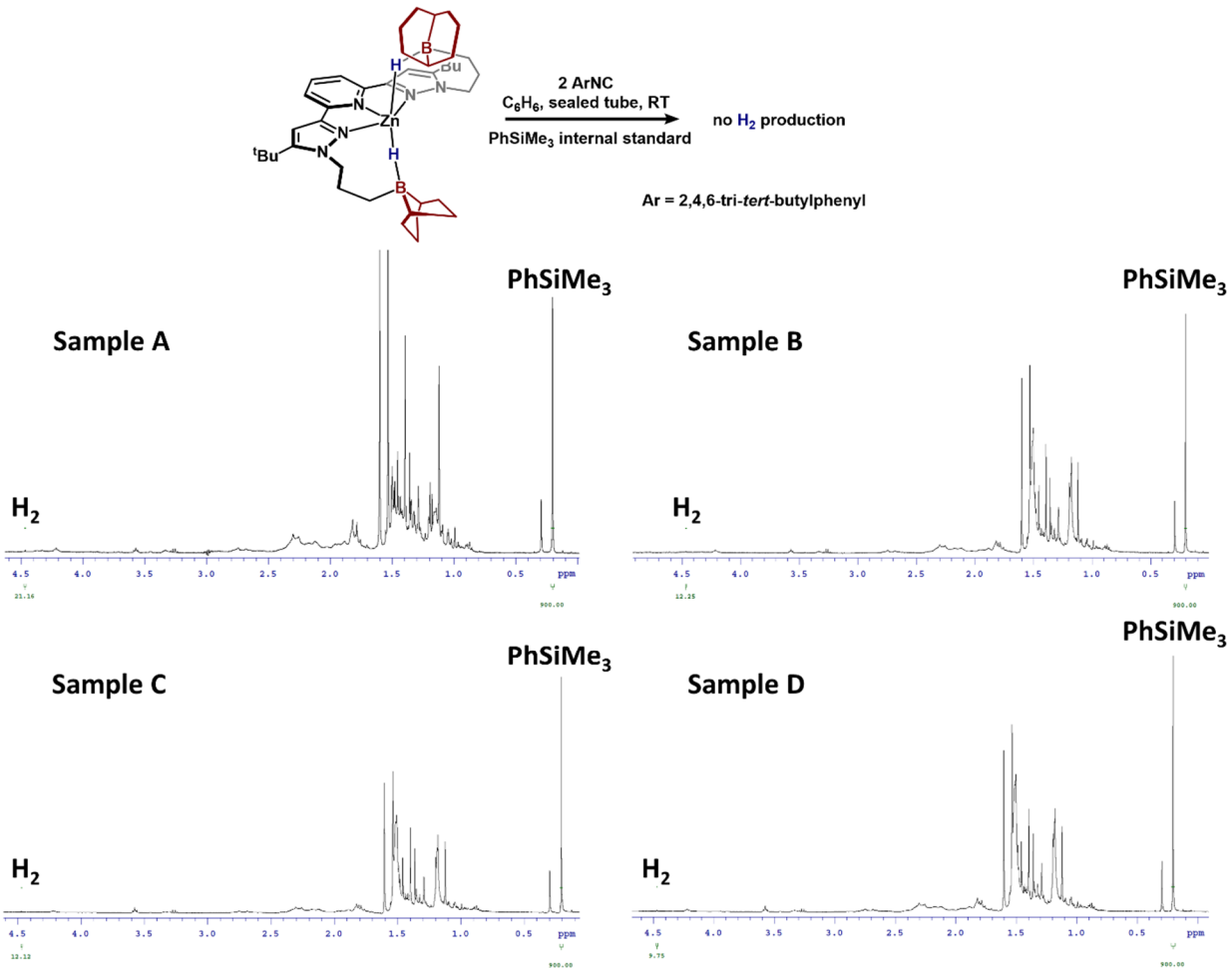


Figure S58. ^{1}H NMR spectra (C_6H_6, 25 °C) of reaction between (^{BBN}PDP^{tBu})ZnH_2 and two equivalents 2,4,6-tri-*tert*-butylphenylisocyanide in a sealed J-Young NMR tube. Details for sample preparation are described above.

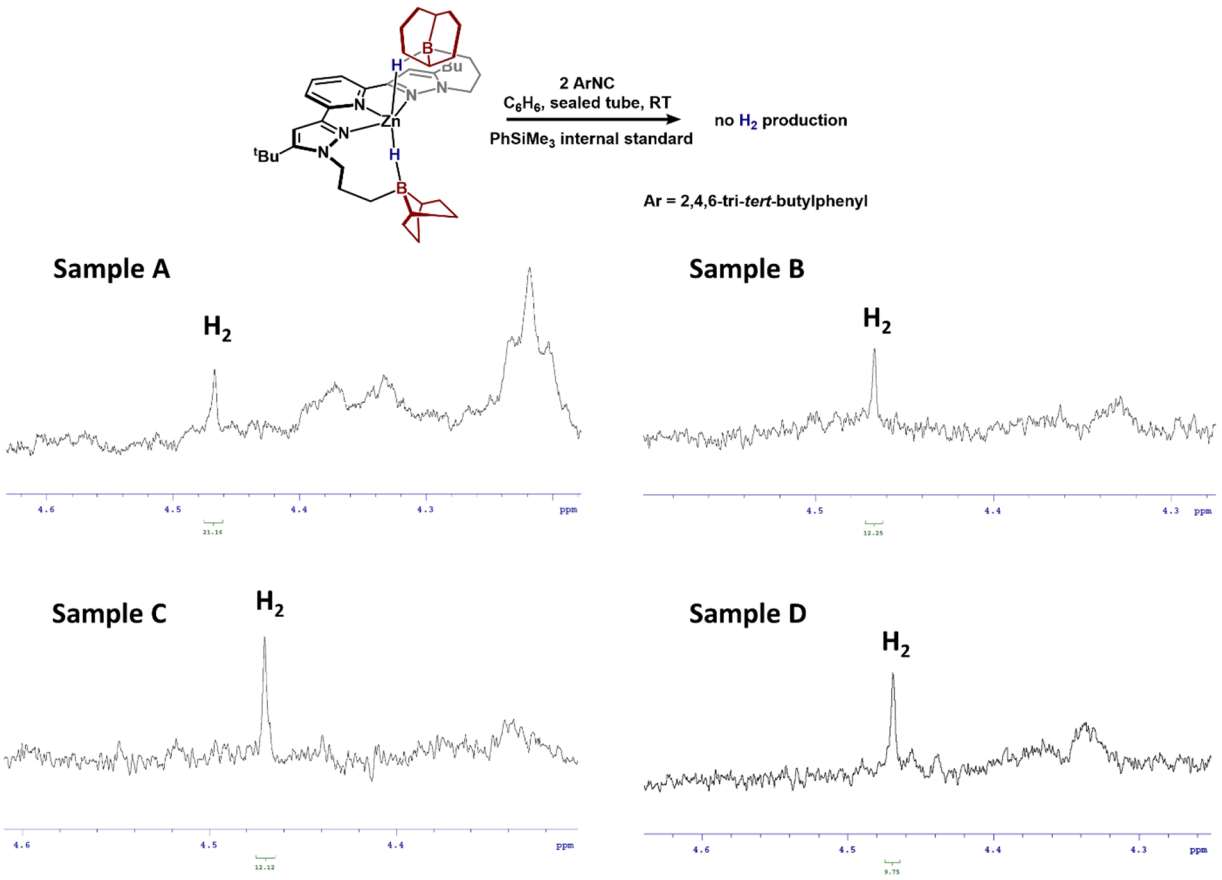


Figure S59. ^{1}H NMR spectra (C_6H_6, 25 °C) of reaction between (^{BBN}PDP^{tBu})ZnH_2 and two equivalents 2,4,6-tri-*tert*-butylphenylisocyanide in a sealed J-Young NMR tube. Spectra are the same as the above figure and are zoomed in on the hydrogen region.

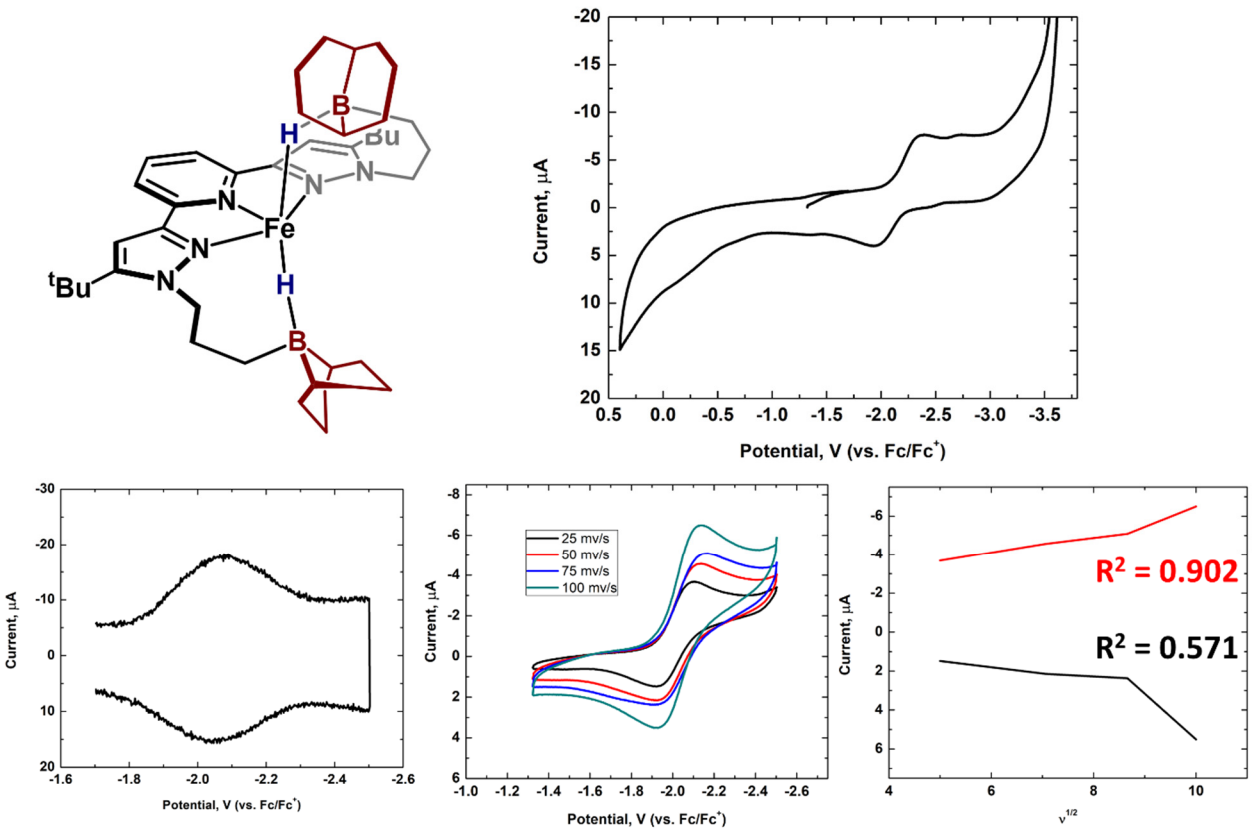


Figure S60. Electrochemical analysis of (^{BBN}PDP^{tBu})FeH_2 (0.47 mM) recorded in THF with 0.2 M $[Bu_4N][PF_6]$ electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.06 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave collected at 25, 50, 75, and 100 mv/s. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

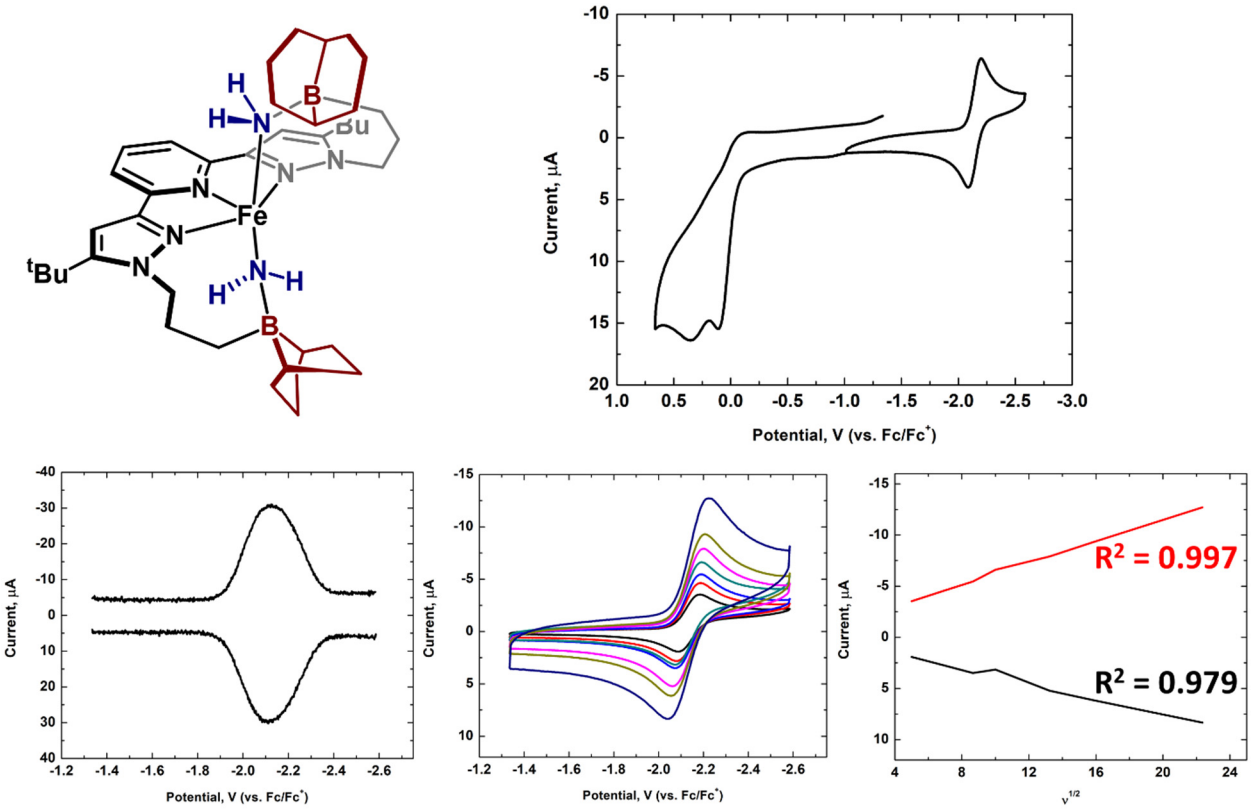


Figure S61. Electrochemical analysis of (^{BBN}PDP^{tBu})Fe(NH_2)$_2$ (0.91 mM) recorded in THF with 0.2 M [Bu_4N][PF_6] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.06 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave collected at 25, 50, 75, 100, 150, 250, and 500 mv/s. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

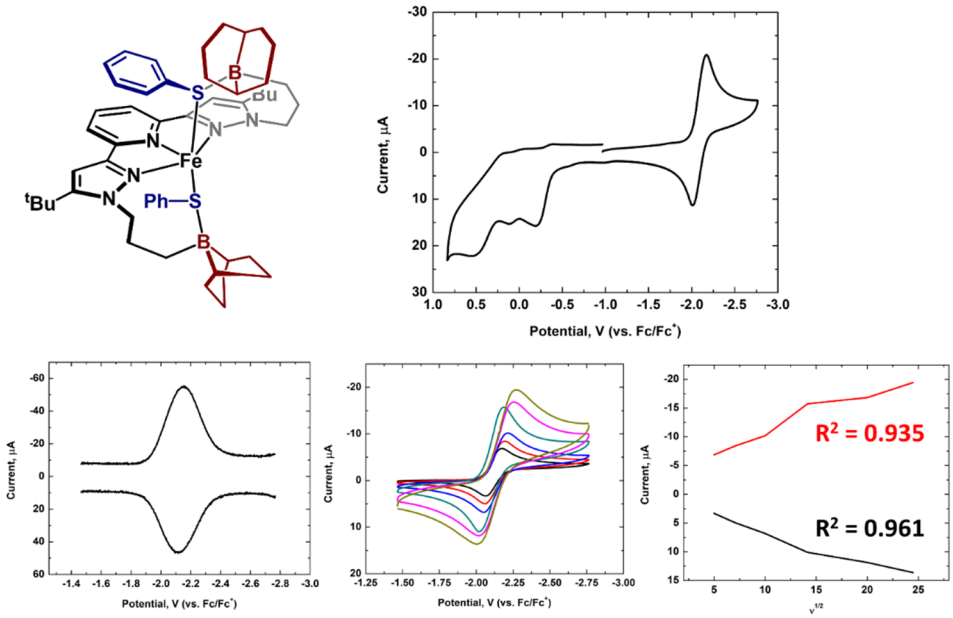


Figure S62. Electrochemical analysis of (^{BBN}PDP^{tBu})Fe(SPh)$_2$ (0.72 mM) recorded in THF with 0.2 M [Bu$_4$N][PF$_6$] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.02 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave collected at 25, 50, 100, 200, 400, and 600 mv/s. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

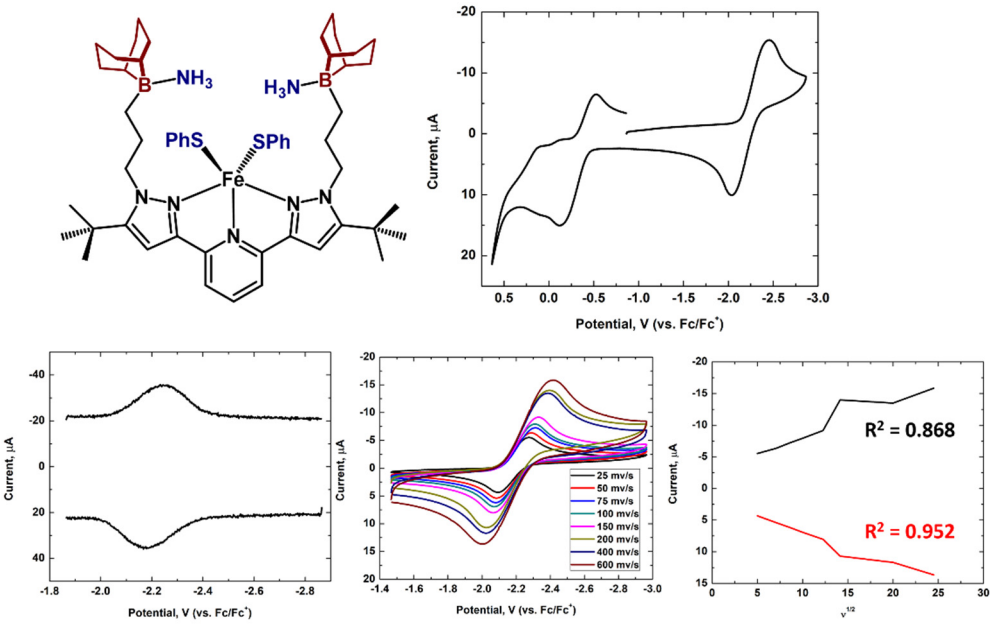


Figure S63. Electrochemical analysis of (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$ (0.70 mM) recorded in THF with 0.2 M [Bu$_4$N][PF$_6$] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.02 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

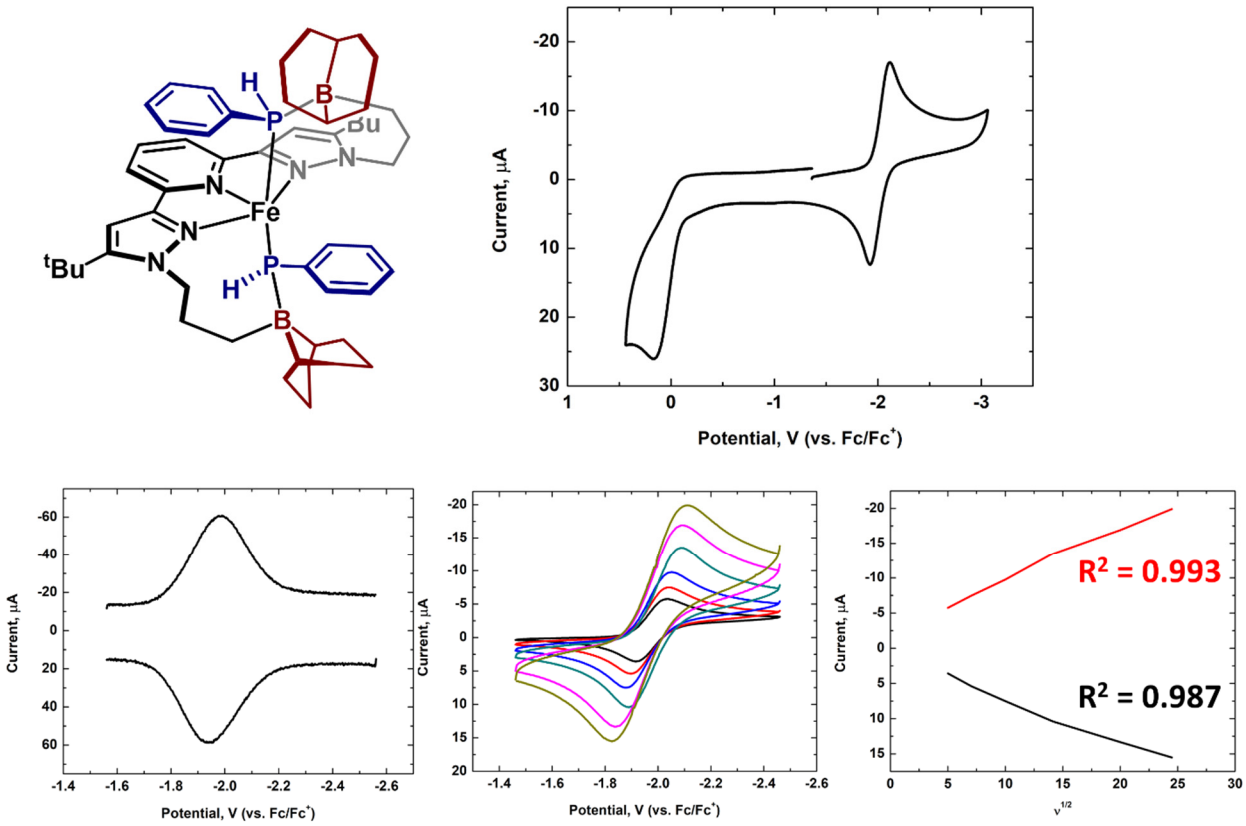


Figure S64. Electrochemical analysis of (^{BBN}PDP^{tBu})Fe(PHPh)$_2$ (0.72 mM) recorded in THF with 0.2 M [Bu$_4$N][PF$_6$] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.02 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave collected at 25, 50, 100, 200, 400, and 600 mv/s. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

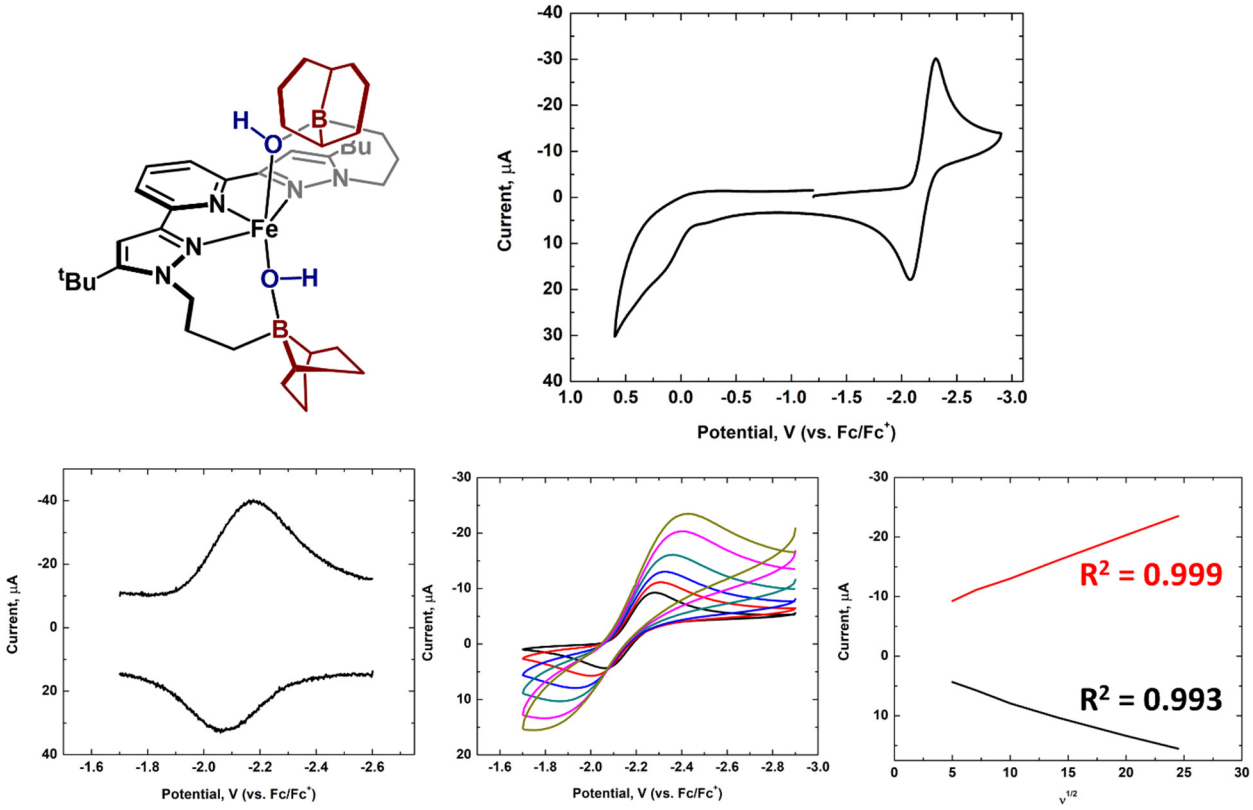


Figure S65. Electrochemical analysis of (^{BBN}PDP^{tBu})Fe(OH)$_2$ (0.90 mM) recorded in THF with 0.2 M [Bu$_4$N][PF$_6$] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.02 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave collected at 25, 50, 100, 200, 400, and 600 mv/s. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

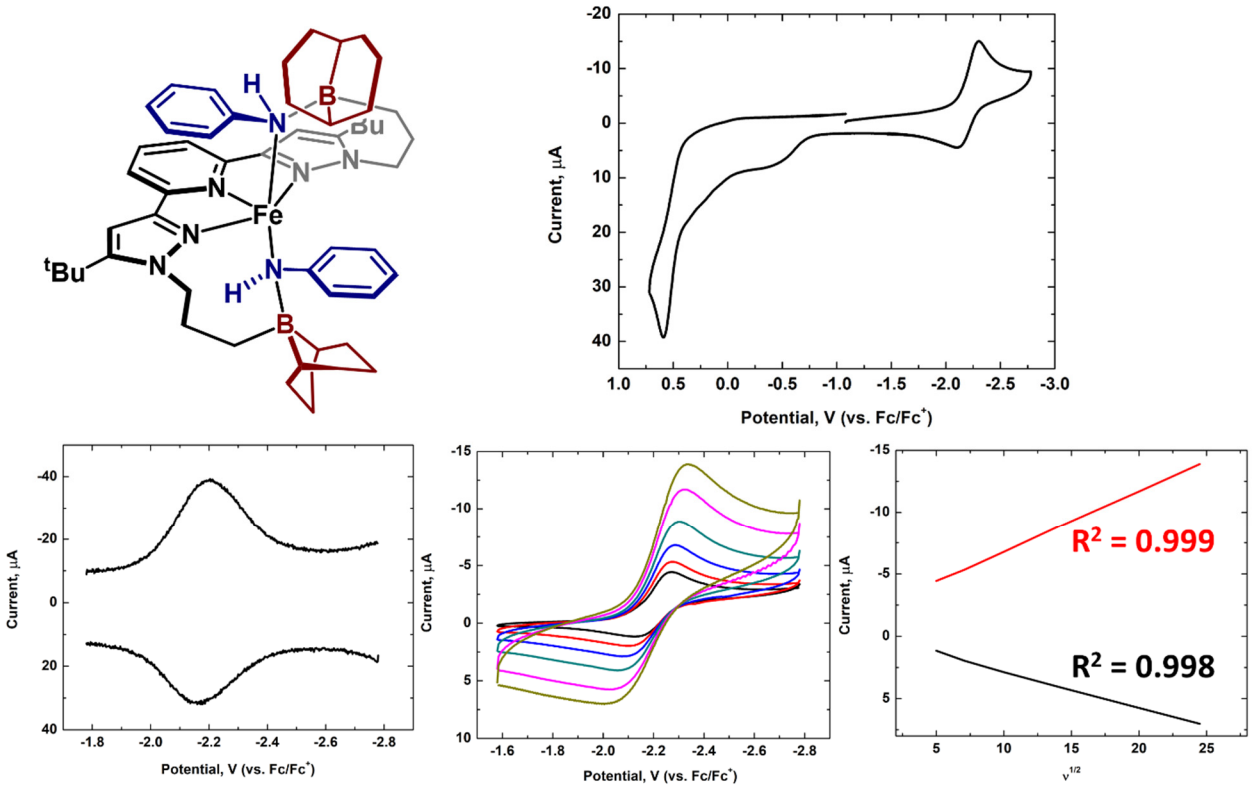


Figure S66. Electrochemical analysis of (^{BBN}PDP^{tBu})Fe(NHPh)$_2$ (0.75 mM) recorded in THF with 0.2 M [Bu_4N][PF_6] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.02 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave collected at 25, 50, 100, 200, 400, and 600 mv/s. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

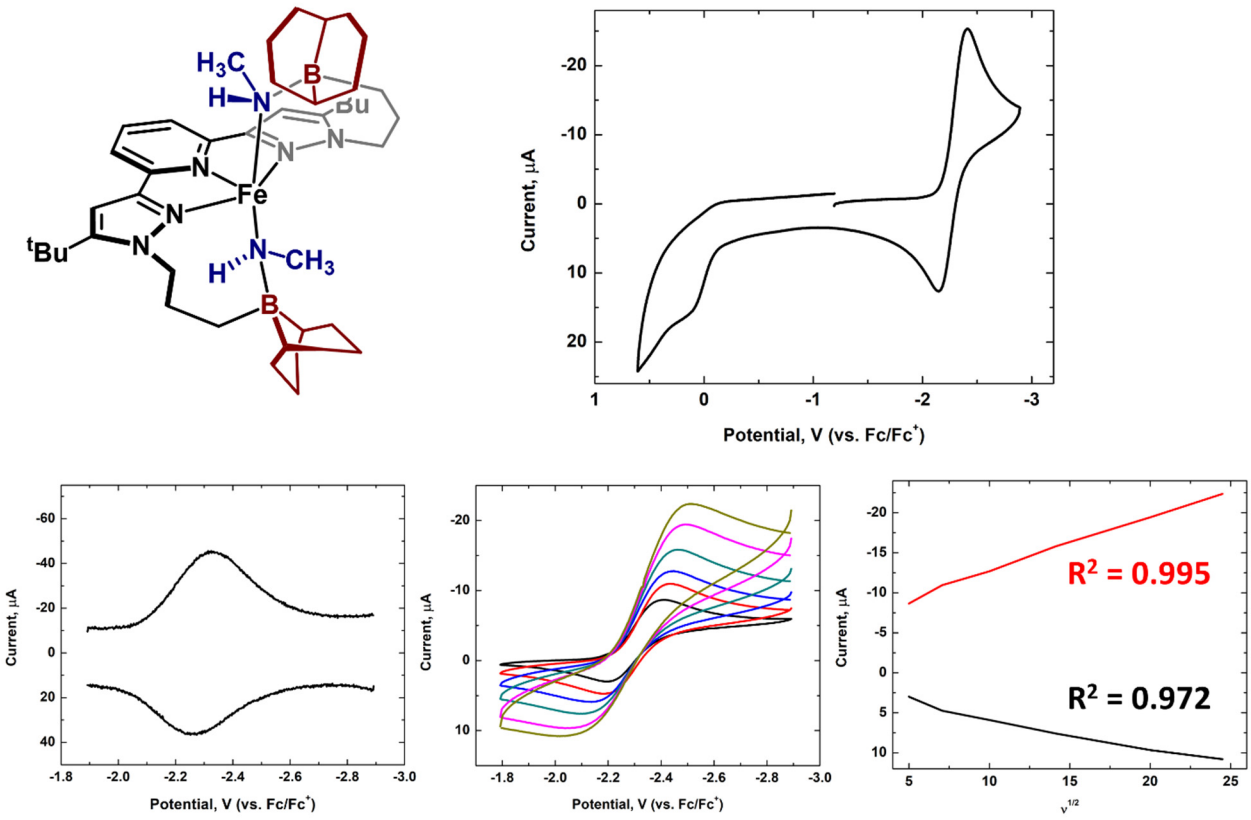


Figure S67. Electrochemical analysis of (^{BBN}PDP^{tBu})Fe(NHMe)$_2$ (0.87 mM) recorded in THF with 0.2 M [Bu_4N][PF_6] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.02 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave collected at 25, 50, 100, 200, 400, and 600 mv/s. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current.

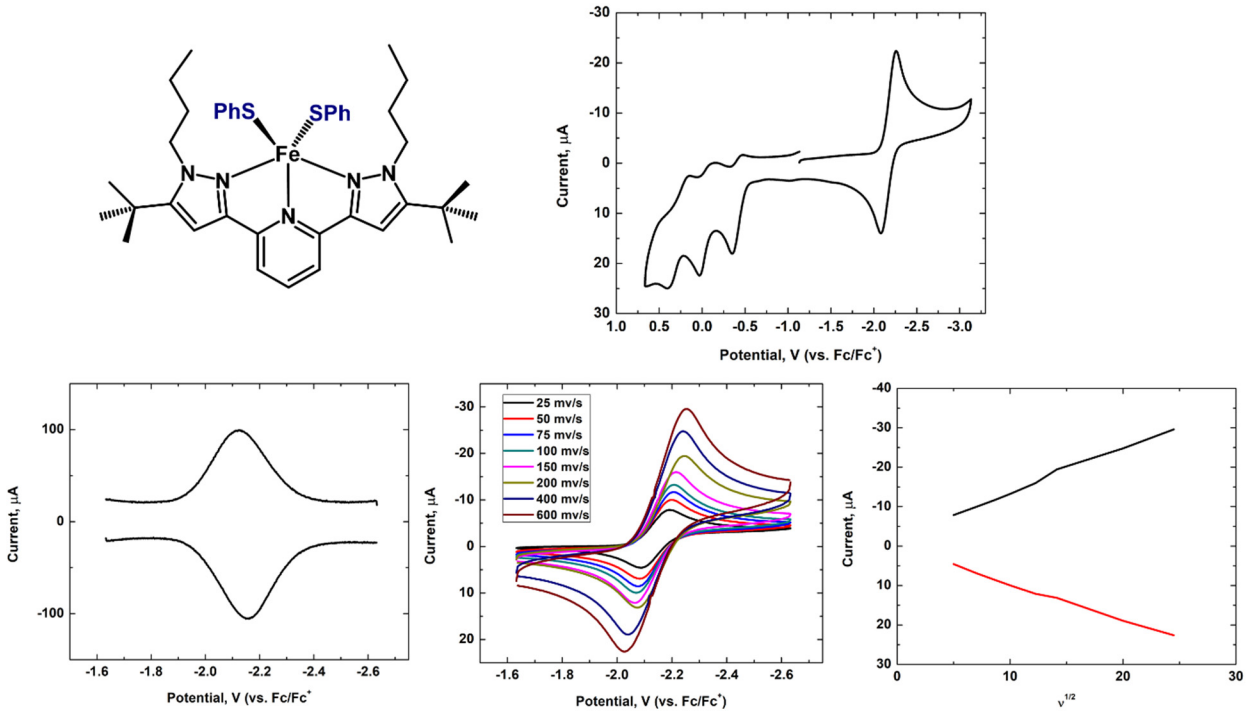


Figure S68. Electrochemical analysis of (^{butyl}PDP^{tBu})Fe(SPh)$_2$ (0.94 mM) recorded in THF with 0.2 M [Bu_4N][PF_6] electrolyte. Top: full scan. Bottom left: square wave voltammogram (parameters: amplitude = 160 mV; period = 0.02 seconds; increment = 2 mV; sampling width = 0.001 seconds). Bottom middle: scan rate dependence of reductive wave. Bottom right: Plot of (scan rate)$^{1/2}$ vs. current. E_{red} determined by square wave voltammetry = -2.14 V (vs. Fc/Fc$^+$).

Table S3. Reduction potentials determined by square wave voltammetry.

Compound	$E_{1/2}$, V (vs. Fc/Fc$^+$)
(^{BBN}PDP^{tBu})FeBr$_2$	-2.14[a]
(^{BBN}PDP^{tBu})FeCl$_2$	-2.07[a]
(^{BBN}PDP^{tBu})FeH$_2$	-2.06
(^{BBN}PDP^{tBu})Fe(NH$_2$)$_2$	-2.12
(^{BBN}PDP^{tBu})Fe(NHMe)$_2$	-2.30
(^{BBN}PDP^{tBu})Fe(NHPh)$_2$	-2.18
(^{BBN}PDP^{tBu})Fe(OH)$_2$	-2.12
(^{BBN}PDP^{tBu})Fe(PHPh)$_2$	-1.96
(^{BBN}PDP^{tBu})Fe(SPh)$_2$	-2.13
(^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH_3)$_2$	-2.21

[a]Values for (^{BBN}PDP^{tBu})FeX$_2$ (X = Cl, Br) taken from ref. 1

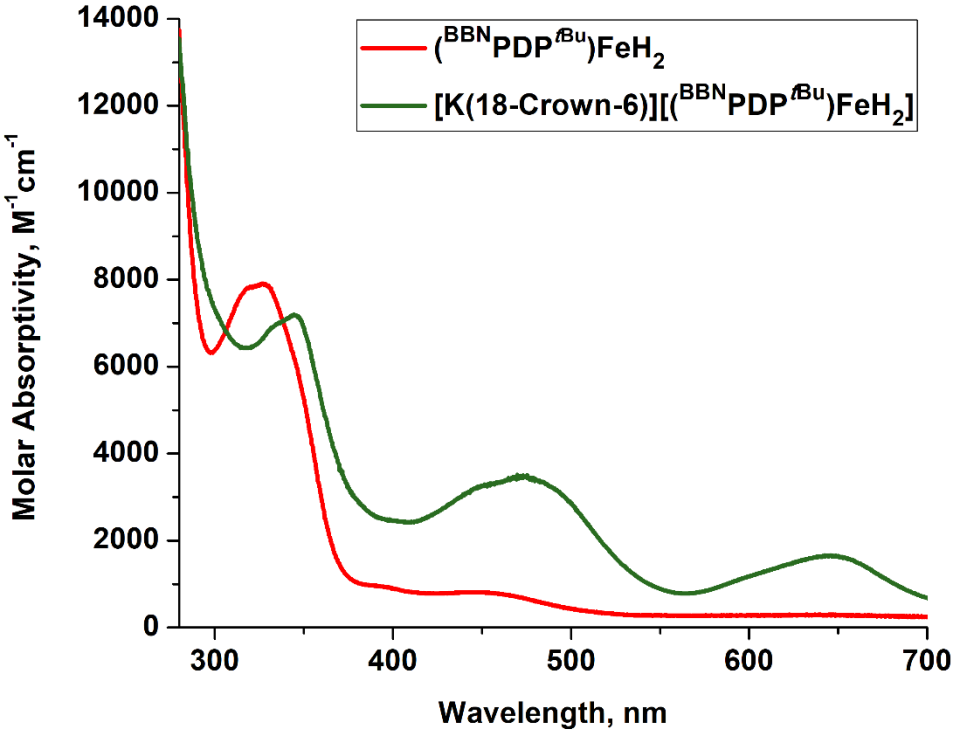


Figure S69. Electronic absorption spectra of ($^{BBN}PDP^{tBu}$)FeH_2 (red) and [K(18-crown-6)][($^{BBN}PDP^{tBu}$)FeH_2] (green) recorded in THF at ambient temperature.

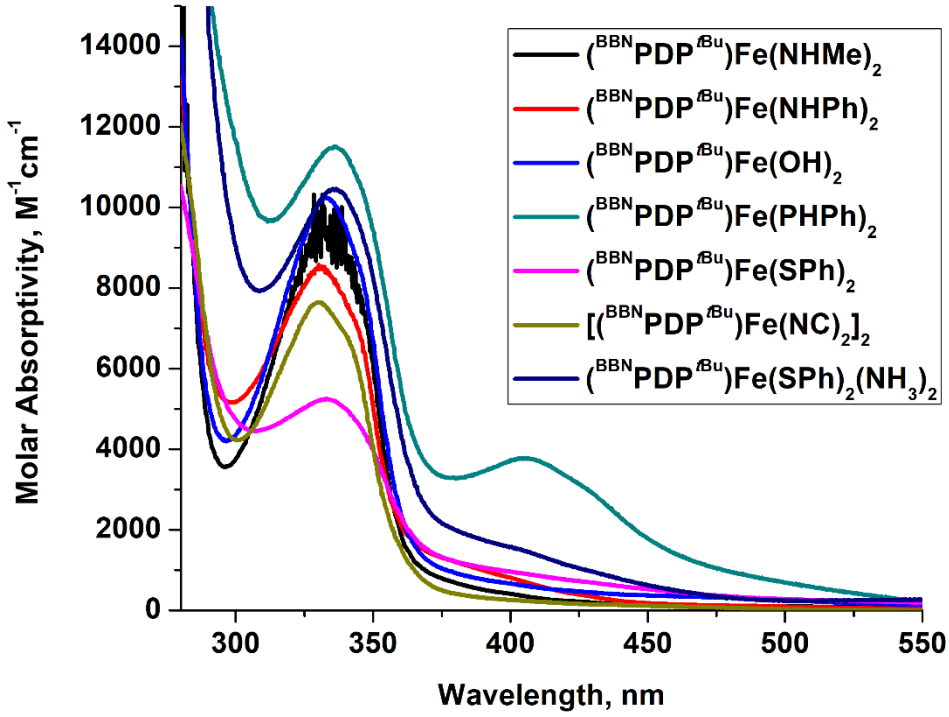


Figure S70. Electronic absorption spectra of iron complexes recorded in THF at ambient temperature.

Compound: (^{BBN}PDP^{tBu})FeH_2

Local Name: jk3155

CCDC 1884221

Table S4. Crystallographic parameters for (^{BBN}PDP^{tBu})FeH_2

Crystal data	
Chemical formula	$C_{41}H_{65}B_2FeN_5 \cdot 0.892(C_7H_8)$
M_r	787.61
Crystal system, space group	Tetragonal, $P4_32_12$
Temperature (K)	150
a, c (Å)	16.0995 (5), 16.3816 (5)
V (Å^3)	4246.0 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.13
Crystal size (mm)	0.12 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.427, 0.526
No. of measured, independent and observed [$I > 2s(I)$] reflections	30458, 4559, 3416
R_{int}	0.070
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.165, 1.00
No. of reflections	4559
No. of parameters	508
No. of restraints	668
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, -0.49
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.390 (10)

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXL2018*/1 (Sheldrick, 2015, 2018), SHELXLE Rev882 (Hübschle *et al.*, 2011).

Refinement details:

The structure is isotypic to its zinc counterpart and was solved by isomorphous replacement, followed by inversion to the enantiomorph space group.

Refined as a 2-component inversion twin.

The ligand side arm and the immediately adjacent part of the chelating ligand (including the *tert*-butyl group) are disordered over two alternative positions, wrapping around the iron center clockwise or anticlockwise. The two disordered moieties were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.554(6) to 0.446(6).

A toluene solvate molecule is partially occupied and disordered around a two-fold axis over four orientations (each two related by the two fold axis). Each benzene ring was constrained to resemble an ideal hexagon (AFIX 66). The methyl C-C bond distance was restrained to 1.53(2) Å. The lesser occupied moiety was restrained to be close to planar, and U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy rates refined to two times 0.333(12) and two times 0.113(12), for a total occupancy for the site of 0.892. No indication for additional electron density at this site was found.

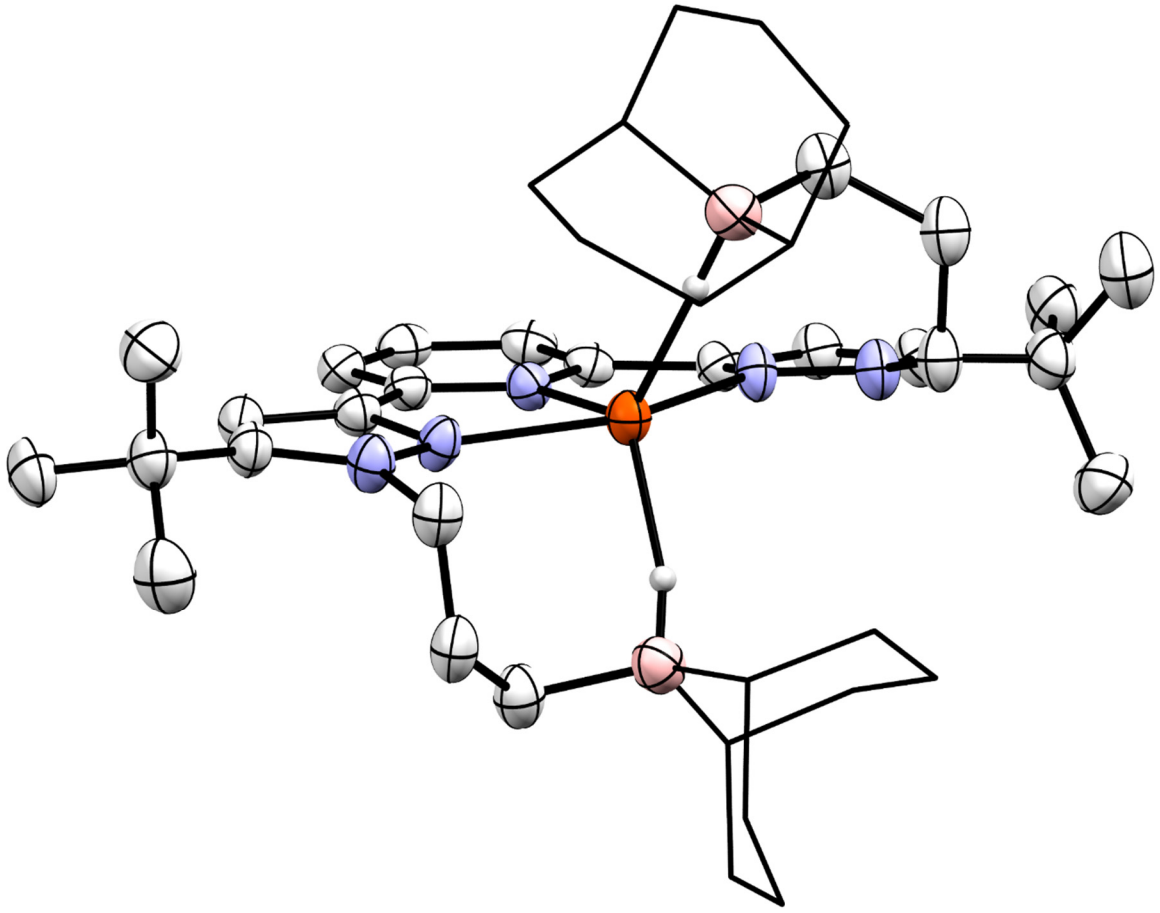


Figure S71. Molecular structure of (^{BBN}PDP^{tBu})FeH_2 displayed with 50% probability ellipsoids. Hydrogen atoms not attached to iron are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$]

Local Name: jk2200

CCDC 1884231

Table S5. Crystallographic parameters for [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$]

Crystal data	
Chemical formula	$C_{18}H_{36}KN_2O_6 \cdot C_{41}H_{65}B_2FeN_5$
M_r	1121.03
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	19.503 (3), 21.623 (3), 22.147 (4)
α, β, γ (°)	67.321 (5), 71.202 (5), 89.815 (4)
V (Å^3)	8079 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.28
Crystal size (mm)	0.39 × 0.22 × 0.06
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). J. Appl. Cryst. 48 3-10.
T_{min}, T_{max}	0.446, 0.563
No. of measured, independent and observed [$I > 2s(I)$] reflections	70366, 70366, 41234
R_{int}	0.053
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.679
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.132, 0.410, 1.07
No. of reflections	70366
No. of parameters	2089
No. of restraints	3477
H-atom treatment	H-atom parameters constrained
	$w = 1/[s^2(F_o^2) + (0.2025P)^2 + 20.270P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.12, -0.52

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2017*/1 (Sheldrick, 2015, 2017), SHELXLE Rev859 (Hübschle *et al.*, 2011).

Refinement details:

The crystal under investigation was found to be slightly non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell Now, with the two components being related by a 180 degree rotation around the real a-axis.

Integration proved problematic due to excessive multiple overlap of reflections, resulting in large numbers of rejected reflections. Attempts were made to adjust integration parameters to avoid excessive rejections (through adjustments to integration queue size, blending of profiles, integration box slicing and twin overlap parameters), which led to less but still substantial numbers of rejected reflections. With no complete data set obtainable through simultaneous integration of both twin domains, the data were instead handled as if not twinned, with only the major domain integrated, and converted into an hklf 5 type format hkl file after integration using the "Make HKLF5 File" routine as implemented in WinGX. The twin law matrix was used as obtained from WinGX and was as follows:

180.0 degree rotation about 1. 0. 0. direct lattice direction:

[1.000 0.000 0.000]

[0.007 -1.000 0.000]

[0.732 0.000 -1.000]

The Overlap R1 and R2 values used were 0.55, i.e. reflections with a discriminator function less or equal to an overlap radius of 0.55 were counted overlapped, all others as single. The discriminator function used was the "delta function on index non-integrality". No reflections were omitted.

The structure was solved using direct methods with the original hklf 4 type file and was refined using the hklf 5 type file, resulting in a final BASF value, after finalizing of structural model and other treatments (see below) of 0.098(2). This is thought to be underestimated due to the use of an after integration created hklf 5 type file.

No Rint value is obtainable for the hklf 5 type file using the WinGX routine. The value from the refinement under omission of twinning is given instead.

The cryptand ligands surrounding the potassium cations were found to be disordered. That around K1A was refined as disordered over two orientations; that around K1B as disordered over three orientations. All disordered moieties were restrained to have similar geometries. The bond distances of C52C to C53C and of C56B to C57B were restrained to a target value of 1.500(1) Angstrom. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.839(5) to 0.161(5) for the first cryptand, and the rates of the second to 0.194(4), 0.551(4) and 0.256(3).

A mild anti bumping restraint was applied to avoid close H...H contacts for disordered atoms.

In addition to disorder and twinning, the structure also exhibits large volume sections consisting of highly disordered solvate molecules. No satisfactory model for the solvate molecules could be developed, and the contribution of the solvate molecules was instead taken into account by reverse Fourier transform methods. The data were first detwinned (using the LIST 8 function of Shelxl2017) and then the cif and hkl files were subjected to the SQUEEZE routine as implemented in the program Platon. The resultant files were used in the further refinement. (Both the hklf 5 type HKL file and the detwinned FAB file are appended to the cif file). A volume of 2821 cubic Å per unit cell (ca 35% of the cell volume) containing 388 electrons was corrected for.

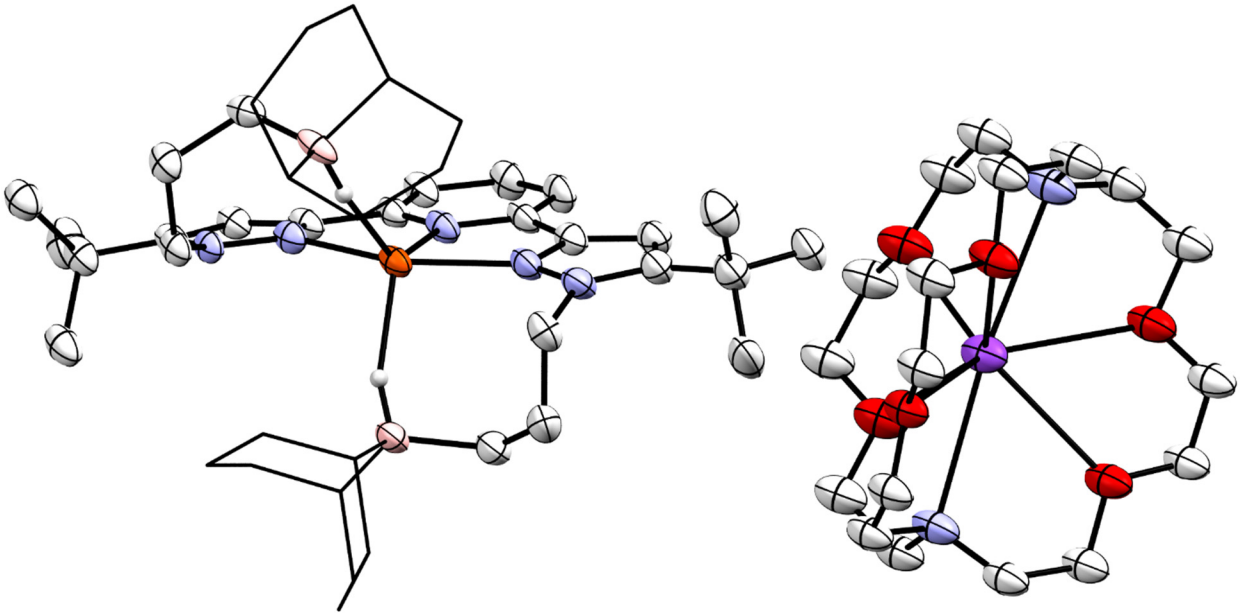


Figure S72. Molecular structure of [K(2,2,2-cryptand)][(^{BBN}PDP^{tBu})FeH$_2$] displayed with 50% probability ellipsoids. Hydrogen atoms not attached to iron are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: $[K(DME)_4][(^{BBN}PDP^{tBu})FeH_2]$

Local Name: jk2177

CCDC 1884224

Table S6. Crystallographic parameters for $[K(DME)_4][(^{BBN}PDP^{tBu})FeH_2]$

Crystal data	
Chemical formula	$4(C_{41}H_{65}B_2FeN_5)\cdot 2.808(C_4H_9O_2)\cdot 3(C_4H_{10}O_2)\cdot 4(K)$
M_r	3498.78
Crystal system, space group	Tetragonal, $I\bar{4}2d$
Temperature (K)	150
a, c (Å)	26.450 (2), 20.9410 (19)
V (Å^3)	14650 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.42 × 0.28 × 0.13
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.486, 0.564
No. of measured, independent and observed [$I > 2s(I)$] reflections	102117, 9087, 6150
R_{int}	0.080
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.094, 0.301, 1.09
No. of reflections	9087
No. of parameters	557
No. of restraints	652
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.20, -0.58
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.48 (4)

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2017*/1 (Sheldrick, 2017), SHELXLE Rev859 (Hübschle *et al.*, 2011).

Substantial disorder is observed for this structure, for both the iron complex as well as solvate molecules and counter-cations. Due to the overall low data quality and the extensive disorder a global similarity restraint was applied to all atom's ADPs: U^{ij} components of ADPs for atoms closer to each other than 2.0 Å were restrained to be similar within an esd of 0.01 $Å^2$.

For the iron complex, the ligand arms are alternatively wrapped around the iron center clockwise or counterclockwise. The disorder extends to the main segment of the ligand, including the *tert*-butyl groups, and the pyrazole fragments were restrained to be coplanar with immediately bonded adjacent atoms. Chemically equivalent bond lengths and angles of *tert*-butyl groups and of some other segments were restrained to be similar. The iron atom was included in the disorder. The two disordered moieties were restrained to have similar geometries. Subject to these conditions the occupancy ratio refined to 0.652(6) to 0.348(6).

Channels around the four-fold inversion axis are occupied by highly disordered potassium ions chelated by DME solvate molecules. One major moiety is relatively well resolved and the K ion and coordinated DME molecules were refined. Occupancies refined to less than half. For the potassium ions, alternative ill-defined positions located on the four-fold inversion axis were included, and the sum of all K ions was constrained based on charge balance considerations. For DME molecules, only the major moiety was taken into consideration. Other remaining DME sites were not resolved and were ignored. Heavily disordered solvate pockets along the channel showed no resolved atoms at all and their electron density was instead included via reverse Fourier transform methods (Squeeze, see below). All refined DME moieties were restrained to have similar geometries and given a common occupancy rate. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy rate refined to 0.351(11).

The structure contains a solvent accessible voids of 2354 $Å^3$. No substantial electron density peaks were found in the solvent accessible voids (2.9 electrons for the largest peak and less than 1.7 electron/$Å^3$ for all others) and the residual electron density peaks were not arranged in an interpretable pattern. The cif and hkl files were subjected to reverse Fourier transform methods using the SQUEEZE routine (van der Sluis, P.; Spek, A. L. *Acta Cryst.* **1990** *A46*, 194-201) 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 the cif file). The Squeeze procedure corrected for 516 electrons within the solvent accessible voids.

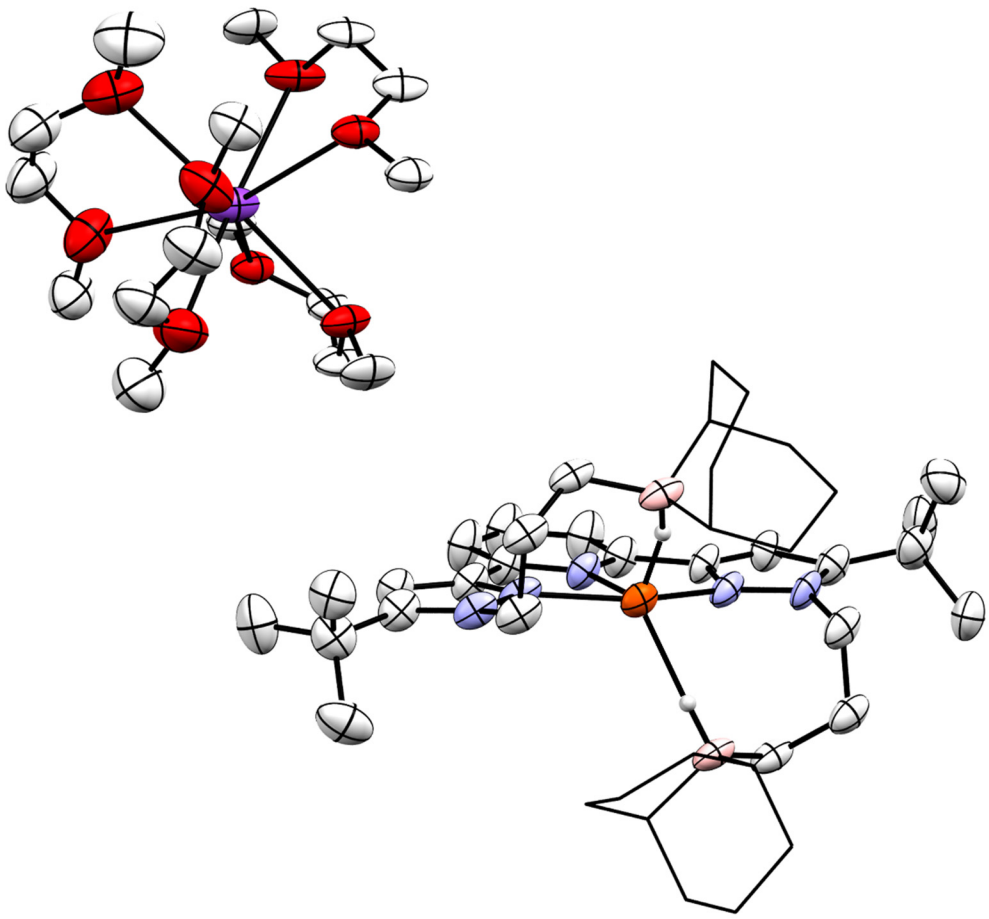


Figure S73. Molecular structure of $[K(DME)_4][(^{BBN}PDP^{tBu})FeH_2]$ displayed with 30% probability ellipsoids. Disordered fragments and hydrogen atoms not attached to iron are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})ZnH_2

Local Name: jk3136

CCDC 1884220

Table S7. Crystallographic parameters for (^{BBN}PDP^{tBu})ZnH_2

Crystal data	
Chemical formula	$C_{41}H_{65}B_2N_5Zn \cdot 0.718(C_7H_8)$
M_r	781.14
Crystal system, space group	Tetragonal, $P4_12_12$
Temperature (K)	150
a, c (Å)	16.1630 (5), 16.4362 (6)
V (Å^3)	4293.8 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.61
Crystal size (mm)	0.26 × 0.24 × 0.14
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.648, 0.746
No. of measured, independent and observed [$I > 2s(I)$] reflections	62259, 6563, 4926
R_{int}	0.088
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.140, 1.03
No. of reflections	6563
No. of parameters	507
No. of restraints	668
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, -0.66
Absolute structure	Flack x determined using 1628 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	-0.010 (4)

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/1 (Sheldrick, 2015, 2018), SHELXLE Rev882 (Hübschle *et al.*, 2011).

Refinement details:

The ligand side arm and the immediately adjacent part of the chelating ligand (including the *tert*-butyl group) are disordered over two alternative positions, wrapping around the zinc center clockwise or anticlockwise. The two disordered moieties were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.600(5) to 0.400(5).

A toluene solvate molecule is partially occupied and disordered around a two-fold axis over four orientations (each two related by the two fold axis). Each benzene ring was constrained to resemble an ideal hexagon (AFIX 66). The methyl C-C bond distance was restrained to 1.53(2) Å. The lesser occupied moiety was restrained to be close to planar, and U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy rates refined to two times 0.216(10) and two times 0.143(9), for a total occupancy for the site of 0.718. No indication for additional electron density at this site was found.

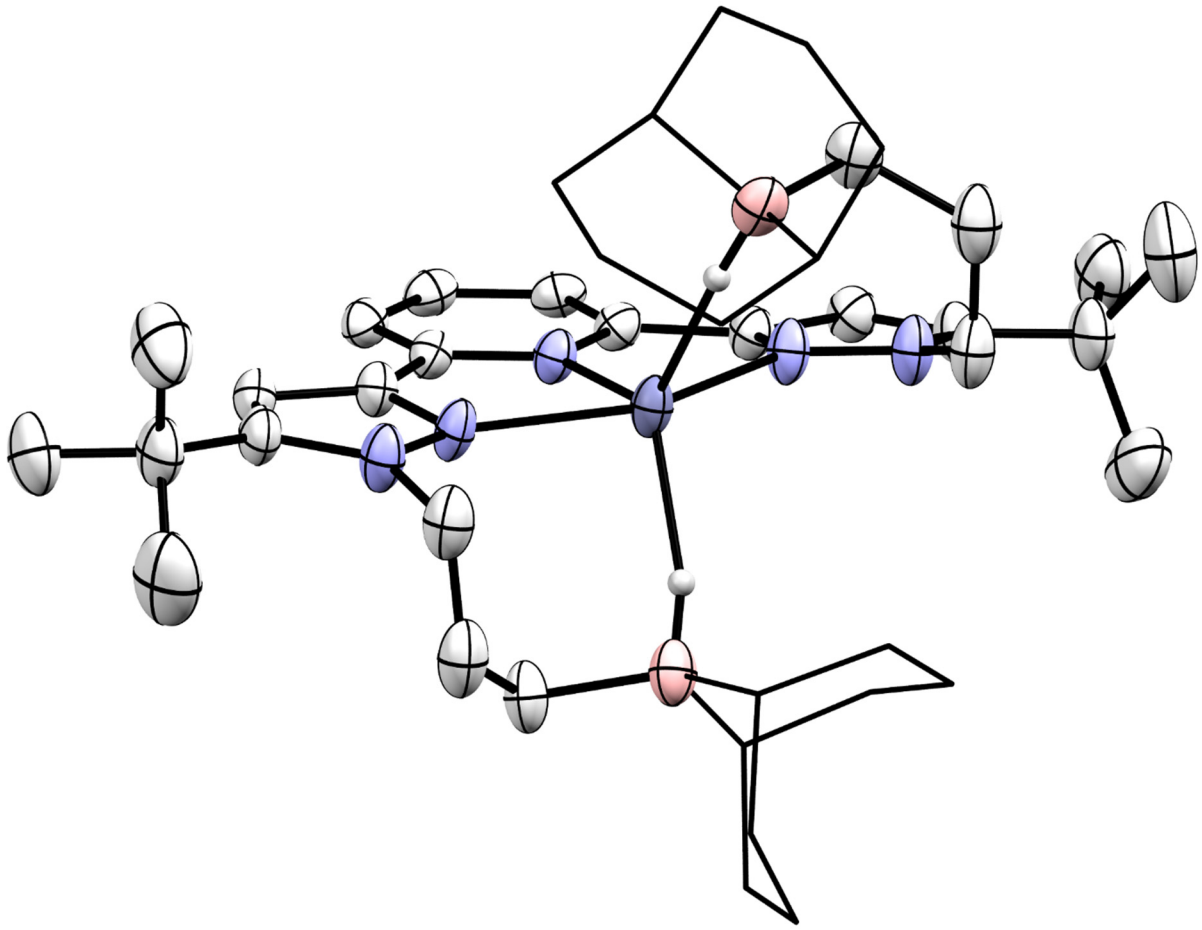


Figure S74. Molecular structure of (^{BBN}PDP^{tBu})ZnH_2 displayed with 50% probability ellipsoids. Hydrogen atoms not attached to zinc are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})Fe(NHMe)$_2$

Local Name: jk2150

CCDC 1884223

Table S8. Crystallographic parameters for (^{BBN}PDP^{tBu})Fe(NHMe)$_2$

Crystal data	
Chemical formula	$C_{43}H_{71}B_2FeN_7 \cdot CH_2Cl_2$
M_r	848.46
Crystal system, space group	Tetragonal, $P4_32_12$
Temperature (K)	150
a, c (Å)	16.4289 (8), 16.7181 (10)
V (Å^3)	4512.4 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.49
Crystal size (mm)	0.23 × 0.21 × 0.16
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.194, 0.263
No. of measured, independent and observed [$I > 2s(I)$] reflections	47133, 5321, 4539
R_{int}	0.080
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.132, 1.08
No. of reflections	5321
No. of parameters	420
No. of restraints	317
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, -0.46
Absolute structure	Flack x determined using 1784 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	-0.050 (6)

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2017*/1 (Sheldrick, 2017), SHELXLE Rev859 (Hübschle *et al.*, 2011).

Refinement details:

The structure was solved by isomorphous replacement based on the Fe-complex without the N-methyl CH_3 group.

The ligand side arm is disordered. The two disordered moieties were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. The nitrogen atoms N4 and N4B as well as the methyl atoms C22 and C22B were constrained to have each identical ADPs. Subject to these conditions the occupancy ratio refined to 0.852(5) to 0.148(5).

The methylene chloride solvate molecule was refined as disordered over three positions located around a two-fold axis. The three disordered moieties were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 1.7 Å were restrained to be similar. Subject to these conditions the occupancy rates refined to 0.072(4), 0.770(4) and two times 0.0791(19) (related by two-fold rotation).

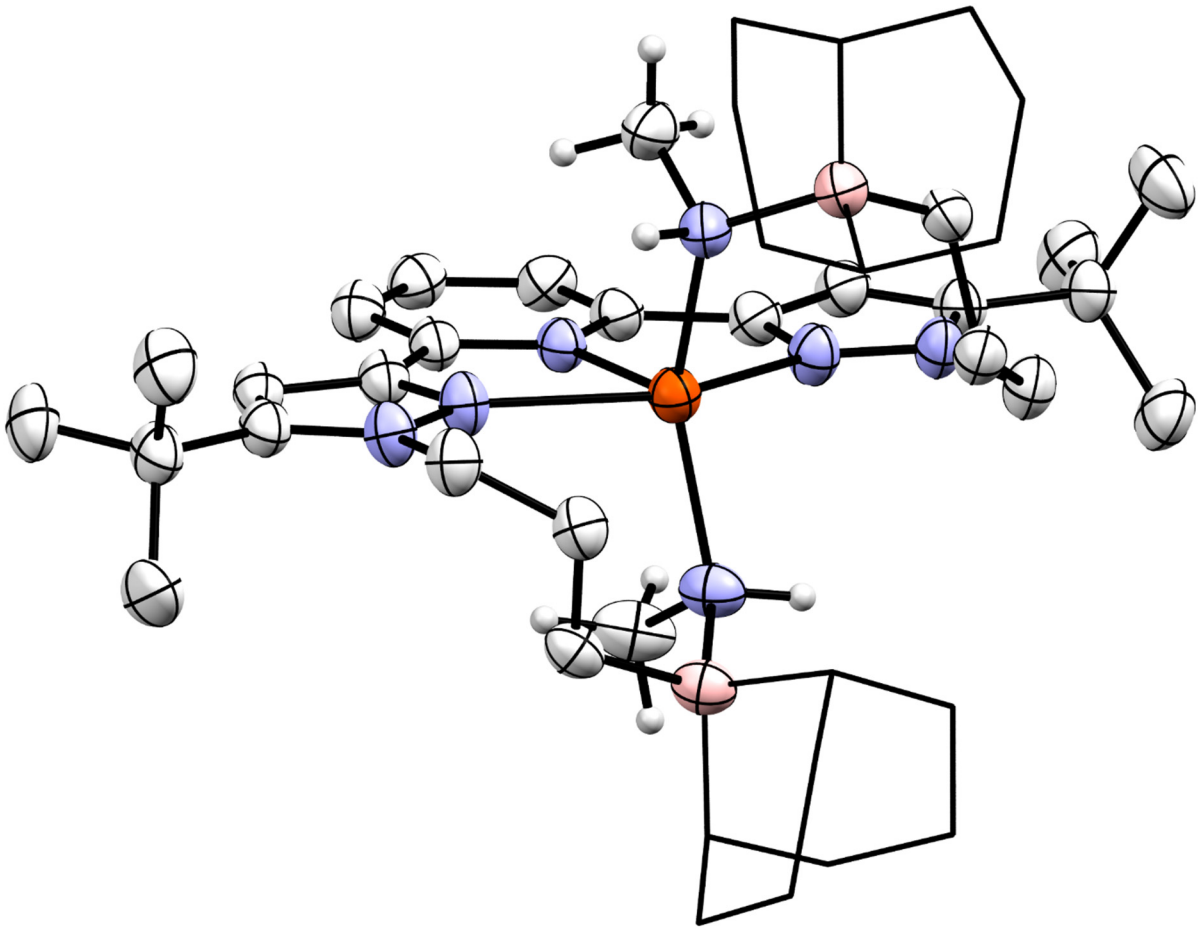


Figure S75. Molecular structure of (^{BBN}PDP^{tBu})Fe(NHMe)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms not attached to nitrogen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})Fe(OH)$_2$

Local Name: jk238

CCDC 1884227

Table S9. Crystallographic parameters for (^{BBN}PDP^{tBu})Fe(OH)$_2$

Crystal data	
Chemical formula	$C_{41}H_{65}B_2FeN_5O_2 \cdot C_5H_{12}$
M_r	809.59
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	13.8891 (4), 17.2913 (6), 19.1228 (7)
β (°)	94.835 (2)
V (Å^3)	4576.2 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.95
Crystal size (mm)	0.25 × 0.23 × 0.17
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.524, 0.754
No. of measured, independent and observed [I > 2s(I)] reflections	32363, 9656, 7951
R_{int}	0.060
(sin θ/λ)$_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.132, 1.06
No. of reflections	9656
No. of parameters	772
No. of restraints	929
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ$_{max}$, Δρ$_{min}$ (e Å^{-3})	0.35, -0.43

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2016*/6 (Sheldrick, 2015, 2016), SHELXLE Rev714 (Hübschle *et al.*, 2011).

Refinement details:

Disorder is observed for the ligand side arms and for one solvate pentane molecule. For both the pentane and ligand side arms, geometries of major and minor moieties were restrained to be similar, and U^{ij} components of ADPs were restrained to be similar for atoms closer to each other than 2.0 Å. The hydroxyl O atoms are shared between disordered moieties, but hydroxyl H atoms were included in the disorder and their positions atoms were refined, with O-H distances restrained to 0.84 Å. The H...B and H...Fe distances of the minor moiety hydroxyl H atoms were restrained to be similar to those of the major moiety. The ligand side arm disorder was extended to the H atoms of the methyl group of C11. Subject to these conditions the pentane occupancy ratio refined to 0.700(5) to 0.300(5), the ligand side arm occupancy ratio to 0.9492(12) to 0.0508(12).

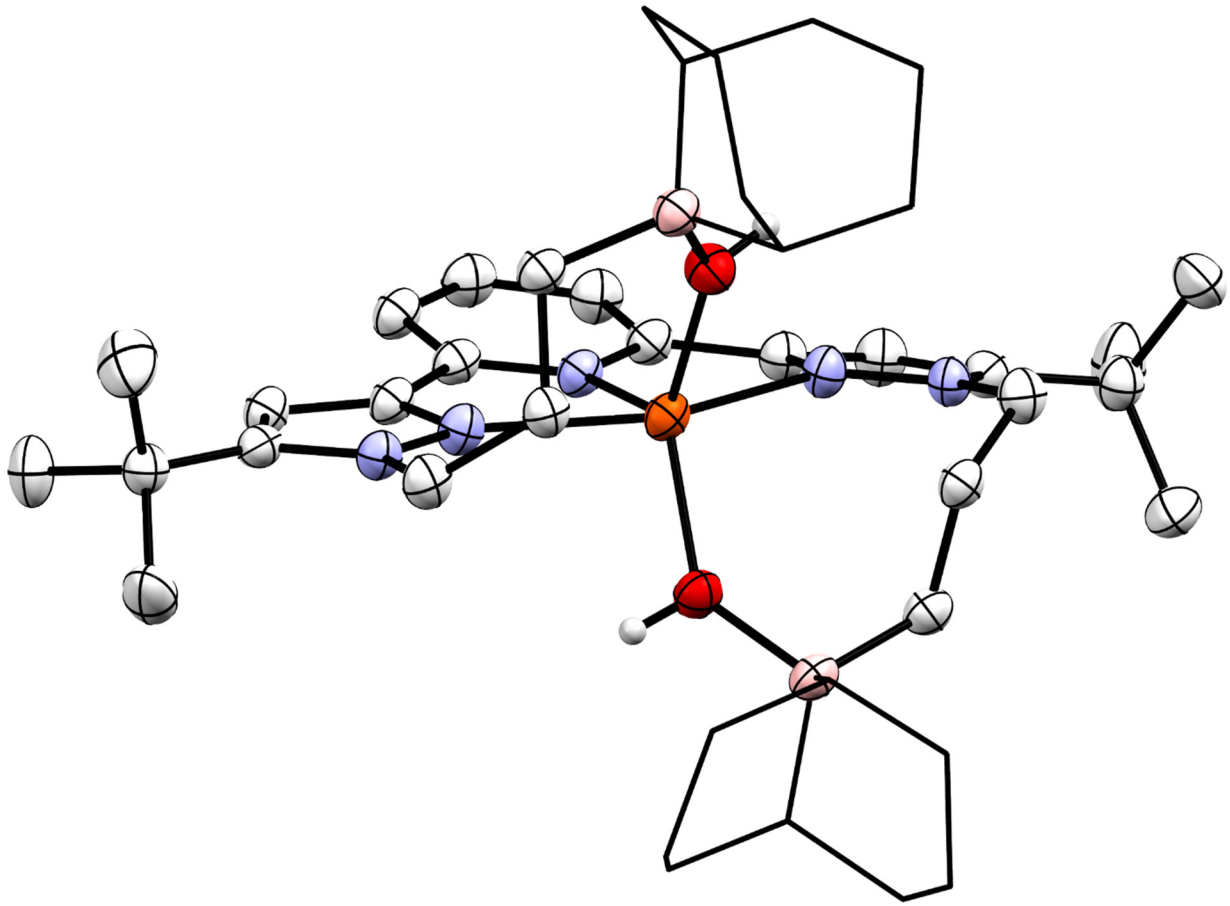


Figure S76. Molecular structure of (^{BBN}PDP^{tBu})Fe(OH)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms not attached to oxygen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})Fe(NHPh)$_2$

Local Name: jk318

CCDC 1884228

Table S10. Crystallographic parameters for (^{BBN}PDP^{tBu})Fe(NHPh)$_2$

Crystal data	
Chemical formula	$C_{53}H_{75}B_2FeN_7 \cdot 3(C_4H_8O)$
M_r	1103.98
Crystal system, space group	Monoclinic, *P*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	12.0303 (5), 11.0429 (4), 22.8724 (9)
β (°)	94.3767 (15)
V (Å^3)	3029.7 (2)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.30
Crystal size (mm)	0.28 × 0.17 × 0.13
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.652, 0.746
No. of measured, independent and observed [$I > 2s(I)$] reflections	22161, 8157, 6386
R_{int}	0.031
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.137, 1.07
No. of reflections	8157
No. of parameters	641
No. of restraints	968
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, -0.51

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2017*/1 (Sheldrick, 2015, 2017), SHELXLE Rev859 (Hübschle *et al.*, 2011).

Refinement details:

The main molecule shows minor disorder of the ligand side arm. The two disordered moieties were restrained to have similar geometries. C11 and C11B were constrained to have positions exactly related by the two fold axis bisecting the molecule. The methyl H atoms around C9 were included in the disorder by a 60 degree rotation between major and minor moiety (AFIX 127). The position of the N-bound H atoms H4 and H4B were refined, and the B...H and Fe...H distances in the two moieties were restrained to be similar. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.9055(19) to 0.0945(19).

Two THF molecules are disordered. One in a general position, and one around a two-fold axis with additional disorder by pseudo-inversion. The disordered moieties of each site were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. A mild anti-bumping restraint was applied to keep minor atoms from approaching main molecule H atoms too closely. Subject to these conditions the occupancy ratios refined to 0.728(10) to 0.272(10) for the THF molecule in the general position, and to two times 0.384(4) and two times 0.116(4) for the THF molecule around the two fold axis.

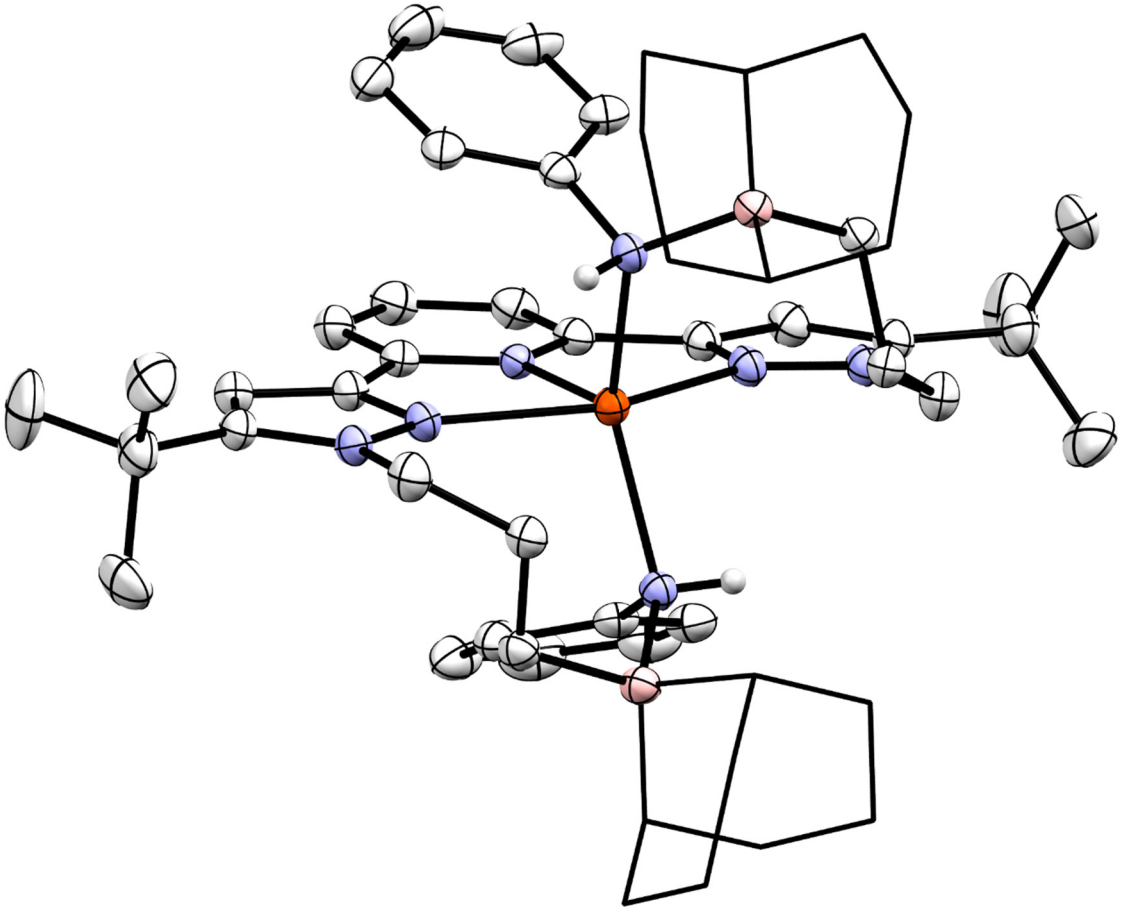


Figure S77. Molecular structure of (^{BBN}PDP^{tBu})Fe(NHPh)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms not attached to nitrogen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})Fe(PHPh)$_2$

Local Name: jk319

CCDC 1884232

Table S11. Crystallographic parameters for (^{BBN}PDP^{tBu})Fe(PHPh)$_2$

Crystal data	
Chemical formula	$C_{53}H_{74}B_2FeN_5P_2 \cdot 3(C_4H_8O)$
M_r	1137.90
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	10.989 (6), 12.928 (6), 24.431 (11)
α, β, γ (°)	92.678 (16), 91.124 (18), 114.185 (16)
V (Å^3)	3160 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.34
Crystal size (mm)	0.20 × 0.18 × 0.15
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.509, 0.745
No. of measured, independent and observed [$I > 2s(I)$] reflections	33481, 11734, 4754
R_{int}	0.142
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.130, 0.447, 1.06
No. of reflections	11734
No. of parameters	806
No. of restraints	401
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.73, -0.87

Computer programs: Apex3 v2017.3-0 (Bruker, 2016), *SAINT* V8.38A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev915 (Hübschle *et al.*, 2011).

Refinement details:

The structure exhibits pseudo-symmetry, nearly emulating a double the volume C-centered monoclinic cell in C2/c. The data can be refined in this setting, but R values are about 1/3 larger than in the primitive setting under inclusion of twinning by the monoclinic pseudosymmetry. The structure was refined as twinned by a two-fold rotation around (2 -1 0), with a twin matrix of 1 0 0, -1 -1 0, 0 0 -1. The final twin ratio refined to 0.810(4) to 0.190(4).

The structure exhibits large thermal libration for all atoms and disorder for several of the THF solvate molecules, leading to an intrinsic low resolution and absence of high angle data, and rather high data R values. Refined model R values are in line with the data quality.

P bound H atoms were located in difference density maps and their positions were refined with a P-H bond distance restraint of 1.00(2) Å.

No attempts were made to refine disorder for the main molecule. ADPs indicate a "swinging motion" around the Fe ion in the plane of the coordinated ligand fragment.

Of the four THF molecule sites two are located on inversion centers and two in general positions. The two molecules on inversion points were refined as 1:1 disordered. The two molecules in the general position are related by pseudo-monoclinic symmetry and disorder is highly correlated. One of the two molecules was refined as disordered, the other as not disordered. All THF moieties were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. The atoms of the molecules around inversion centers were also restrained to be close to isotropic. A mild anti-bumping restraint was applied to keep disordered H atoms from approaching other atoms too closely. Subject to these conditions the occupancy ratio for the disordered THF molecule in the general position refined to 0.217(19) to 0.783(19).

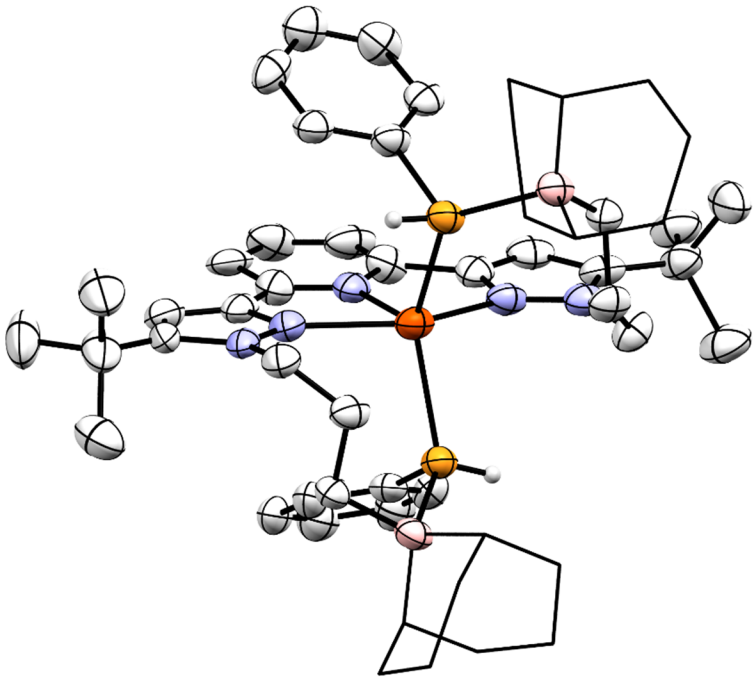


Figure S78. Molecular structure of (^{BBN}PDP^{tBu})Fe(PHPh)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms not attached to phosphorus atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})Fe(SPh)$_2$

Local Name: jk3188

CCDC 1884229

Table S12. Crystallographic parameters for (^{BBN}PDP^{tBu})Fe(SPh)$_2$

Crystal data	
Chemical formula	$C_{53}H_{73}B_2FeN_5S_2$
M_r	921.75
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	23.8853 (10), 11.6376 (5), 19.0401 (8)
β (°)	110.8255 (16)
V (Å^3)	4946.8 (4)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.43
Crystal size (mm)	0.53 × 0.35 × 0.27
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.674, 0.747
No. of measured, independent and observed [$I > 2s(I)$] reflections	35885, 9150, 6037
R_{int}	0.061
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.771
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.141, 1.06
No. of reflections	9150
No. of parameters	289
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, -0.62

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/1 (Sheldrick, 2015, 2018), SHELXLE Rev900 (Hübschle *et al.*, 2011).

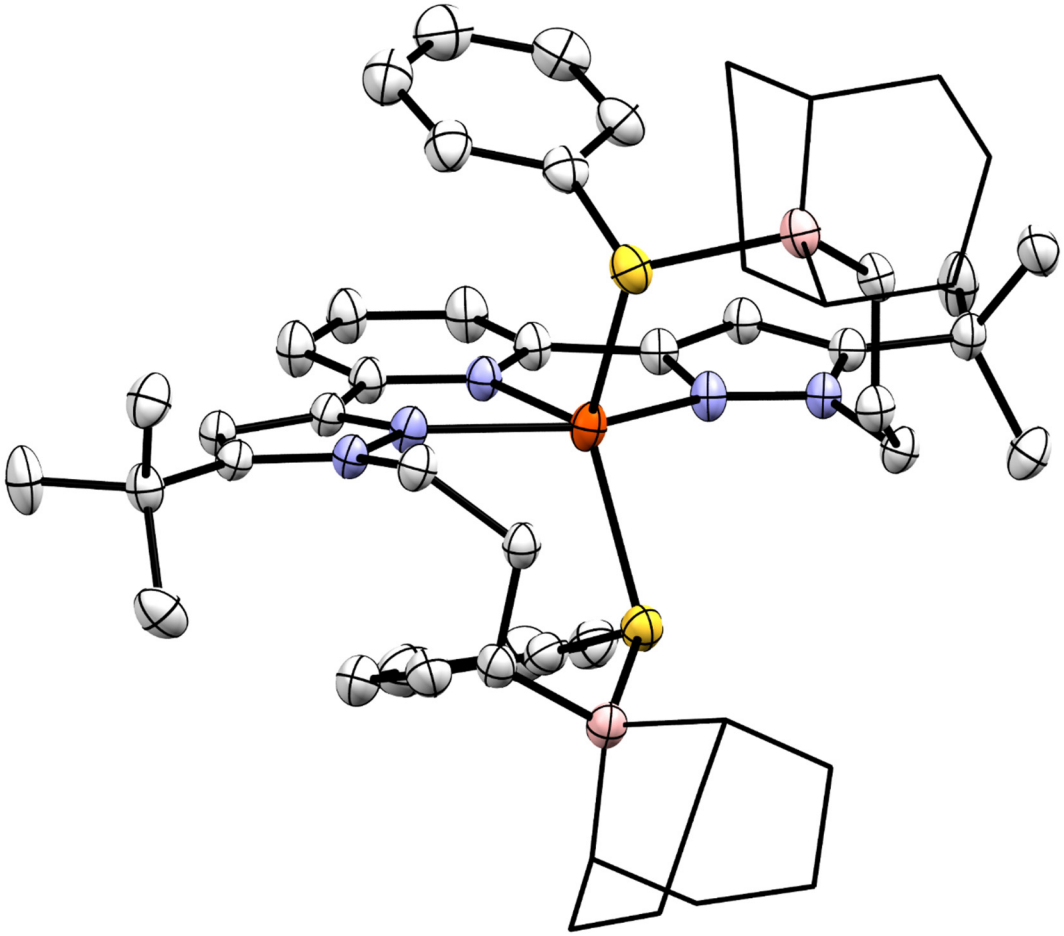


Figure S79. Molecular structure of (^{BBN}PDP^{tBu})Fe(SPh)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$

Local Name: jk4207

CCDC 1884230

Table S13. Crystallographic parameters for (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$

Crystal data	
Chemical formula	$C_{53}H_{79}B_2FeN_7S_2$
M_r	955.82
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	150
a, *b*, *c* (Å)	8.8548 (4), 17.4697 (7), 17.4739 (8)
α, β, γ (°)	92.316 (3), 99.766 (2), 99.769 (2)
V (Å^3)	2618.6 (2)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	3.36
Crystal size (mm)	0.41 × 0.08 × 0.07
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan TWINABS 2012/1: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). J. Appl. Cryst. 48 3-10.
T_{min}, T_{max}	0.131, 0.330
No. of measured, independent and observed [$I > 2s(I)$] reflections	34295, 10649, 8780
R_{int}	0.077
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.119, 0.323, 1.10
No. of reflections	10649
No. of parameters	595
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	3.95, -0.73

Computer programs: Apex3 v2017.3-0 (Bruker, 2017), *SAINT* V8.38A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev937 (Hübschle *et al.*, 2011).

Refinement details:

The crystal under investigation was found to be twinned by both non-merohedry as well as pseudo-merohedry. The orientation matrices for the components related by non-merohedry were identified using the program Cell_Now, with the two components being related by a 180 degree rotation around the real a-axis. The structure was also found to be twinned by perfect pseudo-merohedry, emulating a double volume C-centered lattice. When solved in monoclinic symmetry molecules were systematically disordered in an intricate way with the two moieties related by a two-fold rotation axis. Reduction of symmetry to triclinic (space group group $P\overline{1}$) and application of the twin transformation matrix -1 0 0, 0 0 -1, 0 -1 0 (180 degree rotation around (0 1-1)) resulted in nearly complete disappearance of one of the two disordered moieties ("ghost" electron densities are apparent for the "alternative" positions of the iron and sulfur atoms, but refinement was possible without application of restraints for either geometry or thermal parameters). The triclinic solution, not requiring refinement of disorder, was chosen as the more likely true structure and was used.

Several data processing procedures were tested. In the first procedure, the two components related by non-merohedry were integrated using Saint and corrected for absorption using twinabs, resulting in the following statistics:

14214 data (6765 unique) involve domain 1 only, mean I/sigma 23.0

14181 data (6769 unique) involve domain 2 only, mean I/sigma 16.8

5943 data (3270 unique) involve 2 domains, mean I/sigma 32.7

The exact twin matrix identified by the integration program was found to be:

1.00000 -0.00008 0.00008

-0.67226 -1.00047 -0.00735

-0.66839 0.00736 -0.99948

The structure was solved using direct methods with all non-overlapping reflections of both components. The structure was refined against the same data, under application of the twin matrix -1 0 0, 0 0 -1, 0 -1 0 to account for pseudo-merohedric twinning, resulting in a BASF value of 0.512(3), indicating a close to ideally twinned crystal.

Using the non-overlapping reflections of only the first (major) component gave similar results, but R values and overall quality indicators were slightly worse.

In an alternative approach, the data were integrated as a four component twin, with each of the two moieties related by non-merohedry additionally split by application of the twin matrix for pseudo-merohedric twinning. Results were, however, of substantially lower quality (R1 values were between 18 and 19%, ADPs less well defined and residuals more pronounced), and this approach was abandoned.

The R_{int} value given is for all reflections and is based on agreement between observed single and composite intensities and those calculated from refined unique intensities and twin fractions (TWINABS (Sheldrick, 2012)).

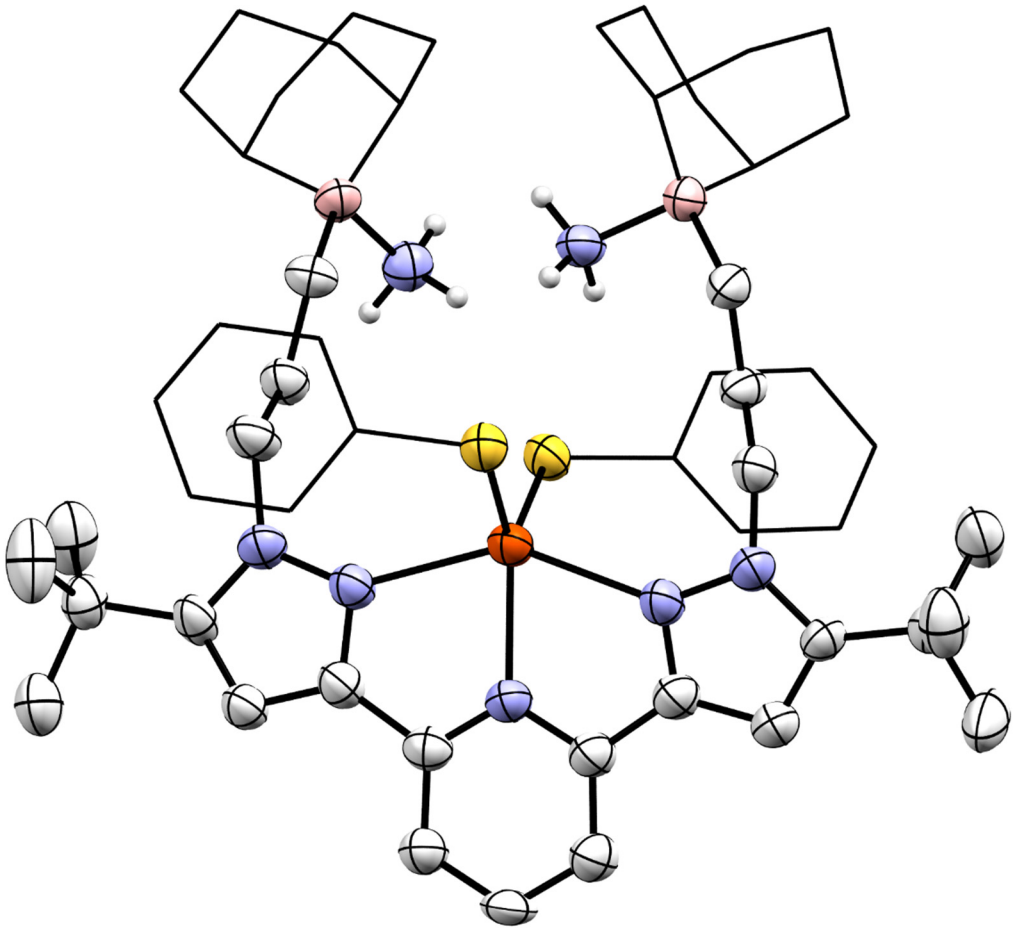


Figure S80. Molecular structure of (^{BBN}PDP^{tBu})Fe(SPh)$_2$(NH$_3$)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms not attached to nitrogen atoms are omitted for clarity. The 9-BBN and phenyl moieties are displayed in wireframe for clarity.

Compound: $[(^{BBN}PDP^{tBu})Fe(NC)_2]_2$

Local Name: jk217

CCDC 1884225

Table S14. Crystallographic parameters for $[(^{BBN}PDP^{tBu})Fe(NC)_2]_2$

Crystal data	
Chemical formula	$C_{86}H_{126}B_4Fe_2N_{14}\cdot 3.272(CH_2Cl_2)$
M_r	1807.60
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	100
a, *b*, *c* (Å)	14.7395(8), 31.7053(18), 22.0966(13)
β (°)	90.451(2)
V (Å^3)	10325.9(10)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.51
Crystal size (mm)	0.54 × 0.52 × 0.39
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.630, 0.747
No. of measured, independent and observed [$I > 2s(I)$] reflections	123502, 24774, 23021
R_{int}	0.043
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.140, 1.13
No. of reflections	24774
No. of parameters	1314
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.63, -0.52

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/1 (Sheldrick, 2015, 2018), SHELXLE Rev900 (Hübschle *et al.*, 2011).

Refinement details:

The structure exhibits pseudo-inversion and pseudo-twofold symmetry emulating space group C2/c. The higher symmetry is broken by ordering of the borabicyclononane of B1 and B3.

Refined as an inversion twin.

Dichloromethane solvate molecules are extensively disordered. All methylene chloride moieties were restrained to have similar geometries. U^{ij} components of ADPs were restrained to be similar for atoms closer to each other than 2.0 Å. A weak anti-bumping restraint was applied to keep solvate H atoms from approaching main moiety H atoms too closely. Atoms Cl8 and C92 and atoms Cl16 and C97 were constrained to share a site and ADP. Due to the extensive and sequential disorder no attempts were made to match occupancy rates and occupancies for all solvate molecules were independently refined. Occupancies refined to values between 0.800(6)and 0.059(5).

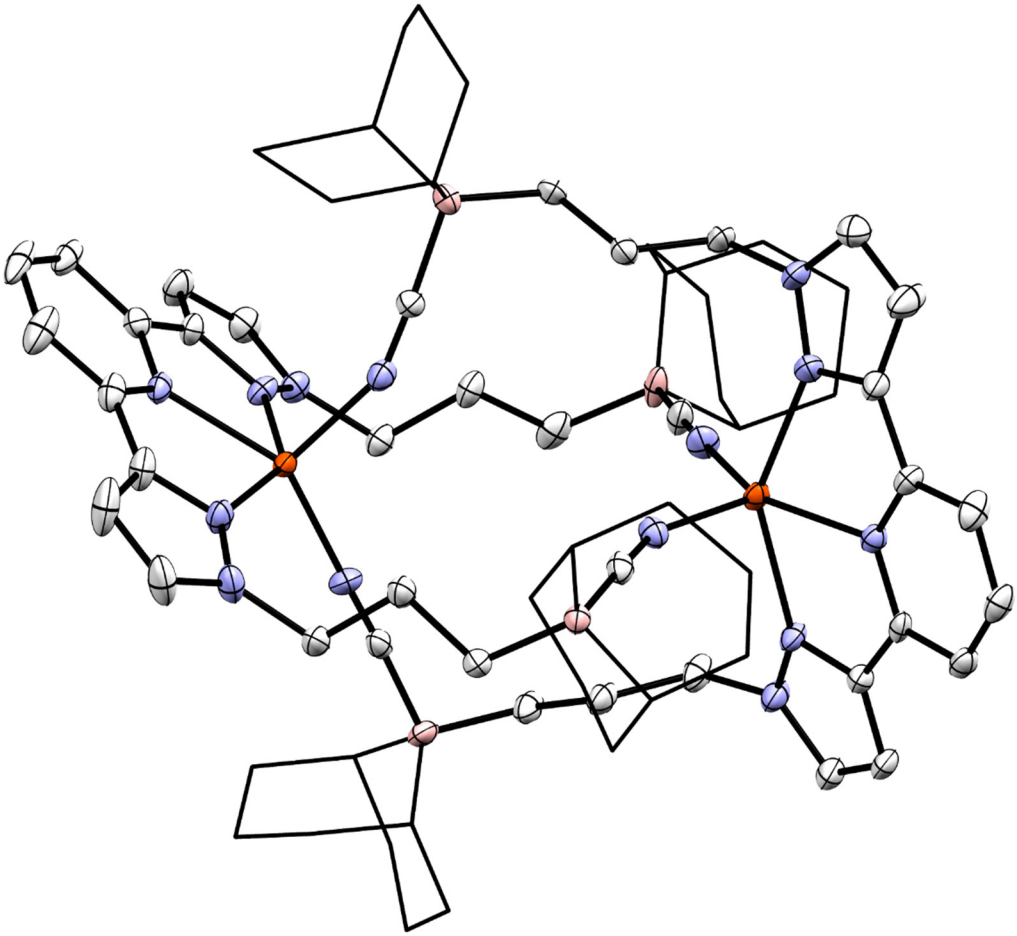


Figure S81. Molecular structure of $[(^{BBN}PDP^{tBu})Fe(NC)_2]_2$ displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: (^{BBN}PDP^{tBu})Zn(SPh)$_2$

Local Name: jk3257

CCDC 1884226

Table S15. Crystallographic parameters for (^{BBN}PDP^{tBu})Zn(SPh)$_2$

Crystal data	
Chemical formula	$C_{53}H_{73}B_2N_5S_2Zn$
M_r	931.27
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	23.8971 (10), 11.5743 (5), 19.0415 (7)
β (°)	110.4440 (14)
V (Å^3)	4935.0 (4)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.62
Crystal size (mm)	0.21 × 0.18 × 0.13
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). J. Appl. Cryst. 48 3-10.
T_{min}, T_{max}	0.718, 0.747
No. of measured, independent and observed [$I > 2s(I)$] reflections	146991, 9441, 7807
R_{int}	0.041
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.771
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.096, 1.05
No. of reflections	9441
No. of parameters	289
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.71, -0.58

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/1 (Sheldrick, 2015, 2017), SHELXLE Rev882 (Hübschle *et al.*, 2011).

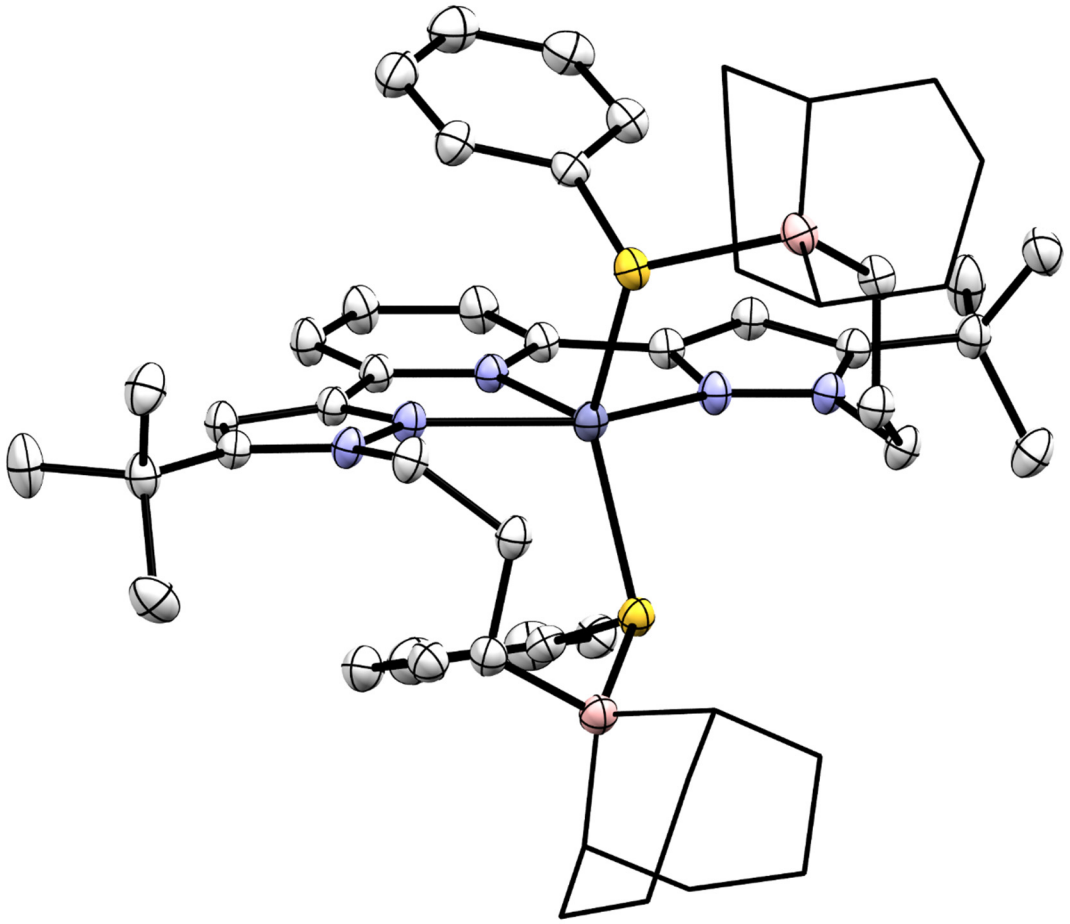


Figure S82. Molecular structure of (^{BBN}PDP^{tBu})Zn(SPh)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.

Compound: $[K(18\text{-crown-6})(THF)]_2[(^{BBN}PDP^{tBu})_2Fe(OPh)_4]$

Local Name: jk337

CCDC 1884222

Table S16. Crystallographic parameters for $[K(18\text{-crown-6})(THF)]_2[(^{BBN}PDP^{tBu})_2Fe(OPh)_4]$

Crystal data	
Chemical formula	$C_{106}H_{146}B_4FeN_{10}O_4{\cdot}2(C_{16}H_{32}KO_7){\cdot}2(C_4H_8O)$
M_r	2618.64
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	33.6410 (7), 16.3704 (3), 27.3584 (6)
β (°)	100.166 (1)
V (Å^3)	14830.2 (5)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	1.84
Crystal size (mm)	0.35 × 0.28 × 0.13
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.442, 0.754
No. of measured, independent and observed [$I > 2s(I)$] reflections	39390, 14541, 13474
R_{int}	0.040
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.073, 0.218, 1.05
No. of reflections	14541
No. of parameters	1109
No. of restraints	1008
H-atom treatment	H-atom parameters constrained
	$w = 1/[s^2(F_o^2) + (0.1402P)^2 + 15.7177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.50, -0.86

Computer programs: Apex3 v2016.9-0 (Bruker, 2016), *SAINT* V8.37A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2017*/1 (Sheldrick, 2015, 2017), SHELXLE Rev859 (Hübschle *et al.*, 2011).

Refinement details:

Two phenoxy groups, one *tert*-butyl group and the two next neighboring carbon atoms, and two THF molecules were refined as disordered. For all disordered moieties, major and minor moieties were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.687(14) to 0.313(14) and 0.790(6) to 0.210(6) for the two phenoxy groups, to 0.596(18) to 0.404(18) for the *tert*-butyl group, and to 0.703(7) to 0.297(7) and 0.605(10) to 0.395(10) for the two THF molecules.

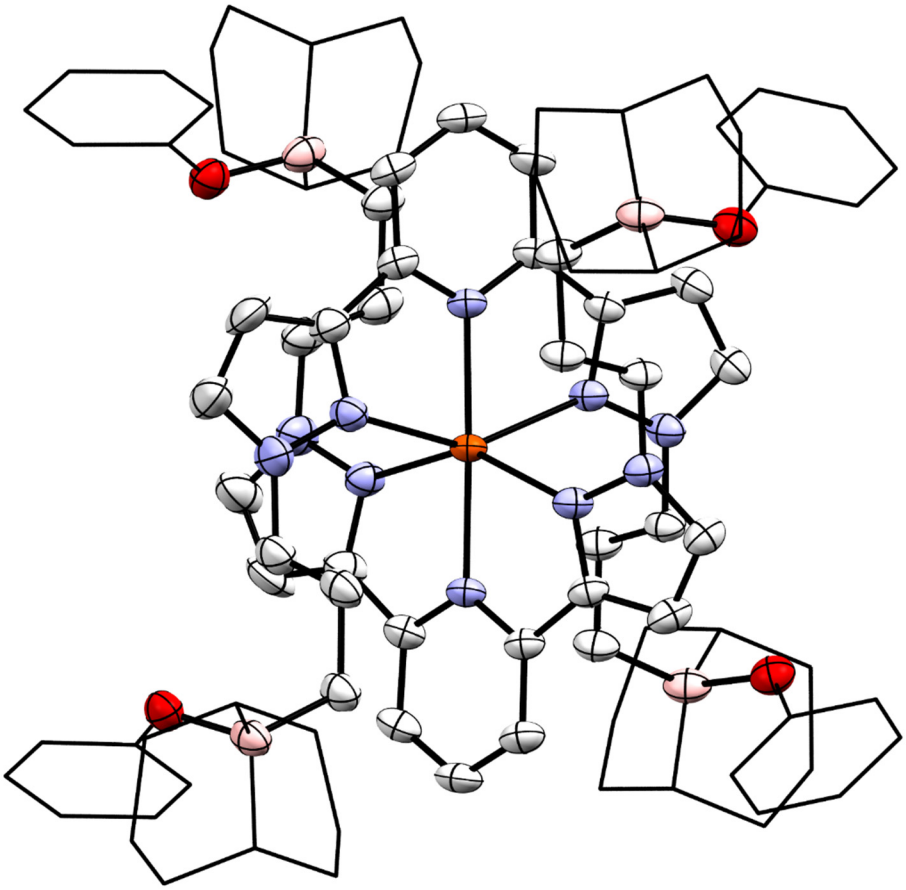


Figure S83. Anionic portion of the molecular structure of $[K(18\text{-crown-6})(THF)]_2[(^{BBN}PDP^{tBu})_2Fe(OPh)_4]$ displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The 9-BBN and phenoxide moieties are displayed in wireframe for clarity.

Compound: (^{butyl}PDP^{tBu})Fe(SPh)$_2$

Local Name: jk566

CCDC 1903500

Table S17. Crystallographic parameters for (^{butyl}PDP^{tBu})Fe(SPh)$_2$

Crystal data	
Chemical formula	$C_{39}H_{51}FeN_5S_2$
M_r	709.81
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	9.2208 (10), 15.9972 (18), 25.443 (3)
β (°)	93.373 (6)
V (Å^3)	3746.5 (7)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.52
Crystal size (mm)	0.21 × 0.06 × 0.02
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.496, 0.754
No. of measured, independent and observed [$I > 2s(I)$] reflections	20041, 7782, 5293
R_{int}	0.058
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.640
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.061, 0.181, 1.03
No. of reflections	7782
No. of parameters	763
No. of restraints	1218
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.94, -0.43

Computer programs: Apex3 v2017.3-0 (Bruker, 2017), *SAINT* V8.38A (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev946 (Hübschle *et al.*, 2011).

Refinement details:

The alkyl chains on both sides of the molecule are disordered, inducing disorder in large sections of the remainder of the molecule. The two moieties are mutually exclusive with their counterparts in neighbouring molecules, thus making exact 1:1 disorder necessary. The various equivalent fragments of the two disordered moieties were restrained to have each similar geometries. Uij components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar.

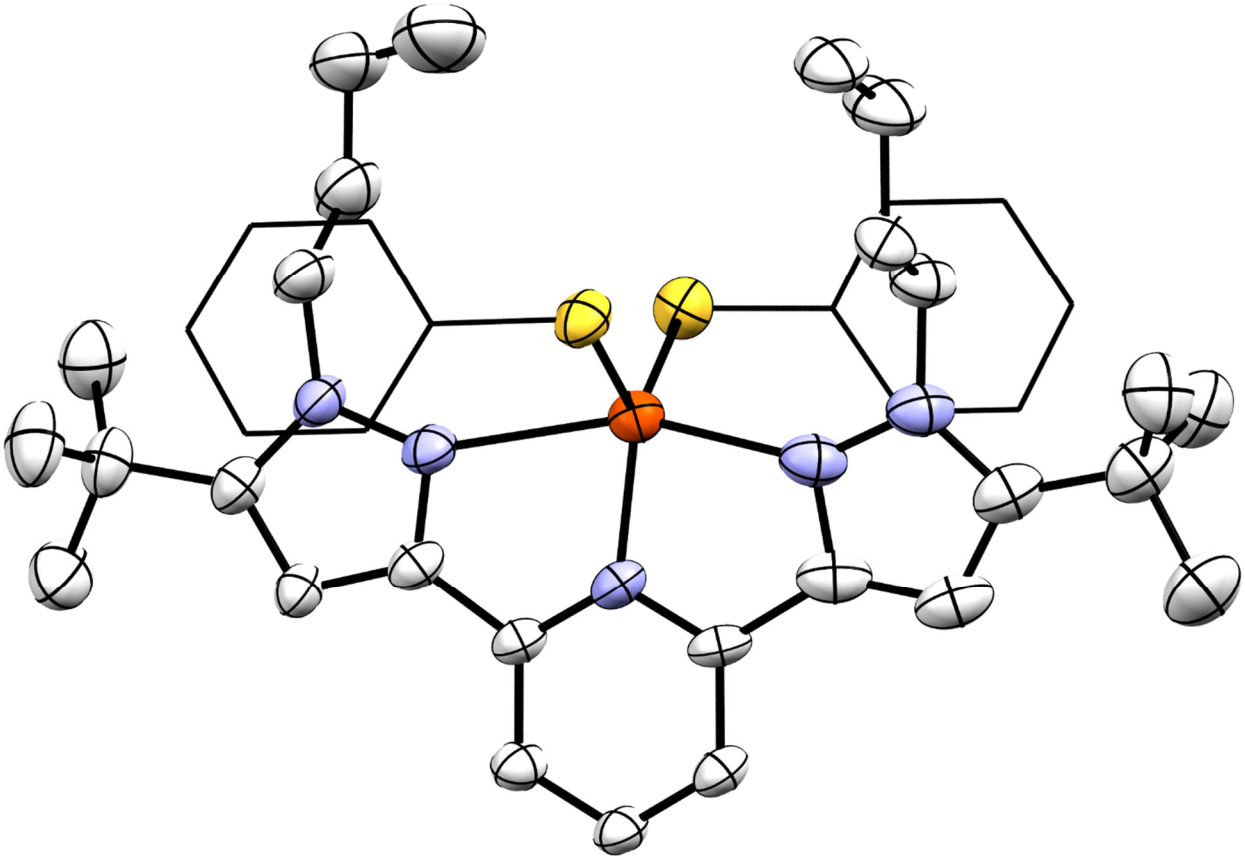


Figure S84. Molecular structure of (^{butyl}PDP^{tBu})Fe(SPh)$_2$ displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The phenyl moieties are displayed in wireframe for clarity.

$(^{Bu}PDP^{tBu})FeBr_2$
$(^{BBN}PDP^{tBu})FeH_2$
$[K(2,2,2\text{-crypt})][(^{BBN}PDP^{tBu})FeH_2]$

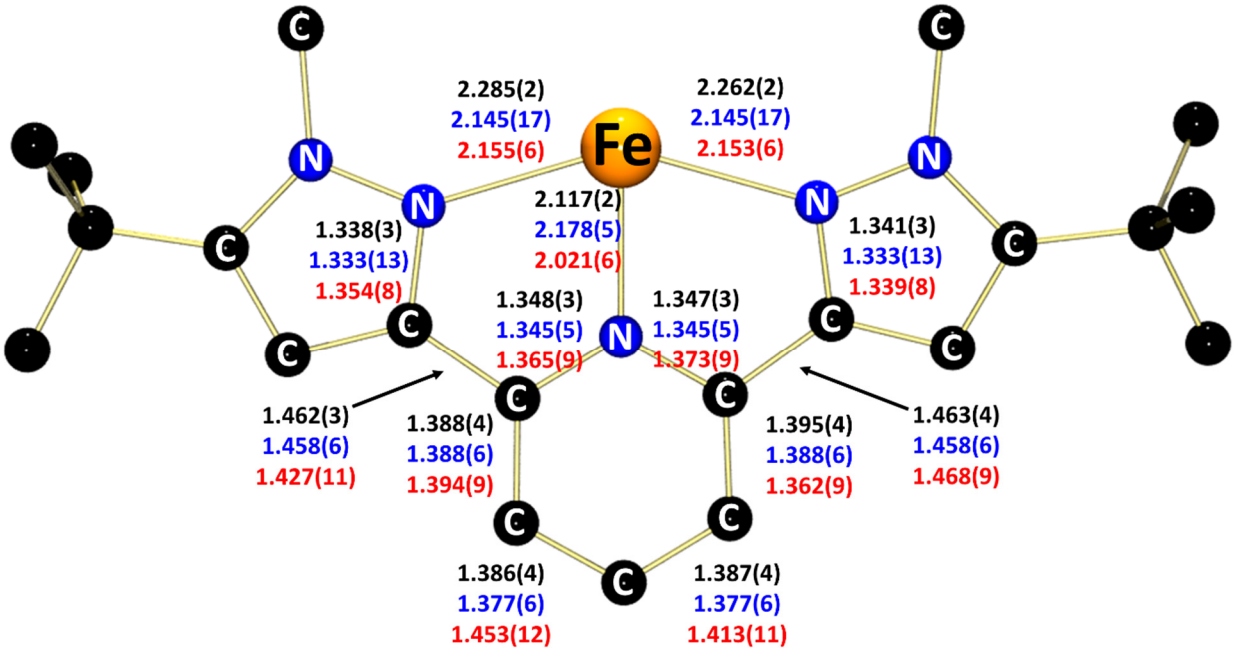


Figure S85. Comparison of intraligand bond distances in $(^{Bu}PDP^{tBu})FeBr_2$, $(^{BBN}PDP^{tBu})FeH_2$, and $[K(2,2,2\text{-crypt})][(^{BBN}PDP^{tBu})FeH_2]$. The data for $(^{Bu}PDP^{tBu})FeBr_2$ is taken from reference 1.

Table S18. Metrical parameters for hydride containing compounds.

	$(^{BBN}PDP^{tBu})FeH_2$	$[K(2,2,2\text{-crypt})][(^{BBN}PDP^{tBu})FeH_2]$	$(^{BBN}PDP^{tBu})ZnH_2$
M-$N_{pyrazole}$ (Å)	2.174(17)	2.155(6)	2.176(13)
M-$N_{pyrazole}$ (Å)	--	2.153(6)	--
M-$N_{pyridine}$ (Å)	2.178(5)	2.021(6)	2.153(4)
M-B (°)	2.970	2.977	2.977
M-B (°)	--	3.060	--
τ_5	0.314	0.363	0.374
IR υ(M-H-B) (cm^{-1})	1839	1866	1775

Table S19. Metrical parameters for complexes **2**.

	2-NH_2	**2-NHMe**	**2-NHPh**	**2-OH**	**2-PHPh**	**2-SPh**
Fe-$N_{pyrazole}$ (Å)	2.2950(18)	2.327(4)	2.2460(14)	2.2604(16)	2.248(11)	2.2148(13)
Fe-$N_{pyrazole}$ (Å)	--	--	--	2.2812(16)	2.304(12)	--
Fe-$N_{pyridine}$ (Å)	2.124(2)	2.168(5)	2.1123(19)	2.1164(15)	2.082(10)	2.1139(18)
Fe-X	2.075(2)	2.111(9)	2.179(3)	1.9812(13)	2.401(3)	2.4134(5)
Fe-X	--	--	--	1.9964(13)	2.414(4)	--
B-X	1.633(3)	1.641(11)	1.666(4)	1.592(2)	2.020(14)	2.0504(19)
B-X	--	--	--	1.595(2)	2.009(13)	--
Fe-B (Å)	3.349	3.329	3.418	3.343	3.907	3.848
Fe-B (Å)	--	--	--	3.340	3.918	--
$\Sigma B_{1\alpha}$ (°)	325.6(2)	326.4(6)	326.54(18)	321.69(16)	323.9(9)	319.57(12)
$\Sigma B_{2\alpha}$ (°)	--	--	--	322.34(16)	320.9(9)	--
τ_5	0.02	0.04	0.14	0.35	0.26	0.27

Table S20. Metrical parameters for ($^{BBN}PDP^{tBu}$)M$(SPh)_2$ species.

	2-SPh	**($^{BBN}PDP^{tBu}$)Fe$(SPh)_2(NH_3)_2$**	**($^{BBN}PDP^{tBu}$)Zn$(SPh)_2$**	**($^{butyl}PDP^{tBu}$)Fe$(SPh)_2$**
M-$N_{pyrazole}$ (Å)	2.2148(13)	2.321(5)	2.2508(9)	2.162(5)
M-$N_{pyrazole}$ (Å)	--	2.346(6)	--	2.407(9)
M-$N_{pyridine}$ (Å)	2.1139(18)	2.114(5)	2.0998(13)	1.897(10)
M-S	2.4134(5)	2.365(2)	2.3510(3)	2.356(4)
M-S	--	2.385(2)	--	2.332(6)
B-X	2.0504(19)	1.670(10)	2.0657(13)	--
B-X	--	1.631(9)	-	--
M-S-Ph (°)	90.06(6)	110.0(3)	91.94(4)	113.8(3)
M-S-Ph (°)	--	111.0(3)	--	114.0(4)
$\Sigma B_{1\alpha}$ (°)	319.57(12)	322.8(6)	319.14(8)	--
$\Sigma B_{2\alpha}$ (°)	--	319.4(6)	--	--
τ_5	0.27	0.30	0.26	0.61

Table S21. Comparison of literature values for Fe-B distances and υ(Fe-H-B) stretching frequencies.

Compound	Fe-B (Å)	υ(Fe-H-B) (cm^{-1})	Reference
$(^{BBN}PDP^{tBu})FeH_2$	2.970	1839	This work
$[(^{BBN}PDP^{tBu})FeH_2]^{1-}$	2.977 / 3.060	1866	This work
$(^{BBN}PDP^{tBu})ZnH_2$	2.977	1775	This work
$(P_2B\text{-}H)FeH(CO)_2$	2.743	2080	*J. Am. Chem. Soc.* **2013**, *135*, 12580.
$(PNP)FeH(CO)(BH_4)$	2.702	2339	*Adv. Synth. Catal.* **2016**, *358*, 820.
$(dmpe)_2FeH(BH_4)$	2.826	2030	*Inorg. Chim. Acta* **1986**, *114*, C27.
$(PhB(^{mes}IM)_3)FeHBEt_3$	2.124	Not reported	*Organometallics* **2015**, *34*, 4560.
$(PNNNP)FeH(CO)(BH_4)$	2.721	Not reported	*Organometallics* **2014**, *33*, 6905.
$(PNP)Fe(CO)H(BH_4)$	2.744	2051	*Angew. Chem. Int. Ed.* **2013**, *52*, 14162.
$(P_2B\text{-}H)Fe(N_2R_2)$	2.860	2000	*J. Am. Chem. Soc.* **2013**, *135*, 4938.
$(P_2B\text{-}H)Fe(N_2R'_2)$	2.833	2100	*J. Am. Chem. Soc.* **2013**, *135*, 4938.
$(P_3B\text{-}H)FeH(CN^tBu)$	2.673	Not reported	*Organometallics* **2013**, *32*, 3053.
$(P_3B\text{-}H)FeH(N_2)$	2.602	Not reported	*Organometallics* **2013**, *32*, 3053.
$(P_3B\text{-}H)FeH(H_2)$	2.628	Not reported	*Organometallics* **2013**, *32*, 3053.
$(PNP)FeH(CO)(BH_4)$	2.864	Not reported	*Chem. Sci.* **2015**, *6*, 4291.
$(P_2B\text{-}H)Fe(SPh)$	3.018	1949	*Organometallics* **2015**, *34*, 4741.
$(P_2B\text{-}H)Fe(C\text{-}N_{chelate})$	2.334	2270	*Organometallics* **2015**, *34*, 4741.
$(P_2B\text{-}H)Fe(NH\text{-}N_{chelate})$	2.966	2130 / 2000	*Organometallics* **2015**, *34*, 4741.
$(PNP)FeH(CO)(BH_4)$	2.667	2028	*Chem. Eur. J.* **2012**, *18*, 7196.
$(Tm^{Ph})_2Fe$	3.15	2448	*Polyhedron* **2001**, *20*, 1891.
$(Tm^{tBu})_2Fe$	3.152	Not assigned	*Inorg. Chem.* **2006**, *45*, 7056.
$[\kappa^3\text{-}H,S,S\text{-}Tm^{tBu}]FeCl(py)$	2.994	Not assigned	*Inorg. Chem.* **2006**, *45*, 7056.
$[P_3{}^B(\mu\text{-}H)Fe(H)(CO)]^{2-}$	2.785	1760/1824	*J. Am. Chem. Soc.* **2017**, *139*, 2561.
$[P_3{}^B(\mu\text{-}H)Fe(H)_2(CO)]^{1-}$	2.667	1826/1862	*J. Am. Chem. Soc.* **2017**, *139*, 2561.
$(P_3{}^B\text{-}H)Fe(CO)$	2.650	2588	*J. Am. Chem. Soc.* **2017**, *139*, 2561.
$(PNP)FeH(CO)(BH_4)$	2.708 / 2.700	2360	*Catal. Sci. Technol.* **2016**, *6*, 4768.
$(H_2B(L)_2)FeH(L\text{-}H)$	2.658	2385	*Chem. Eur. J.* **2018**, *24*, 1358.
$(PNP)FeH(CO)(BH_4)$	2.745	1896	*Inorg. Chem.* **2014**, *53*, 2133.
$(PNP)FeH(CO)(BH_4)$	2.749	2038	*J. Am. Chem. Soc.* **2014**, *136*, 7869.
$[P_3{}^B(\mu\text{-}H)Fe(H)(NNR)]^{1-}$	2.791	2078	*Chem. Sci.* **2018**, *9*, 6264.
$P_3{}^B(\mu\text{-}H)Fe(NHNR_2)(CNR)$	2.885	2090	*Chem. Sci.* **2018**, *9*, 6264.
$[(P_3{}^B\text{-}H)Fe(CNR)]^{1+}$	2.763 / 2.769	2483	*Chem. Sci.* **2018**, *9*, 6264.
$(P_2)Fe(HBR_2R')$	2.436	Not reported	*Organometallics* **2017**, *37*, 729.
$[(L\text{-}H)(H_3BL)FeH(CN)]^{1-}$	2.649	2360/2340	*Chem. Eur. J.* **2018**, *24*, 12346.

DFT Calculations

Calculations were performed using Gaussian 09 revision D.01.[8] Calculations of all compounds were performed using the B3LYP functional and an ultrafine integration grid for all atoms. Optimizations were performed in the gas phase with the 6-31g(d) basis set for all atoms followed by vibrational frequency analysis to confirm that local minima were obtained through the absence of imaginary vibrational frequency modes.[9] Natural bonding orbital analysis and Wiberg bond index analysis were performed using NBO version 3.1.[10] Becke orbital composition analysis[11] was performed using Multiwfn version 3.5.[12] Solvation corrections were determined for thermodynamic profiles by the integral-equation-formalism polarizable continuum model (IEFPCM) using a SMD solvation model of THF.[13]

Table S22. Spin state configurations

Complex	H(gas)	G(gas)
1 S=0	-3187.480914	-3187.602773
1 S=1	-3187.501231	-3187.627250
1 S=2	-3187.523920	-3187.654000
1 S=3	-3187.462148	-3187.590482
1$^-$ S=1/2	-3187.563635	-3187.687652
1$^-$ S=3/2	-3187.707423	-3187.707423
1$^-$ S=5/2	-3187.698959	-3187.568936
Zn$^-$ S= 1/2	-3703.098298	-3703.226102

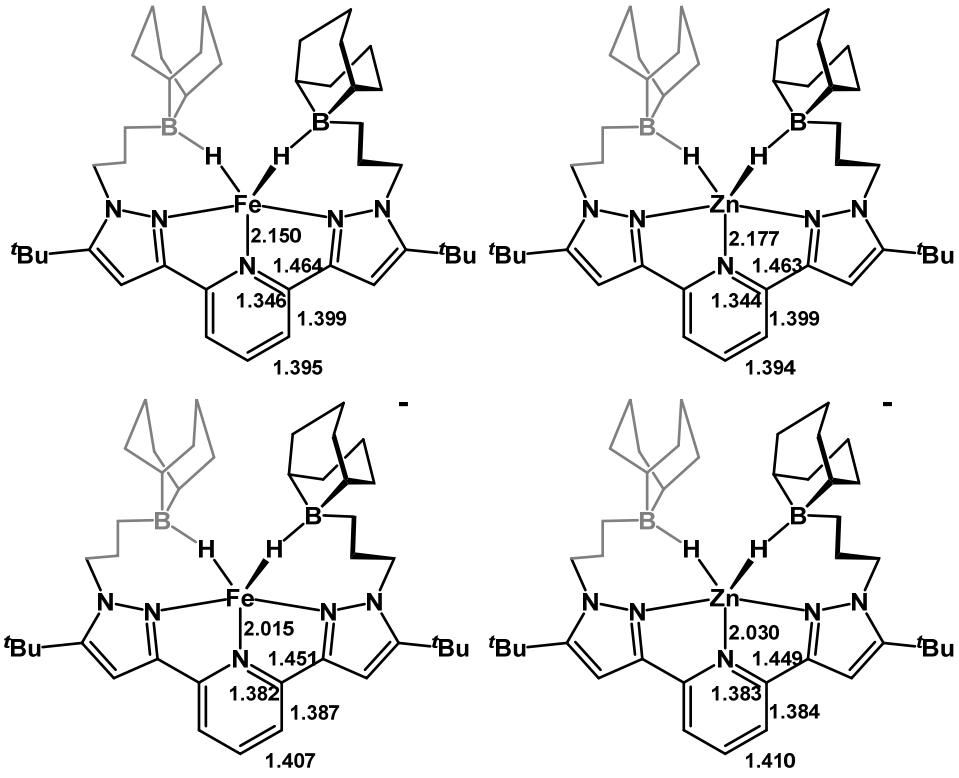


Figure S86. Summary of key bond parameters for the optimized geometries of **1**, **1-K(crypt)**, (**^{BBN}PDP^{tBu}**)**ZnH$_2$**, and (**^{BBN}PDP^{tBu}**)**ZnH$_2^-$**

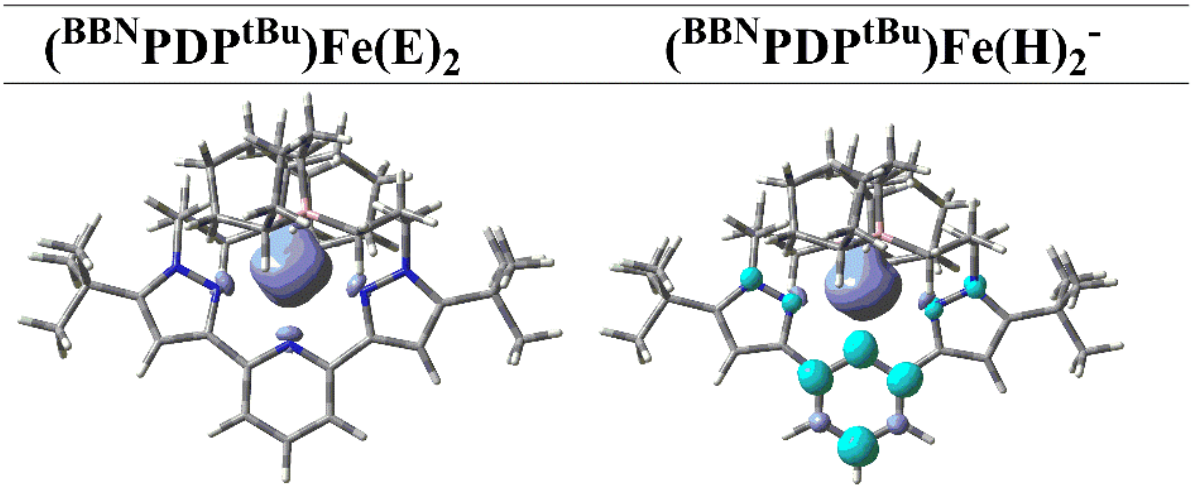


Figure S87. Spin density plots for **1** and **1**$^-$.

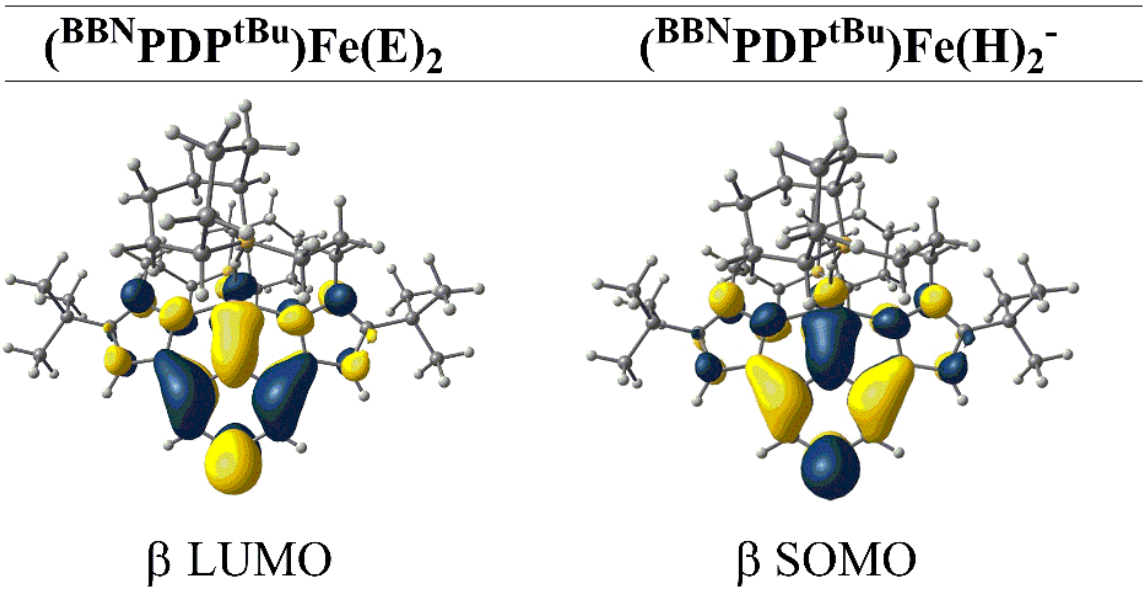


Figure S88. β LUMO at 0.03 au for **1**, and β SOMO for **1**$^-$.

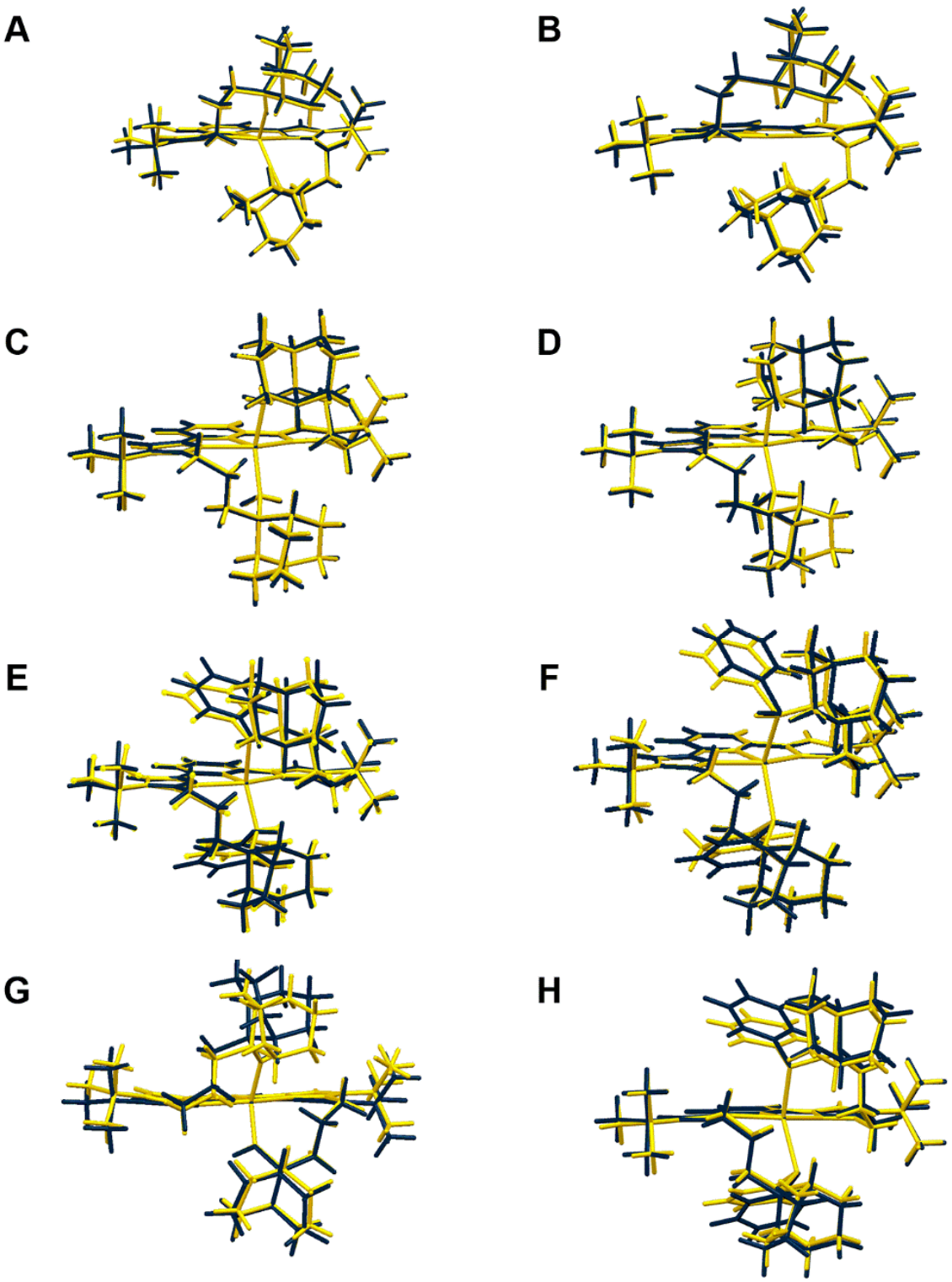
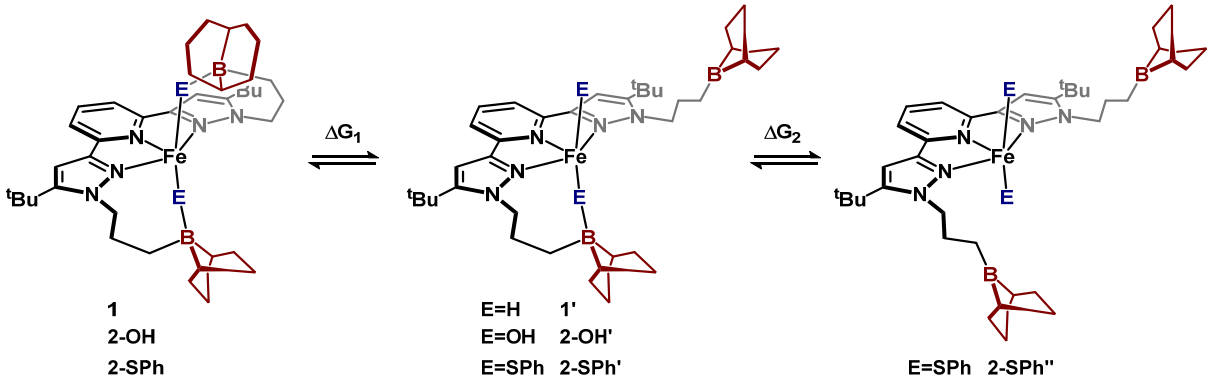


Figure S89. Overlay of XRD (yellow) and optimized geometries (blue) for a) **1**, b) **1-K(crypt)**, c) **2-NH$_2$** d) **2-NHMe**, e) **2-NHPh**, f) **2-PHPh** g) **2-OH** h) **2-SPh**

Table S23. Summary of thermodynamics for E-BBN binding



Compound	' (kcal/mol)	'' (kcal/mol)
1	2.3	
2-OH	10.3	
2-SPh	-8.6	-18.4

Table S24. Summary of NBO charge analysis

Compound	M	E	B	N(Py)
1	1.327	-0.254	0.421	-0.565
1^-	1.256	-0.212	0.361	-0.687
(^{BBN}PDP^{tBu})ZnH_2^-	1.291	-0.287	0.461	-0.553
(^{Me}PDP^{tBu})FeH_2	0.742	-0.419		-0.537
H-BBN(CH_3)$^-$		-0.081	0.214	
BBN(CH_3)			1.005	
2-NH_2	1.342	-1.196	0.684	-0.560
2-NHMe	1.372	-1.013	0.684	-0.568
2-NHPh	1.384	-0.966	0.694	-0.573
2-PHPh	1.135	0.264	0.318	-0.565
2-OH	1.359	-0.989	0.800	-0.563
2-SPh	1.160	-0.146	0.650	-0.567
1'	1.045	-0.217	0.389	-0.541
		-0.458	1.031	
2-OH'	1.295	-0.978	0.798	-0.544
		-1.117	1.030	
2-SPh'	1.120	-0.127	0.608	-0.561
		-0.404	1.032	

Table S25. Summary of Wiberg bond index analysis

Compound	M-E	E-B	M-N(Py)	Total Valence E	Total Valence B	% B-H	% M-H
1	0.18	0.70	0.17	0.91	3.48	74%	19 %
1^-	0.14	0.77	0.30	0.95	3.53	81%	14%
(^{BBN}PDP^{tBu})ZnH_2	0.22	0.65	0.18	0.92	3.48	71%	24%
(^{Me}PDP^{tBu})FeH_2	0.65		0.23	0.73			89%
H-BBN(CH_3)$^-$		0.95		0.99	3.59		
BBN(CH_3)					2.83		
2-NH_2	0.24	0.66	0.16	2.61	3.28		
2-NHMe	0.18	0.64	0.12	2.72	3.28		
2-NHPh	0.16	0.60	0.13	2.80	3.27		
2-PHPh	0.43	0.85	0.17	3.38	3.57		
2-OH	0.24	0.55	0.16	1.60	3.15		
2-SPh	0.38	0.60	0.16	2.25	3.31		
1'	0.18	0.73	0.19	0.94	3.51		
	0.66	0.00		0.76	2.81		
2-OH'	0.25	0.57	0.17	1.63	3.16		
	0.45	0.00		1.31	2.82		
2-SPh'	0.36	0.64	0.17	2.28	3.36		
	0.50	0.00		1.80	2.81		
(^{Me}PDP^{tBu})Fe(NH_2)$_2$	0.55		0.35	2.34			
(^{Me}PDP^{tBu})Fe(NHMe)$_2$	0.54		0.41	2.62			
(^{Me}PDP^{tBu})Fe(NHPh)$_2$	0.40		0.18	2.66			
(^{Me}PDP^{tBu})Fe(PHPh)$_2$	0.55		0.18	2.73			
(^{Me}PDP^{tBu})Fe(OH)$_2$	0.40, 0.52		0.21	1.34			
(^{Me}PDP^{tBu})Fe(SPh)$_2$	0.50, 0.57		0.18	1.86			

Table S26. Frontier orbital energies (eV) and Becke orbital composition for **1** and **2**-**E** and analogous (^{Me}PDP^{tBu})Fe(E)$_2$ complexes.

		α		β		Orbital Composition β LUMO		
	E	**HOMO**	**LUMO**	**HOMO**	**LUMO**	**Fe %**	**E%**	**E%**
(^{BBN}PDP^{tBu})Fe(E)$_2$	**H**	-5.303	-2.231	-5.204	-2.485	17.1	0.1	0.1
	NH_2	-4.918	-2.184	-4.917	-2.346	9.6	0.3	0.3
	NHMe	-4.865	-2.163	-4.879	-2.327	10.4	0.1	0.1
	NHPh	-5.048	-2.041	-5.067	-2.294	15.9	0.1	0.1
	PHPh	-5.067	-2.171	-5.222	-2.506	9.5	0.6	0.6
	OH	-4.925	-2.171	-4.893	-2.332	20.4	0.6	0.6
	SPh	-4.346	-1.766	-4.193	-1.976	15.3	0.4	0.4
	SPh (2-SPh'')	-4.535	-1.795	-4.415	-1.997	13.6	0.9	0.9
(^{Me}PDP^{tBu})Fe(E)$_2$	**H**	-3.930	-1.196	-3.320	-1.492	20.5	0.1	0.1
	NH_2	-4.437	-0.766	-2.736	-0.877	59.7	4.7	4.7
	NHMe	-4.264	-0.754	-2.784	-0.653	21.5	2.7	1.4
	NHPh	-3.630	-1.668	-3.589	-1.859	7.9	1.0	0.2
	PHPh	-3.831	-0.490	-3.812	-1.929	12.0	1.4	1.1
	OH	-5.423	-1.018	-3.078	-0.890	14.7	0.4	0.5
	SPh	-5.532	-1.725	-5.031	-2.376	10.6	1.3	0.3

Computational analysis of reduction potentials:

To avoid the reliance on a computational investigation of the reduced forms of synthetically intractable compounds, an analysis of LUMO energies was used as a surrogate for computationally obtained E^0 values.[14] A single case of each heteroatom (excluding the fluctional **2-SPh**) was analyzed by a computationally determined E^0.[15] A correction of -0.56 V was used to correct from potentials vs SCE to Fc.[16]

The trend in DFT calculated E^0 values for the investigated subset shows β LUMO as a fair surrogate for the calculated E^0 (Figure S90). High level dispersion corrected DFT calculations for the compounds were cost prohibitive and the relative position of E^0 (DFT) is higher than anticipated by experiment. This a common problem for anions without modeled dispersion.[15] The relative differences in E^0 (DFT) are more illustrative of the analysis and provide similar output to the β LUMO (Figures S91 and S92). The experimental $E^{1/2}$ of **2-OH** is quasireversable and presents a second source of uncertainty and could be a potential source of disagreement in the relative ordering of **2-NH$_2$** and **2-OH**.

Table S27. Energies for the calculation of E^0 vs Fc for **1** and **2-E**.

Molecule	Charg.	H(SCF) (eV)	G(Solv) (kcal/mol)	H(SCF) + G(Solv) (eV)	Δ (eV)	ZPE-Entropy correction (eV)	E^0 (calc) V (vs. Fc/Fc^+)	$E_{1/2}$, V (vs. Fc/Fc^+)
$(^{BBN}PDP^{tBu})Fe(H)_2$	0	-86736.988	25.50	-86735.892				
	-1	-86738.493	6.83	-86738.200	-2.308	-0.088	-2.594	-2.06
$(^{BBN}PDP^{tBu})Fe(NH_2)_2$	0	-89750.909	29.07	-89749.659				
	-1	-89752.085	11.91	-89751.573	-1.913	-0.130	-2.947	-2.12
$(^{BBN}PDP^{tBu})Fe(OH)_2$	0	-90833.656	30.76	-90832.333				
	-1	-90834.880	10.91	-90834.410	-2.077	-0.116	-2.797	-2.12
$(^{BBN}PDP^{tBu})Fe(PHPh)_2$	0	-117916.663	41.65	-117914.872				
	-1	-117918.282	24.62	-117917.224	-2.351	-0.112	-2.527	-1.96

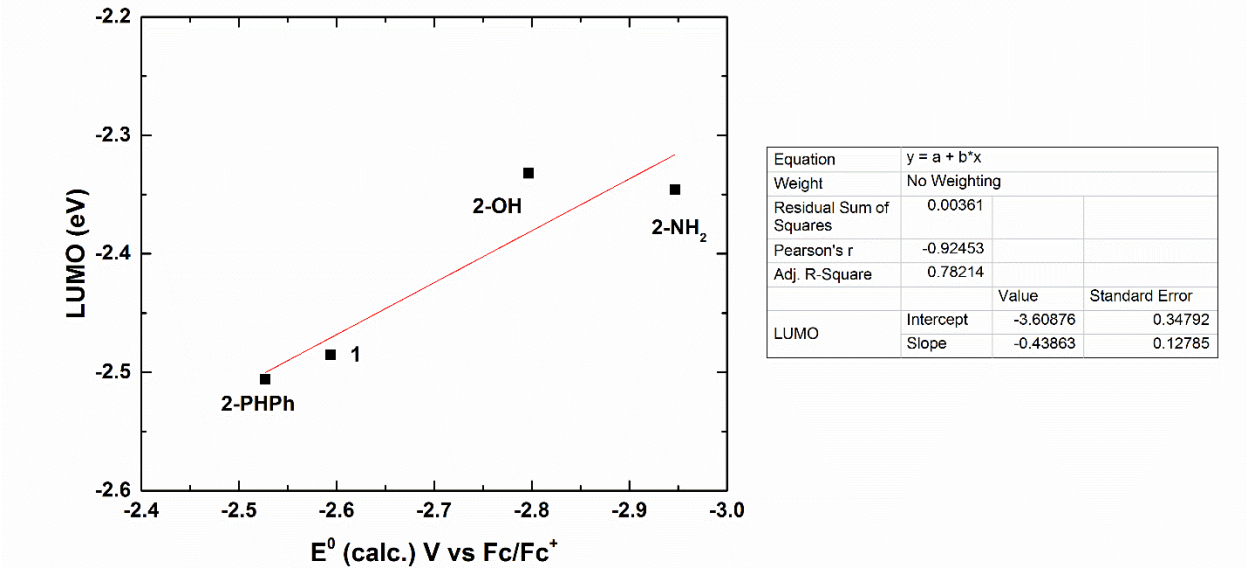
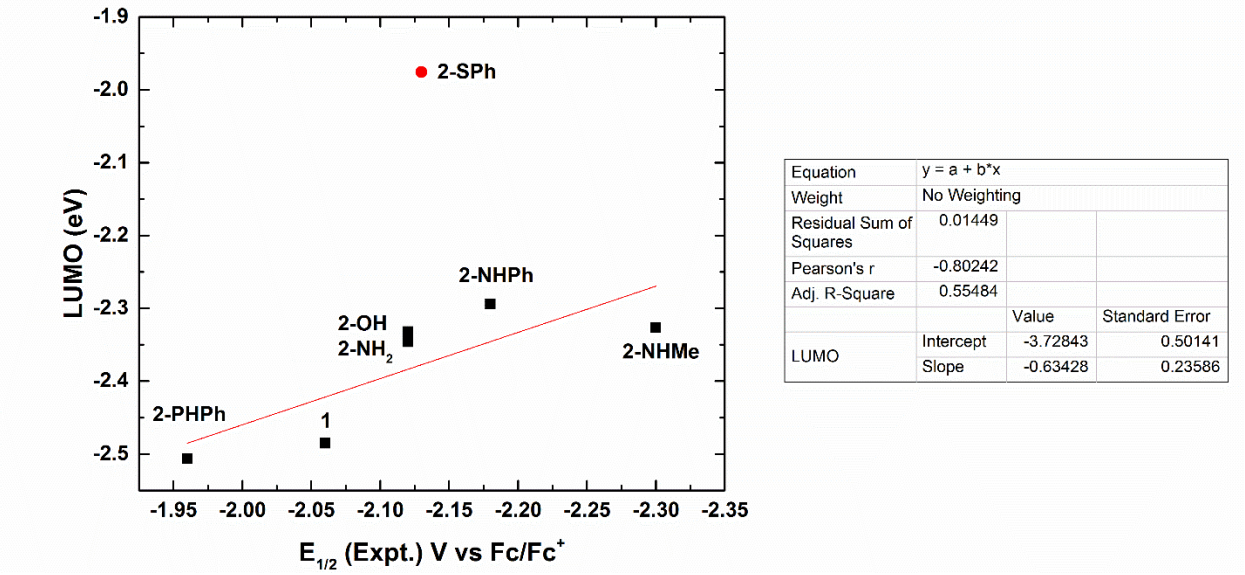
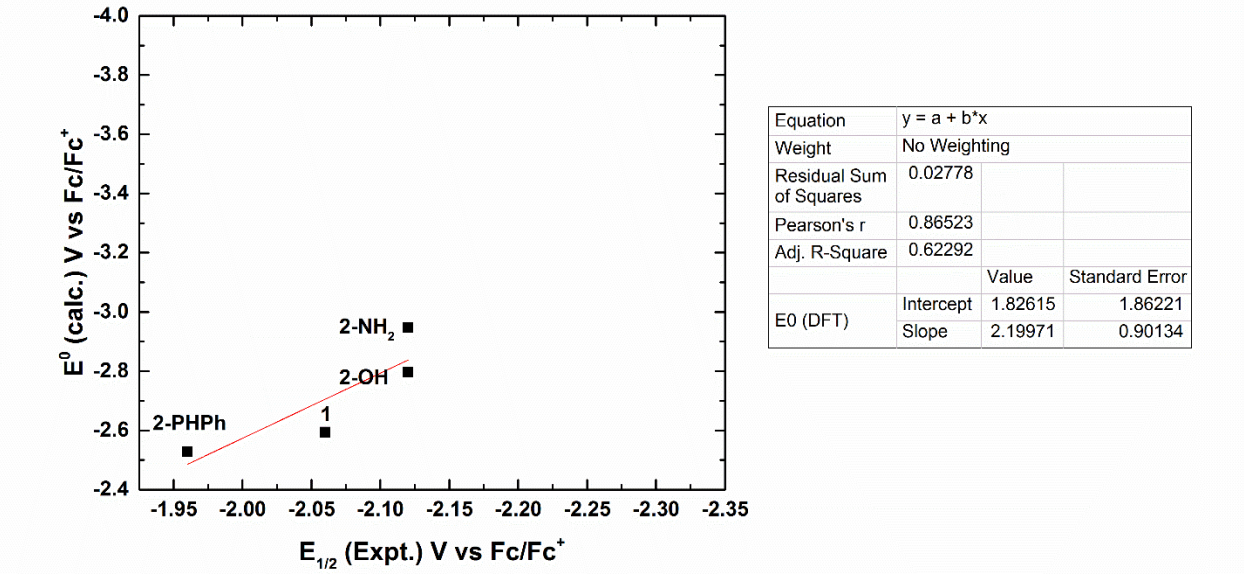


Figure S90. LUMO β energy (eV) vs E^0 (calc) V (vs. Fc/Fc^+) for **1** and **2-E**.



Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.01449		
Pearson's r	-0.80242		
Adj. R-Square	0.55484		
		Value	Standard Error
LUMO	Intercept	-3.72843	0.50141
	Slope	-0.63428	0.23586

Figure S91. LUMO β energy (eV) vs $E_{1/2}$ (expt.) V (vs. Fc/Fc^+) for **1** and **2**-**E**.



Equation	y = a + b*x		
Weight	No Weighting		
Residual Sum of Squares	0.02778		
Pearson's r	0.86523		
Adj. R-Square	0.62292		
		Value	Standard Error
E0 (DFT)	Intercept	1.82615	1.86221
	Slope	2.19971	0.90134

Figure S92. E^0 (calc) V (vs. Fc/Fc^+) vs $E_{1/2}$ (expt.) V (vs. Fc/Fc^+) for **1** and **2**-**E**.

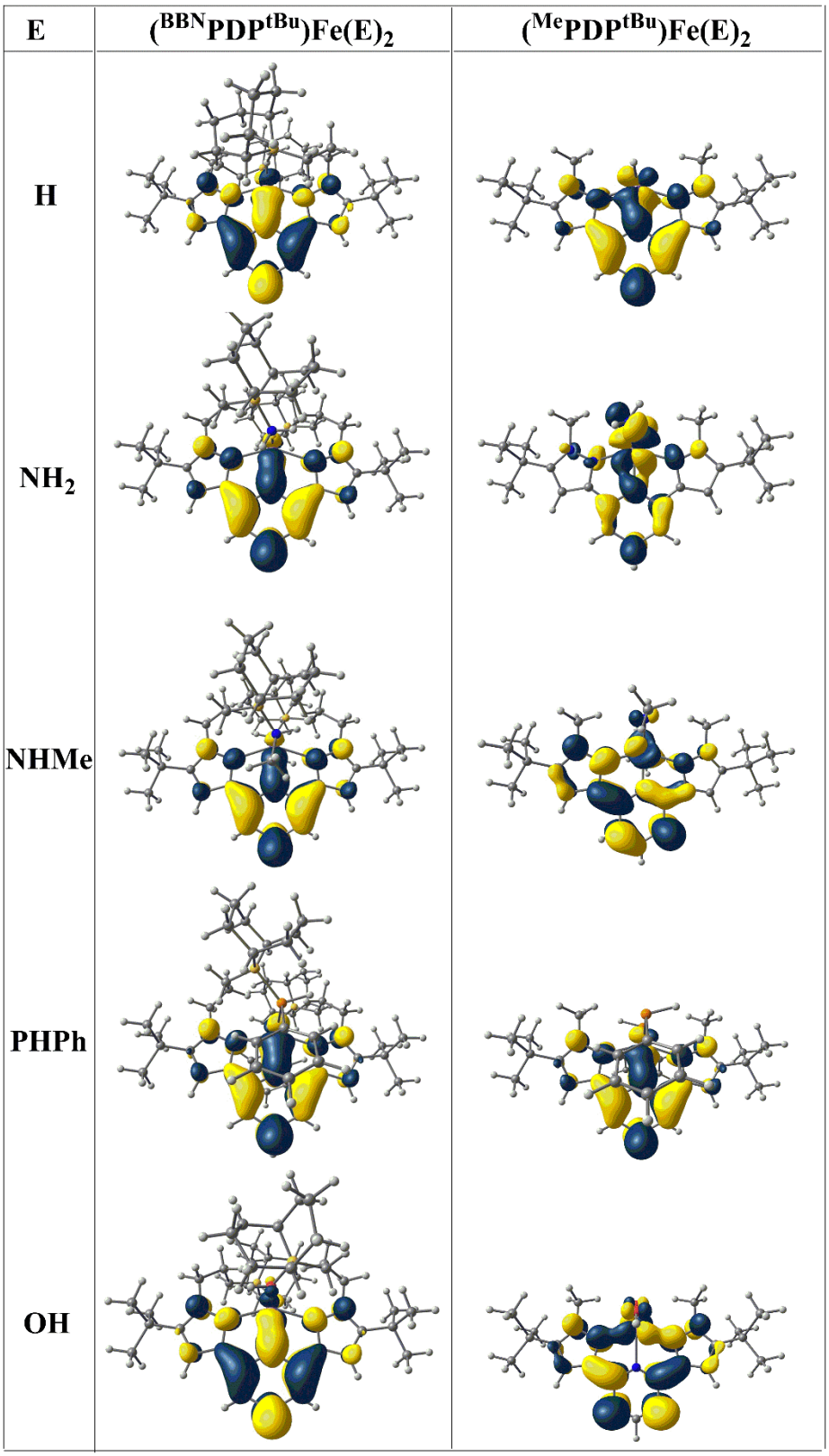


Figure S93. Figure of β LUMO at 0.03 au for **1**, **2**-**E** and analogous (^{Me}PDP^{tBu})M(E)$_2$ complexes.

Optimized Geometries

1 S=2

Fe	8.59011200	10.67666900	-0.71950800
N	10.11120900	12.19601300	-0.71848500
C	10.14848600	13.09116300	0.28581700
C	11.11999900	14.09672700	0.31534000
H	11.14679800	14.81470100	1.12757500
C	12.05747000	14.13987200	-0.71711400
H	12.82597400	14.90743100	-0.71657400
C	9.12648500	12.86075300	1.30933600
C	8.75630600	13.55234100	2.47141800
H	9.14715200	14.49151200	2.82942500
C	7.74651900	12.79412000	3.06397400
C	6.90801300	13.15284600	4.28764300
C	7.44232600	14.47526600	4.88036400
H	6.84231400	14.75064200	5.75391100
H	7.37697400	15.29793600	4.16023000
H	8.48402800	14.37985800	5.20680300
C	5.43631700	13.37994900	3.86083800
H	4.84340900	13.68949700	4.72935800
H	4.97566900	12.47735100	3.44881500
H	5.36589200	14.16519800	3.10080500
C	6.97986300	12.07924700	5.39818500
H	6.44988300	12.44184700	6.28637700
H	8.01710900	11.87317200	5.68386100
H	6.51576700	11.13571300	5.10323100
N	8.38680300	11.74675000	1.18422000
N	7.57061400	11.70116700	2.25193800
C	6.84548100	10.43255800	2.44719800
H	6.54416500	10.11027900	1.44930600
H	5.93782500	10.64798000	3.01257700
C	7.69333000	9.35223800	3.14098900
H	7.04501900	8.46698800	3.19486000
H	7.86394300	9.66700700	4.17969600
C	9.03032800	8.97596100	2.47052700
H	9.52760100	8.30420000	3.18646900
H	9.68189300	9.86389700	2.44753600
B	9.01923800	8.21196800	1.02228200
H	8.71823000	9.10986100	0.06712400
C	7.92691000	7.01763900	0.83298300
H	6.90079900	7.33889900	1.08080700
C	8.28409500	5.88935300	1.83914900
H	8.12705700	6.27774000	2.85629100
H	7.58726700	5.04154200	1.73503700
C	9.72985000	5.34962900	1.74019000
H	9.79079500	4.63365200	0.91386000
H	9.95466100	4.76290900	2.64297000

C	10.81931900	6.43323400	1.56107900
H	11.75562900	5.93949400	1.25233100
H	11.03337000	6.87897800	2.54251600
C	10.45904700	7.58078600	0.57877400
H	11.27805400	8.31846700	0.65396100
C	10.41377000	7.11784200	-0.89664900
H	11.36185500	6.63507600	-1.18875600
H	10.33241200	8.01804500	-1.52277500
C	9.25065000	6.16378400	-1.25429600
H	9.14867900	6.11496500	-2.34992100
H	9.51473700	5.14485600	-0.95309300
C	7.88378800	6.53969000	-0.63689900
H	7.43744800	7.35324600	-1.22912800
H	7.20117100	5.68210200	-0.75510700
C	11.00712200	12.23288300	-1.72212100
C	12.01390000	13.20317700	-1.75025400
H	12.73248500	13.22965700	-2.56196000
C	10.77620200	11.21186100	-2.74650400
C	11.46822600	10.84159300	-3.90829600
H	12.40815100	11.23152100	-4.26532400
C	10.70921800	9.83313300	-4.50210000
C	11.06782600	8.99504700	-5.72609400
C	12.39134000	9.52815900	-6.31745400
H	12.66663600	8.92842200	-7.19121500
H	13.21339100	9.46129800	-5.59675200
H	12.29744900	10.57020500	-6.64323600
C	11.29281500	7.52277100	-5.30017600
H	11.60232100	6.93011700	-6.16888300
H	10.38934000	7.06291400	-4.88919300
H	12.07738500	7.45084800	-4.53958200
C	9.99513800	9.06900600	-6.83738000
H	10.35774500	8.53921300	-7.72568100
H	9.79055000	10.10670800	-7.12247000
H	9.05081600	8.60585900	-6.54345500
N	9.66119400	10.47346700	-2.62272300
N	9.61542600	9.65804100	-3.69101900
C	8.34611000	8.93453500	-3.88771700
H	8.02276200	8.63282000	-2.89029100
H	8.56088000	8.02707500	-4.45365300
C	7.26729300	9.78419400	-4.58162200
H	6.38143800	9.13683300	-4.63698600
H	7.58319600	9.95557200	-5.61985900
C	6.89174400	11.12085400	-3.91008200
H	6.22095200	11.61946600	-4.62600100
H	7.78025500	11.77158700	-3.88580400
B	6.12674500	11.10899100	-2.46237500
H	7.02380500	10.80653000	-1.50686800
C	4.93154500	10.01732100	-2.27483400

H	5.25225600	8.99121000	-2.52337200
C	3.80415600	10.37618600	-3.28141500
H	4.19308600	10.21978400	-4.29844800
H	2.95579900	9.67985000	-3.17846900
C	3.26536300	11.82222700	-3.18152700
H	2.54887800	11.88293100	-2.35561900
H	2.67940200	12.04824800	-4.08449700
C	4.34960700	12.91078300	-3.00072300
H	3.85631300	13.84715800	-2.69145800
H	4.79613900	13.12540800	-3.98167700
C	5.49626500	12.54883800	-2.01799400
H	6.23456200	13.36740100	-2.09196700
C	5.03232900	12.50255900	-0.54291700
H	4.55003600	13.45071700	-0.25027000
H	5.93207200	12.42001400	0.08371500
C	4.07723000	11.33978200	-0.18694200
H	4.02761000	11.23686700	0.90855900
H	3.05868700	11.60484400	-0.48858200
C	4.45260600	9.97321100	-0.80530400
H	5.26546400	9.52578100	-0.21293800
H	3.59447000	9.29108100	-0.68826800

1 S=0

Fe	8.32216900	10.40822400	-0.71927500
N	9.64600400	11.73345200	-0.71993100
C	9.68449200	12.63497900	0.29368000
C	10.65650100	13.63583400	0.31491600
H	10.68100600	14.35504400	1.12635100
C	11.59273200	13.68123700	-0.72049300
H	12.36023100	14.44914100	-0.72071000
C	8.64332500	12.35063100	1.27052300
C	8.20716800	12.88996800	2.49272200
H	8.57320600	13.77848100	2.98173000
C	7.18112100	12.06237200	2.93831200
C	6.29233000	12.24983000	4.16336700
C	6.77208400	13.49997000	4.93232600
H	6.13216200	13.65727400	5.80689800
H	6.71703000	14.40143500	4.31283400
H	7.80210100	13.38412100	5.28755600
C	4.82849800	12.48916500	3.71992100
H	4.19762600	12.66026300	4.60012400
H	4.41418900	11.63553200	3.17480100
H	4.75402300	13.36655200	3.06913700
C	6.35578100	11.04695200	5.13300200
H	5.81024200	11.29133900	6.05171100
H	7.38963200	10.80828800	5.40443200
H	5.89828800	10.14833900	4.71269600
N	7.91142800	11.26147500	0.97598800
N	7.04037400	11.07648600	1.98290300
C	6.39302400	9.75552100	1.99305000
H	6.20754500	9.53005400	0.93876600
H	5.41609700	9.84774600	2.47126300
C	7.25635100	8.66108800	2.65383700
H	6.87590500	7.70003600	2.28179400
H	7.04524100	8.66995900	3.73034900
C	8.78003200	8.76355100	2.42837600
H	9.21657200	8.10930700	3.19569100
H	9.11429900	9.76857800	2.72851000
B	9.48065800	8.30967100	1.02421100
H	9.16376500	9.17938600	0.02750900
C	9.09451100	6.82516400	0.47184900
H	8.00735200	6.68174900	0.33482700
C	9.52634200	5.80947500	1.56733300
H	8.89138500	5.96517500	2.45037200
H	9.32161100	4.77883900	1.23446900
C	11.01127600	5.89519500	1.99767400
H	11.62150200	5.34055500	1.27767500
H	11.13632900	5.35756300	2.94879900
C	11.58201400	7.32807600	2.15315500
H	12.68239500	7.26327100	2.15923000

H	11.30775100	7.71009200	3.14543200
C	11.10912700	8.35951400	1.08921700
H	11.47550000	9.34348100	1.42873700
C	11.73237000	8.10375600	-0.30122900
H	12.83357900	8.09652400	-0.24280800
H	11.47090700	8.94988700	-0.95112400
C	11.27122100	6.80013900	-0.98696300
H	11.56744600	6.82698900	-2.04641400
H	11.81692600	5.95194400	-0.56161600
C	9.75139400	6.53512700	-0.89930600
H	9.25812600	7.16841300	-1.64693200
H	9.55748400	5.49533600	-1.21180500
C	10.54720300	11.77214800	-1.73382000
C	11.54754700	12.74467100	-1.75561000
H	12.26651800	12.76932200	-2.56725100
C	10.26316500	10.73054000	-2.71028800
C	10.80214200	10.29471800	-3.93276600
H	11.69013800	10.66134700	-4.42226900
C	9.97493300	9.26817700	-4.37794000
C	10.16235900	8.37948400	-5.60307400
C	11.41165600	8.86018300	-6.37281000
H	11.56891200	8.22036400	-7.24746500
H	12.31354900	8.80583300	-5.75387800
H	11.29479600	9.89010400	-6.72798600
C	10.40312600	6.91587600	-5.15965400
H	10.57428900	6.28508000	-6.03989800
H	9.55010700	6.50091300	-4.61406800
H	11.28090900	6.84216800	-4.50931200
C	8.95885800	8.44189700	-6.57199500
H	9.20313100	7.89646700	-7.49079800
H	8.71921200	9.47553400	-6.84337500
H	8.06085900	7.98373100	-6.15111200
N	9.17462000	9.99796600	-2.41518200
N	8.98958600	9.12687300	-3.42206800
C	7.66910800	8.47850000	-3.43144200
H	7.44427800	8.29304600	-2.37703400
H	7.76187000	7.50154900	-3.90950100
C	6.57360400	9.34079000	-4.09186200
H	5.61307100	8.96006500	-3.71877000
H	6.58167800	9.12897200	-5.16824400
C	6.67547600	10.86464600	-3.86744300
H	6.02076700	11.30052000	-4.63474000
H	7.68027300	11.19916600	-4.16808400
B	6.22179800	11.56551400	-2.46340400
H	7.08948900	11.24491100	-1.46590700
C	4.73640800	11.18104800	-1.91209300
H	4.59153000	10.09400100	-1.77587300
C	3.72182500	11.61499500	-3.00777200

H	3.87678400	10.98005000	-3.89094900
H	2.69073500	11.41184300	-2.67533900
C	3.81014300	13.09992000	-3.43765100
H	3.25611600	13.71086100	-2.71778300
H	3.27321700	13.22610100	-4.38902700
C	5.24400500	13.66842000	-3.59219900
H	5.18092000	14.76890200	-3.59823600
H	5.62626600	13.39360400	-4.58423000
C	6.27393400	13.19383100	-2.52754900
H	7.25864000	13.55912800	-2.86611000
C	6.01772600	13.81700900	-1.13713900
H	6.01147400	14.91823800	-1.19538400
H	6.86320100	13.55474800	-0.48676000
C	4.71331200	13.35687300	-0.45219100
H	4.74000500	13.65264800	0.60738700
H	3.86583600	13.90359000	-0.87767400
C	4.44674600	11.83737300	-0.54062700
H	5.07932900	11.34294500	0.20687300
H	3.40667300	11.64441700	-0.22847900

1 S=1

Fe	8.62326100	10.71963300	-0.75006800
N	10.08144900	12.06207500	-0.70746500
C	10.11242600	12.96589400	0.29114000
C	11.12310100	13.93360700	0.33339500
H	11.15110100	14.66946700	1.12925800
C	12.09409500	13.91337400	-0.66741800
H	12.89462800	14.64715400	-0.65228100
C	9.03486100	12.72915800	1.23620700
C	8.60067500	13.34127100	2.41864300
H	8.98299000	14.24641100	2.86216400
C	7.55244400	12.55990600	2.89415900
C	6.64124800	12.86263900	4.08244800
C	7.15878200	14.13991100	4.78075000
H	6.50703200	14.37903700	5.62737200
H	7.15431800	15.00198900	4.10525400
H	8.17487600	14.00551900	5.16854600
C	5.20440000	13.14234500	3.57739000
H	4.56444800	13.42136000	4.42269400
H	4.75576600	12.26951500	3.09453600
H	5.19456000	13.96314800	2.85295800
C	6.61434300	11.73357000	5.13807200
H	6.05034600	12.07414300	6.01395900
H	7.62520100	11.47067600	5.46766100
H	6.12863200	10.82733000	4.77060100
N	8.28476200	11.63318200	0.98022400
N	7.40866900	11.52362500	1.99816700
C	6.69986100	10.23808400	2.10527300
H	6.52573800	9.92315500	1.07652400
H	5.72858500	10.42154600	2.56779400
C	7.51382700	9.18243000	2.87045700
H	6.94628600	8.24637500	2.78035800
H	7.50749800	9.44067900	3.93677400
C	8.95704000	8.97321800	2.37632000
H	9.43016000	8.32529900	3.12756300
H	9.50791200	9.92342700	2.46494000
B	9.18050300	8.27625500	0.91417000
H	8.69894600	9.11211300	-0.03925100
C	8.37987500	6.86722100	0.70219500
H	7.29461100	6.96740200	0.87359700
C	8.89742300	5.87103600	1.77774900
H	8.56513500	6.22886700	2.76224500
H	8.42293200	4.88433700	1.64795300
C	10.43254700	5.67035400	1.81784300
H	10.71770600	4.93897600	1.05441900
H	10.70521500	5.20157000	2.77477500
C	11.27760700	6.95483900	1.63034100
H	12.31241100	6.65629600	1.39340400

H	11.33818100	7.48131000	2.59217800
C	10.74451100	7.95217200	0.56428100
H	11.38628900	8.84910200	0.63804100
C	10.90328900	7.41083300	-0.87633000
H	11.95118400	7.12612800	-1.07335000
H	10.68179800	8.23236200	-1.56913600
C	9.99668400	6.21238500	-1.23633700
H	9.99359200	6.07766700	-2.32871300
H	10.43837700	5.29143400	-0.84243800
C	8.54042300	6.33284900	-0.73731500
H	7.99272700	7.01337400	-1.40457000
H	8.05098200	5.35112200	-0.85086500
C	11.00486800	12.04026100	-1.68948800
C	12.05147500	12.96137000	-1.69337800
H	12.80306100	12.94437800	-2.47465900
C	10.69830000	11.00547500	-2.67330600
C	11.31390000	10.54479000	-3.84023900
H	12.26257300	10.85837700	-4.24494900
C	10.46416100	9.57242200	-4.36732800
C	10.72105900	8.68139300	-5.58120700
C	12.06463500	9.10019800	-6.21860800
H	12.26993000	8.46046300	-7.08302500
H	12.89860700	8.98824200	-5.51757200
H	12.04024900	10.13797300	-6.56964400
C	10.84648000	7.20505200	-5.13183200
H	11.09489700	6.57761600	-5.99571700
H	9.91913500	6.82012400	-4.69825200
H	11.63684600	7.08770400	-4.38342100
C	9.62875600	8.81073100	-6.66813100
H	9.93495800	8.24365100	-7.55457800
H	9.48616500	9.85473900	-6.96724100
H	8.66397100	8.41442800	-6.34472400
N	9.53565700	10.34651600	-2.47520800
N	9.39265800	9.49638000	-3.51163500
C	8.06235600	8.88622400	-3.67052100
H	7.71723500	8.66407200	-2.65997000
H	8.18707300	7.93862200	-4.19622200
C	7.07871800	9.81917200	-4.39244900
H	6.12391700	9.27757200	-4.42023600
H	7.40139700	9.92244200	-5.43674500
C	6.87497400	11.20374400	-3.74979600
H	6.25742600	11.76368800	-4.46605400
H	7.83268600	11.74781300	-3.75060200
B	6.12136300	11.28521100	-2.29758800
H	6.95628800	10.80870700	-1.32698500
C	4.75939700	10.38855700	-2.19098500
H	4.93147000	9.32552500	-2.43139700
C	3.76904900	10.92027000	-3.26560900

H	4.18237000	10.69225600	-4.25819800
H	2.81445700	10.37158000	-3.21115700
C	3.46357300	12.43609600	-3.19650400
H	2.69928900	12.61242400	-2.43259400
H	2.99718000	12.74891100	-4.14222100
C	4.68459500	13.34497900	-2.91369100
H	4.31445500	14.33852100	-2.61108000
H	5.22718700	13.51015300	-3.85417100
C	5.68820100	12.79960700	-1.86005900
H	6.54367700	13.49919300	-1.86219500
C	5.10370100	12.82097500	-0.42810500
H	4.74991200	13.83292800	-0.16617500
H	5.92202000	12.60156800	0.26748300
C	3.95404200	11.82180900	-0.16430500
H	3.79938600	11.72841200	0.92197400
H	3.01612400	12.24033300	-0.54329300
C	4.16414000	10.41457300	-0.76641800
H	4.84216700	9.84598900	-0.11534400
H	3.20320700	9.87479800	-0.73230300

1 S=3

Fe	8.69898900	10.78525800	-0.71820800
N	10.13489400	12.21804300	-0.71435000
C	10.17812800	13.16638000	0.29822000
C	11.14344800	14.15682400	0.30904500
H	11.15389100	14.88785900	1.11205300
C	12.11633100	14.19545000	-0.70891200
H	12.88383600	14.96138200	-0.70681500
C	9.16091300	12.92802100	1.28893800
C	8.73120900	13.58502900	2.45410500
H	9.09435400	14.52596500	2.83506000
C	7.71626800	12.80668500	2.99955900
C	6.83988700	13.14114000	4.20466200
C	7.30737900	14.48944100	4.79593100
H	6.67544600	14.74961000	5.65160000
H	7.22931500	15.30051300	4.06441400
H	8.34344700	14.43805400	5.14841400
C	5.36840500	13.30494900	3.74980500
H	4.74879400	13.60383200	4.60341200
H	4.94928700	12.37989500	3.34318200
H	5.28197400	14.07625200	2.97732400
C	6.93282700	12.08354300	5.32983000
H	6.37486000	12.43638200	6.20482700
H	7.97225600	11.92157900	5.63539000
H	6.50923500	11.11916700	5.04068300
N	8.42591000	11.80047300	1.11603900
N	7.55754600	11.72295600	2.16907400
C	6.91794600	10.42204900	2.39578600
H	6.62131800	10.04985700	1.41280200
H	6.00099000	10.59581500	2.96084000
C	7.81808400	9.40172900	3.11329700
H	7.19736400	8.50572200	3.25202600
H	8.03139000	9.78181600	4.12098100
C	9.12975800	9.01892000	2.40261800
H	9.66446200	8.35899900	3.10367700
H	9.77741200	9.90399400	2.32687900
B	9.05887100	8.21202700	0.99284200
H	8.75618900	9.20868800	0.00139000
C	7.89767400	7.10065700	0.80001900
H	6.89763000	7.46556600	1.08491600
C	8.24248700	5.95527700	1.79997800
H	8.13256300	6.34894900	2.82058700
H	7.50338500	5.14313400	1.71247800
C	9.65923000	5.35448200	1.65438400
H	9.66474100	4.63963300	0.82564700
H	9.88487100	4.75712900	2.54941000
C	10.78715100	6.39156200	1.44670500
H	11.69200000	5.86518900	1.10360700

H	11.05015100	6.82677700	2.42033700
C	10.44642400	7.55679200	0.46987600
H	11.29216400	8.26200200	0.52331000
C	10.33485600	7.09219800	-1.00106500
H	11.25251300	6.56689700	-1.31233800
H	10.28024900	7.99103700	-1.62884000
C	9.12173400	6.18911900	-1.32215400
H	8.98485600	6.14646700	-2.41339200
H	9.34796000	5.15924200	-1.02860900
C	7.79174400	6.62484400	-0.66637300
H	7.36157800	7.45499200	-1.24661200
H	7.06839100	5.79898500	-0.75802300
C	11.08609700	12.26210900	-1.72415200
C	12.07851800	13.22541200	-1.72964700
H	12.81177300	13.23655800	-2.53061600
C	10.84845400	11.24801100	-2.71826100
C	11.50802800	10.81980100	-3.88249900
H	12.45088800	11.18183500	-4.25973600
C	10.72904400	9.80799500	-4.43288800
C	11.06513300	8.93400400	-5.63927300
C	12.41595300	9.40040200	-6.22564300
H	12.67724400	8.77017100	-7.08222500
H	13.22487000	9.31887000	-5.49212100
H	12.36753100	10.43747500	-6.57557900
C	11.22489400	7.46106700	-5.18769000
H	11.52498100	6.84304900	-6.04202900
H	10.29792800	7.04266400	-4.78469900
H	11.99388000	7.37122800	-4.41329000
C	10.01083400	9.03182900	-6.76711600
H	10.36502700	8.47540400	-7.64254800
H	9.85171100	10.07233900	-7.07048500
H	9.04484800	8.60936400	-6.48172800
N	9.71871600	10.51516100	-2.55065800
N	9.64244900	9.64969000	-3.60611500
C	8.34115000	9.01276400	-3.83791700
H	7.96579800	8.71438700	-2.85667000
H	8.51498200	8.09691900	-4.40473700
C	7.32425600	9.91632500	-4.55600200
H	6.42756100	9.29746400	-4.69855200
H	7.70736500	10.13136000	-5.56217300
C	6.94183700	11.22694300	-3.84317600
H	6.28473000	11.76453600	-4.54466900
H	7.82784900	11.87283800	-3.76346600
B	6.13110500	11.15394300	-2.43573600
H	7.12477200	10.84615200	-1.44261100
C	5.01704600	9.99438400	-2.24876900
H	5.38078000	8.99439600	-2.53536500
C	3.87485000	10.34398100	-3.25070500

H	4.27090200	10.23602400	-4.27060300
H	3.06110100	9.60618500	-3.16721300
C	3.27637800	11.76147000	-3.10284900
H	2.55952700	11.76616400	-2.27583700
H	2.68164600	11.99061300	-3.99873000
C	4.31510700	12.88684300	-2.88967000
H	3.78962600	13.79182700	-2.54556200
H	4.75326600	13.15149900	-3.86153400
C	5.47724100	12.54137100	-1.91080100
H	6.18417500	13.38591100	-1.96029300
C	5.00874200	12.42689400	-0.44132300
H	4.48436600	13.34473100	-0.12901900
H	5.90588500	12.36901400	0.18857900
C	4.10258700	11.21464600	-0.12563100
H	4.05704100	11.07497500	0.96513300
H	3.07385700	11.44362700	-0.42104100
C	4.53733900	9.88553600	-0.78385600
H	5.36517600	9.45219300	-0.20268200
H	3.70982700	9.16358000	-0.69619400

1⁻ S=3/2

Fe	16.75353600	11.33465700	0.61330200
N	18.02429900	12.73454900	-0.08490600
N	17.07838000	10.77536700	-1.45951100
N	16.69462500	9.79941800	-2.32243200
N	17.06921600	12.66049000	2.30333200
N	16.67165600	12.77169700	3.59730400
C	18.55635200	12.63852400	-1.35659900
C	19.44683200	13.57871600	-1.85307600
C	19.81831600	14.67505800	-1.05421600
C	19.27596800	14.78122400	0.23966600
C	18.40088000	13.80861700	0.69873100
C	18.03504900	11.49460800	-2.08084200
C	18.27941500	10.94466000	-3.35760600
C	17.41654600	9.86402400	-3.49168000
C	17.36910500	8.84272300	-4.62444400
C	18.37741400	9.26157400	-5.71608100
C	17.79512200	7.45192200	-4.09263200
C	15.97683000	8.74609700	-5.29055900
C	15.46976200	9.07966300	-1.95815300
C	14.17462300	9.81855400	-2.33724500
C	13.96399900	11.21921500	-1.72367400
C	12.78377800	10.23526600	0.58841300
C	11.36255100	10.38805800	-0.01467300
C	10.74100900	11.79949700	0.10466700
C	11.71187200	12.96494100	-0.20193200
C	13.14352200	12.80375200	0.37119800
C	13.19068900	12.92896200	1.91179000
C	12.52616800	11.76896900	2.68998500
C	12.81317500	10.35649100	2.12881100
C	17.81384800	13.74849500	2.02468100
C	17.86605900	14.58295100	3.16199800
C	17.13450900	13.94219400	4.15413100
C	16.76404800	14.48209400	5.53231200
C	17.20968500	13.55435900	6.68564100
C	15.23446300	14.71141300	5.60656800
C	17.46074600	15.84469100	5.73712500
C	16.10361000	11.55036800	4.18008400
C	17.15230800	10.55324700	4.70714600
C	18.24732700	10.10290100	3.71658400
C	19.15269400	8.55057000	1.64415900
C	19.95932800	7.62173200	2.58809200
C	19.14234200	6.49372100	3.26311500
C	17.74269600	6.91726400	3.76843000
C	16.93685500	7.82726100	2.80450500
C	16.49093600	7.10916700	1.50967500
C	17.62697500	6.75059000	0.52335400
C	18.70389500	7.84556600	0.34305100

B	13.76478400	11.35650300	-0.09690500
H	14.92459600	11.24064000	0.49836800
B	17.84884000	9.14053200	2.44652600
H	17.14787500	9.83229600	1.57917900
H	19.01491500	11.27351700	-4.07529000
H	19.84028200	13.46881700	-2.86057100
H	20.50902200	15.42453400	-1.42847800
H	19.54647900	15.61154600	0.88715600
H	18.35269300	15.54283200	3.24007500
H	18.55141800	15.74664100	5.69713200
H	17.15339800	16.57105800	4.97737800
H	17.19294400	16.25101300	6.71943900
H	18.28271400	13.34135600	6.62679000
H	17.01065400	14.04195600	7.64850500
H	16.67738000	12.60092900	6.68267800
H	14.96443800	15.14557900	6.57799700
H	14.90704700	15.39844700	4.81904700
H	14.67201200	13.78086700	5.48706600
H	19.39930600	9.30211100	-5.32441000
H	18.35898500	8.53219400	-6.53440700
H	18.13017300	10.24409900	-6.13353700
H	18.79495300	7.49744200	-3.64807700
H	17.11180900	7.07339300	-3.32693500
H	17.81483000	6.72441800	-4.91445300
H	16.02484800	8.06189400	-6.14726000
H	15.21240000	8.36857300	-4.60825500
H	15.64735700	9.72544100	-5.65503600
H	15.51959400	11.09681600	3.37731700
H	15.40609400	11.83697400	4.97190000
H	17.61315800	10.98528700	5.60758900
H	16.57891800	9.68006800	5.05275300
H	18.79311600	10.99323500	3.36786900
H	18.98271600	9.55976800	4.33177900
H	19.84359200	9.35684000	1.34126500
H	18.30666600	8.61814800	-0.32801700
H	19.56483100	7.39919800	-0.18692600
H	18.10618200	5.81919100	0.84733100
H	17.18685100	6.51412800	-0.45896000
H	15.92479600	6.18808800	1.73609700
H	15.78028200	7.77588100	0.99990200
H	16.00888200	8.09571300	3.33857600
H	17.17426700	6.00382400	4.01850200
H	17.86737100	7.45757200	4.71869600
H	19.03319800	5.65797500	2.56269100
H	19.72088900	6.08562000	4.10711800
H	20.81004100	7.16125600	2.05507700
H	20.40733500	8.24345200	3.37599000
H	15.50409000	8.09098900	-2.42230800

H	15.52186100	8.93596000	-0.87705600
H	14.12088900	9.87087300	-3.43520900
H	13.35571000	9.15272400	-2.02710400
H	14.77021700	11.88185600	-2.07353300
H	13.05992200	11.61049700	-2.21769700
H	13.73241100	13.64776700	-0.02903100
H	13.10458500	9.20394100	0.35916600
H	11.41682900	10.12551700	-1.08167500
H	10.66124700	9.66250400	0.43470200
H	9.87233000	11.86744800	-0.56955800
H	10.32857800	11.92664900	1.11205800
H	11.79082300	13.07170200	-1.29311600
H	11.24910700	13.90319200	0.15268900
H	14.24760100	12.98664100	2.20247300
H	12.73250200	13.87637600	2.24932500
H	12.85004300	11.80921000	3.74254300
H	11.44256900	11.93004600	2.72412200
H	12.11011600	9.64740600	2.60136100
H	13.81457200	10.04273000	2.45750100

1⁻ S=1/2

Fe	16.84706500	11.41971600	0.57291100
N	17.98932000	12.77559900	-0.09260600
N	17.11147100	10.80236700	-1.28164700
N	16.69730700	9.76393500	-2.06159800
N	17.03066500	12.56515200	2.16973700
N	16.57808300	12.57464200	3.45555500
C	18.52024800	12.68267100	-1.36697800
C	19.36893700	13.65811100	-1.86730000
C	19.68110100	14.77801900	-1.07536300
C	19.13336400	14.87967100	0.21635800
C	18.30702600	13.87191500	0.68930600
C	18.01528200	11.49967400	-2.01420100
C	18.19513300	10.87362500	-3.26251600
C	17.35016900	9.77411800	-3.27702500
C	17.27198800	8.68422800	-4.34390900
C	18.22249000	9.05949200	-5.50191100
C	17.75239900	7.33535900	-3.75491400
C	15.85769200	8.51369200	-4.94536100
C	15.48766500	9.06580100	-1.61962200
C	14.18809200	9.75538500	-2.06130100
C	14.02262800	11.21463400	-1.59965600
C	12.72636000	10.53993400	0.73661900
C	11.35710700	10.80699100	0.05642100
C	10.90774100	12.28818700	0.02699700
C	12.02495000	13.31161900	-0.29549700
C	13.40079800	13.02591700	0.36207700
C	13.38348200	13.25727100	1.89095000
C	12.53766800	12.24854100	2.70167500
C	12.69202100	10.77469200	2.26289400
C	17.69728700	13.73203600	1.98628000
C	17.63856700	14.49995900	3.16489500
C	16.92558500	13.75017400	4.08835300
C	16.46209800	14.19209300	5.47470800
C	16.95309600	13.26524700	6.61089700
C	14.91677800	14.28391100	5.50931900
C	17.02584700	15.60218200	5.75610900
C	16.11394500	11.29106100	3.98723600
C	17.24809100	10.40545100	4.52442600
C	18.35545400	10.05905200	3.51187600
C	19.25828900	8.58629300	1.38601500
C	20.15656900	7.73376100	2.32053800
C	19.43726800	6.57813500	3.05852100
C	18.02612400	6.91877800	3.59514800
C	17.13366100	7.75082300	2.63629600
C	16.69995500	6.95909200	1.38298900
C	17.82680100	6.65011900	0.37071400
C	18.81761300	7.81121100	0.12307600

B	13.85791000	11.48792300	0.01110000
H	15.00799000	11.24836300	0.61953700
B	17.95210900	9.11752100	2.22845800
H	17.17828000	9.80201900	1.40338500
H	18.88182300	11.17184000	-4.03905100
H	19.77662500	13.55484300	-2.86947100
H	20.33713600	15.55473300	-1.45650500
H	19.35946900	15.73265100	0.85074500
H	18.03976400	15.49087400	3.30769600
H	18.12165400	15.60477900	5.74748900
H	16.67407100	16.33008800	5.01753400
H	16.69511700	15.93966100	6.74528900
H	18.04230600	13.15032000	6.58299600
H	16.68100700	13.69986200	7.58127300
H	16.50818800	12.26942600	6.55961500
H	14.58542200	14.66715400	6.48325900
H	14.54948400	14.95809700	4.72872500
H	14.44050200	13.31203200	5.35257700
H	19.25900500	9.14373100	-5.15904100
H	18.18514400	8.28206500	-6.27375300
H	17.93422500	10.00974700	-5.96525700
H	18.76420900	7.42727200	-3.34689800
H	17.10489200	6.98211700	-2.94758200
H	17.76217300	6.56623700	-4.53821800
H	15.89608900	7.79472100	-5.77368700
H	15.13667300	8.13757500	-4.21671200
H	15.47809900	9.46408400	-5.33653800
H	15.60985600	10.79826900	3.15465300
H	15.36330200	11.49045300	4.75618900
H	17.67649700	10.88729500	5.41485600
H	16.76601700	9.48389000	4.88224800
H	18.83774100	10.99200200	3.18185700
H	19.13393800	9.54420100	4.09584800
H	19.88698200	9.42359600	1.03579500
H	18.34848600	8.53048400	-0.55749100
H	19.69191700	7.40642700	-0.41909400
H	18.38060100	5.76503900	0.70483400
H	17.37434600	6.35100500	-0.58865200
H	16.21418800	6.00628400	1.66103000
H	15.92355300	7.54832300	0.87720200
H	16.20572700	7.96825100	3.19347700
H	17.52728300	5.97404100	3.87619700
H	18.13872600	7.48335800	4.53165800
H	19.36597600	5.71221700	2.39077500
H	20.06724900	6.23920900	3.89647300
H	21.00864800	7.30740000	1.76168600
H	20.60267200	8.40127200	3.07044500
H	15.53625300	8.03500400	-1.97984600

H	15.55030700	9.03825800	-0.53080400
H	14.10798900	9.68310000	-3.15537800
H	13.37013200	9.14274500	-1.65541500
H	14.84128500	11.81671300	-2.02272100
H	13.12209900	11.58383800	-2.11400900
H	14.10229600	13.76730500	-0.05891600
H	12.93076200	9.46351200	0.59928400
H	11.41152300	10.44020700	-0.97867700
H	10.55814000	10.21510000	0.53781700
H	10.09374100	12.40149400	-0.70665500
H	10.45565900	12.54246100	0.99218000
H	12.16501200	13.34285900	-1.38471400
H	11.66008000	14.31648500	-0.01727100
H	14.41960600	13.20559100	2.24359200
H	13.02995700	14.27628200	2.13343000
H	12.79679500	12.33456500	3.76950100
H	11.48045900	12.53280600	2.64656700
H	11.88747900	10.18564200	2.73917900
H	13.63002200	10.38051500	2.67592100

1⁻ S=5/2

Fe	16.80276100	11.36124400	0.60196900
N	18.04333500	12.83982600	-0.11155500
N	17.14094000	10.84686900	-1.48583600
N	16.79021300	9.85423300	-2.35036200
N	17.14731600	12.67733600	2.30612100
N	16.75129100	12.77134800	3.60594000
C	18.54745200	12.77359700	-1.39792600
C	19.38727100	13.75384700	-1.89830800
C	19.72995100	14.85770400	-1.08848500
C	19.20870500	14.92879300	0.22170200
C	18.38441300	13.91779600	0.68440300
C	18.05591700	11.61486600	-2.11782300
C	18.30489500	11.08065500	-3.40063800
C	17.49043800	9.96326800	-3.52978600
C	17.47454500	8.94858800	-4.66948100
C	18.45899200	9.41275000	-5.76465500
C	17.95571100	7.57140300	-4.14968700
C	16.08281200	8.80340200	-5.32827800
C	15.58565300	9.09925000	-1.99103600
C	14.26688300	9.80173800	-2.36238100
C	14.01083900	11.18724600	-1.73308500
C	12.86244900	10.15962500	0.58259900
C	11.43142200	10.29632800	-0.00129000
C	10.79120400	11.69765300	0.13802100
C	11.74080900	12.88004800	-0.17064400
C	13.18175200	12.73592000	0.38436900
C	13.24766500	12.84742100	1.92544500
C	12.61014300	11.67131600	2.70132400
C	12.91361300	10.26930000	2.12370000
C	17.82032900	13.81264300	2.01654700
C	17.82922300	14.65086500	3.15218500
C	17.14577500	13.97105300	4.15190400
C	16.75852100	14.49078700	5.53361400
C	17.30808700	13.61422400	6.68300800
C	15.21735700	14.59468000	5.64255400
C	17.34221200	15.90897200	5.71338000
C	16.28468500	11.52286000	4.21709800
C	17.41655900	10.59609400	4.69705500
C	18.40640900	10.09312700	3.62563500
C	19.02381100	8.33775200	1.59282100
C	19.76993200	7.36327100	2.54037300
C	18.86516200	6.37000700	3.30775000
C	17.55623500	6.97947800	3.86301900
C	16.80755700	7.93806700	2.89961200
C	16.20375300	7.22956900	1.66635500
C	17.23053900	6.68479100	0.64698400
C	18.42145400	7.62899200	0.35633000

B	13.81126100	11.30220400	-0.10743500
H	14.98593200	11.19660100	0.47218200
B	17.84652600	9.11523000	2.43098700
H	17.19420700	9.84880500	1.55855900
H	19.01566300	11.44587500	-4.12553900
H	19.76592100	13.67574100	-2.91456600
H	20.38256500	15.63864400	-1.46638300
H	19.46092800	15.76259400	0.87228600
H	18.25063600	15.64178800	3.22061500
H	18.43599800	15.90291300	5.64851600
H	16.95717200	16.60016900	4.95629000
H	17.06391500	16.29916900	6.69936800
H	18.39554000	13.50451600	6.60666300
H	17.07982900	14.08551400	7.64757200
H	16.87054400	12.61355900	6.69281400
H	14.81543200	15.23565700	4.85076000
H	14.72863600	13.61998800	5.55643800
H	14.93685800	15.02627000	6.61212200
H	19.48074200	9.49185000	-5.37854500
H	18.46450100	8.68774600	-6.58708900
H	18.17042500	10.38686900	-6.17515700
H	18.95737700	7.65078000	-3.71400200
H	17.29349600	7.16465300	-3.38004800
H	17.99453900	6.84974900	-4.97594100
H	16.15264600	8.13061800	-6.19249400
H	15.33852500	8.38836900	-4.64547500
H	15.71255400	9.77263000	-5.68041500
H	15.68472000	11.02374300	3.45352400
H	15.61554500	11.77776700	5.04282500
H	17.95683100	11.10798600	5.50744300
H	16.91441500	9.73658200	5.16482600
H	18.93712600	10.95933500	3.20189200
H	19.18272300	9.54789300	4.18666500
H	19.78552500	9.04004500	1.21063300
H	18.08528800	8.41112200	-0.33677900
H	19.19249600	7.05526000	-0.18886000
H	17.60979300	5.71747000	0.99671900
H	16.71170900	6.45920400	-0.29852300
H	15.53791300	6.40025500	1.96436700
H	15.55768400	7.95992500	1.15775300
H	15.95105400	8.33755100	3.47015900
H	16.90015200	6.15245300	4.18785000
H	17.79928700	7.54131300	4.77743100
H	18.61899900	5.52619800	2.65346400
H	19.43736700	5.92976000	4.13981500
H	20.53132500	6.78341100	1.98907000
H	20.32962300	7.96092200	3.27398100
H	15.64625800	8.11589000	-2.46389800

H	15.64207600	8.94537000	-0.91152800
H	14.21190300	9.86571000	-3.45945900
H	13.46954000	9.10627700	-2.06082900
H	14.79395500	11.88044000	-2.07600900
H	13.09273500	11.55525300	-2.21887600
H	13.75288600	13.59166700	-0.01649900
H	13.19611400	9.13597500	0.33952400
H	11.47657700	10.04296400	-1.07104100
H	10.74710300	9.55669700	0.45083900
H	9.91350100	11.75857500	-0.52495700
H	10.38957200	11.81016300	1.15144500
H	11.80591000	12.99638900	-1.26175000
H	11.26880900	13.80848200	0.19685300
H	14.30742700	12.91661900	2.20446600
H	12.78194500	13.78567900	2.27716900
H	12.94702100	11.70733700	3.74978000
H	11.52476300	11.81529800	2.75018500
H	12.23127300	9.54314300	2.60000000
H	13.92564500	9.97233900	2.43520100

(^{BBN}PDP^{tBu})ZnH$_2$

Zn	6.76348900	8.29746300	19.60320700
N	5.22352100	6.75910100	19.60343400
C	5.18957800	5.85415300	18.61007400
C	4.22087300	4.84551500	18.58218200
H	4.20485900	4.12119900	17.77538600
C	3.27269100	4.81035100	19.60375700
H	2.50425300	4.04273300	19.60388400
C	6.20562500	6.07500200	17.58157000
C	6.57543600	5.37666000	16.42132400
H	6.19209200	4.43085000	16.07279100
C	7.57025500	6.14255400	15.81700300
C	8.39890700	5.79445100	14.58400900
C	7.88849200	4.45401300	14.01105800
H	8.48237900	4.18471000	13.13138500
H	6.84023500	4.52126400	13.69898800
H	7.98367900	3.64046600	14.73818900
C	9.88302400	5.60737700	14.98604000
H	10.46772900	5.30334400	14.11000200
H	9.98576500	4.83172600	15.75221500
H	10.32962800	6.52451600	15.38097800
C	8.27945000	6.85664800	13.46623900
H	8.80807900	6.50392100	12.57321800
H	8.71748700	7.81682500	13.74746500
H	7.23234100	7.02805800	13.19378100
N	6.92989700	7.19349300	17.69322400
N	7.73925100	7.24269000	16.62454100
C	8.43557000	8.52285000	16.40730100
H	9.32572600	8.32314200	15.80964500
H	8.76870400	8.85316800	17.39231100
C	7.54582300	9.58669000	15.74231400
H	7.33241700	9.25882200	14.71539700
H	8.18112600	10.47803800	15.64968500
C	6.23419900	9.95691300	16.46582700
H	5.58666800	9.06804500	16.51270700
H	5.70772000	10.62816100	15.77038900
B	6.29199200	10.72390300	17.90926300
H	6.53595400	9.80038400	18.88197500
C	7.44354500	11.85750500	18.09831900
H	8.45083400	11.49063600	17.83763700
C	7.12955900	13.00609300	17.09904600
H	7.86947800	13.81693100	17.19828800
H	7.25484400	12.61456700	16.07881900
C	5.71397900	13.61662600	17.21615600
H	5.50980700	14.21858900	16.31861200
H	5.69682500	14.32998000	18.04666100
C	4.57541900	12.58617200	17.40046400
H	4.32984400	12.15736700	16.41886700

H	3.66713000	13.12164400	17.72243900
C	4.89028700	11.41731000	18.37369100
H	4.03842900	10.71859500	18.30347200
C	4.97216600	11.87103500	19.85024000
H	4.05141600	12.39874000	20.15127500
H	5.01389000	10.96576400	20.47191500
C	6.18327600	12.76633200	20.20076200
H	6.29812000	12.80459300	21.29542100
H	5.96636500	13.79845500	19.90709800
C	7.52437300	12.32836400	19.56824400
H	8.24839400	13.15183900	19.68070800
H	7.93902700	11.49249400	20.15189700
C	4.31869800	6.72629100	20.59694600
C	3.30903300	5.75866700	20.62516800
H	2.58483000	5.74356500	21.43208400
C	4.54079400	7.74228500	21.62523400
C	3.84305700	8.11302400	22.78554800
H	2.89691400	7.73072400	23.13432500
C	4.61009100	9.10716200	23.38953900
C	4.26308000	9.93643600	24.62241500
C	2.92224900	9.42749500	25.19575800
H	2.65373600	10.02183500	26.07536600
H	2.98850700	8.37923400	25.50802600
H	2.10864300	9.52335700	24.46878200
C	4.07741600	11.42065100	24.22010100
H	3.77417800	12.00585500	25.09608000
H	3.30169000	11.52400200	23.45408400
H	4.99491100	11.86624100	23.82484400
C	5.32538800	9.81613800	25.73999300
H	4.97337400	10.34530400	26.63297700
H	6.28595100	10.25314700	25.45848700
H	5.49579600	8.76891100	26.01262800
N	5.66001200	8.46538500	21.51323900
N	5.71024100	9.27488700	22.58176200
C	6.99117700	9.96987000	22.79871900
H	6.79249700	10.86034100	23.39624500
H	7.32174200	10.30248300	21.81361000
C	8.05412900	9.07907800	23.46372200
H	7.72608000	8.86604600	24.49065800
H	8.94612100	9.71349000	23.55629000
C	8.42304000	7.76706600	22.74024200
H	7.53356100	7.12035500	22.69353100
H	9.09389500	7.24000600	23.43561700
B	9.18983400	7.82406600	21.29666700
H	8.26631500	8.06848000	20.32409600
C	10.32425100	8.97474900	21.10720200
H	9.95818400	9.98235300	21.36779700
C	11.47281100	8.66007400	22.10628900

H	12.28416900	9.39938400	22.00676900
H	11.08158900	8.78579800	23.12657900
C	12.08227900	7.24402900	21.98926700
H	12.68429000	7.03955500	22.88671000
H	12.79543600	7.22622000	21.15860700
C	11.05094300	6.10620400	21.80537000
H	10.62216100	5.86112000	22.78710100
H	11.58567000	5.19745900	21.48344200
C	9.88211000	6.42177200	20.83233400
H	9.18277900	5.57044500	20.90284100
C	10.33557900	6.50307600	19.35567500
H	10.86253600	5.58188900	19.05467200
H	9.43019900	6.54537100	18.73418600
C	11.23170200	7.71346600	19.00477200
H	11.26982100	7.82810900	17.91009000
H	12.26372400	7.49583200	19.29825500
C	10.79486900	9.05499300	19.63716900
H	11.61886500	9.77837600	19.52442400
H	9.95919300	9.47019000	19.05362700

(^{BBN}PDP^{tBu})ZnH$_2^-$ S=1/2

Zn	16.77942800	11.33623000	0.61242200
N	18.00050200	12.79257000	-0.10064000
N	17.12642300	10.79586300	-1.49228300
N	16.78188000	9.80729900	-2.35677300
N	17.11357200	12.67698000	2.32665400
N	16.72432200	12.78564800	3.62295000
B	13.84123200	11.30173500	-0.11090800
H	15.03561500	11.23065100	0.45701900
B	17.85401800	9.15517400	2.42207800
H	17.23287300	9.90458900	1.52349100
C	18.51894400	12.71994900	-1.38076800
C	19.36004300	13.69730400	-1.88463100
C	19.69318600	14.81329100	-1.09011200
C	19.15856700	14.89261700	0.21213000
C	18.33584700	13.88285400	0.68111100
C	18.04396400	11.56107000	-2.10887100
C	18.30562900	11.03223100	-3.39372500
C	17.49006800	9.91849000	-3.53385900
C	17.47197300	8.91020500	-4.67853800
C	18.47493900	9.36610800	-5.76023500
C	17.92697900	7.52250100	-4.16343800
C	16.08491800	8.79123100	-5.35274000
C	15.56422800	9.06603000	-2.01453800
C	14.25959200	9.79832000	-2.37639900
C	14.03146400	11.18437600	-1.73629300
C	12.92322500	10.14658100	0.59538700
C	11.48377600	10.26084400	0.02489600
C	10.82261200	11.65195400	0.16651900
C	11.75010700	12.84757500	-0.15652700
C	13.19838500	12.72624300	0.38508100
C	13.27518000	12.84365000	1.92506800
C	12.66455700	11.65994800	2.71098800
C	12.98692500	10.26165800	2.13510600
C	17.77739800	13.80406800	2.01562700
C	17.79412800	14.66152700	3.13950400
C	17.12234600	13.99378000	4.15331300
C	16.75033000	14.52372500	5.53476600
C	17.33092100	13.66595100	6.68335500
C	15.21025000	14.61044500	5.66921400
C	17.31928200	15.95082300	5.68963500
C	16.28296100	11.53893200	4.25551600
C	17.43436800	10.62197200	4.70651400
C	18.41059200	10.13474700	3.61490900
C	19.02854100	8.36187200	1.59816800
C	19.74784500	7.37740600	2.55686100
C	18.81888300	6.39887500	3.31324200
C	17.51231400	7.02941900	3.84960500

C	16.78974500	7.99763600	2.87430800
C	16.19309900	7.29341400	1.63564900
C	17.22603700	6.73188900	0.63189200
C	18.43278400	7.65976700	0.35496500
H	19.02295500	11.39961400	-4.11106000
H	19.74520900	13.60373300	-2.89701600
H	20.34546200	15.59258800	-1.47167000
H	19.39866100	15.73267600	0.85910800
H	18.21369300	15.65434400	3.19025300
H	18.41198100	15.95714400	5.60878700
H	16.91501000	16.62796300	4.92987000
H	17.05059900	16.34937000	6.67501400
H	18.41840300	13.57109000	6.58954300
H	17.11192000	14.14248300	7.64754700
H	16.90835500	12.65900400	6.70933000
H	14.94076700	15.04846100	6.63907200
H	14.78766200	15.23865800	4.87792800
H	14.73158300	13.62933200	5.60099300
H	19.49284300	9.43062300	-5.36142900
H	18.48090900	8.64477200	-6.58596400
H	18.20384800	10.34572000	-6.16952800
H	18.92482000	7.58435800	-3.71629300
H	17.25065700	7.11978900	-3.40399300
H	17.96451800	6.80594200	-4.99424400
H	16.15148600	8.12016400	-6.21861200
H	15.32583300	8.38768600	-4.67921600
H	15.73586400	9.76820500	-5.70514300
H	15.65945500	11.03095300	3.51706000
H	15.64020900	11.79567600	5.10134600
H	17.98593000	11.13730600	5.50729000
H	16.95146000	9.75579900	5.18225900
H	18.92602900	11.00768400	3.18830300
H	19.20058500	9.59374000	4.16078200
H	19.80377100	9.05377700	1.22619900
H	18.11657700	8.44480300	-0.34355300
H	19.20348900	7.07454800	-0.17811100
H	17.58689800	5.76044800	0.98939200
H	16.71707800	6.51058100	-0.31984500
H	15.51218200	6.47468500	1.92820400
H	15.56338000	8.03115200	1.11788300
H	15.93177200	8.40871800	3.43405000
H	16.83835100	6.21389200	4.16610900
H	17.75178800	7.58854900	4.76649200
H	18.56923400	5.55736500	2.65753000
H	19.37289500	5.95215700	4.15407400
H	20.50724100	6.78621800	2.01517400
H	20.30743100	7.96711700	3.29694500
H	15.60881500	8.09180700	-2.50750900

H	15.61292700	8.88741100	-0.93864800
H	14.20473700	9.87379500	-3.47292300
H	13.44840200	9.11635900	-2.08077800
H	14.82164100	11.86727700	-2.08131600
H	13.11503400	11.56870300	-2.21263600
H	13.75424900	13.58761500	-0.02348500
H	13.26787700	9.12698500	0.35137300
H	11.52268600	10.00540300	-1.04445800
H	10.81654000	9.51136200	0.48590200
H	9.93715900	11.69581100	-0.48741600
H	10.42983400	11.76163700	1.18361400
H	11.80167900	12.96142200	-1.24857300
H	11.26882800	13.77014900	0.21334200
H	14.33519900	12.93243600	2.19496100
H	12.79566700	13.77494500	2.27645500
H	13.01070700	11.70546300	3.75596800
H	11.57740300	11.78482200	2.77012600
H	12.32215500	9.52473300	2.61930800
H	14.00682100	9.98252900	2.43667700

(^{Me}PDP^{tBu})FeH$_2$ S= 3/2

Fe	8.52906400	10.61564600	-0.71900400
N	10.04694600	12.13257700	-0.71936700
C	10.10692900	13.03904700	0.28664300
C	11.07843800	14.04296500	0.31274500
H	11.10239000	14.75812200	1.12843900
C	12.01422100	14.09956600	-0.72009300
H	12.78228000	14.86751800	-0.72038200
C	9.08596200	12.85360200	1.31399600
C	8.77115300	13.54446500	2.50210400
H	9.26582100	14.41236700	2.90942000
C	7.68221000	12.88014100	3.05440900
C	6.92707100	13.19618900	4.33888600
C	7.66452200	14.32993900	5.08327000
H	7.13819000	14.56032100	6.01598500
H	7.70043100	15.24743700	4.48598300
H	8.69061400	14.04225700	5.33683500
C	5.49348500	13.69004900	4.02419200
H	4.98120100	13.96408000	4.95416100
H	4.88471400	12.93002600	3.52552400
H	5.52076200	14.57274300	3.37633300
C	6.87840100	11.96657700	5.27678500
H	6.39484200	12.24120800	6.22159000
H	7.88866900	11.60892100	5.50443900
H	6.31412300	11.13296600	4.85027400
N	8.24075600	11.82900300	1.14443500
N	7.39397500	11.85088400	2.18800000
C	6.39025400	10.79340000	2.21821300
H	6.19905100	10.51517000	1.17880700
H	5.47170500	11.15266100	2.68031100
H	8.84610000	9.05454800	-0.15160000
C	10.95305500	12.19205300	-1.72572600
C	11.95710200	13.16339600	-1.75256500
H	12.67196000	13.18694000	-2.56853300
C	10.76709700	11.17071900	-2.75263400
C	11.45759800	10.85530800	-3.94079000
H	12.32551400	11.34962200	-4.34850800
C	10.79288600	9.76630700	-4.49251500
C	11.10836500	9.01063900	-5.77681900
C	12.24191400	9.74767000	-6.52192500
H	12.47185200	9.22097100	-7.45454200
H	13.15965900	9.78367300	-5.92502200
H	11.95426500	10.77370900	-6.77574200
C	11.60219100	7.57712100	-5.46175700
H	11.87576300	7.06442700	-6.39163600
H	10.84232100	6.96863400	-4.96250800
H	12.48516700	7.60456200	-4.81429100
C	9.87837500	8.96176400	-6.71421100

H	10.15252900	8.47768800	-7.65888900
H	9.52085000	9.97200000	-6.94221800
H	9.04480700	8.39788700	-6.28709000
N	9.74233400	10.32583000	-2.58250000
N	9.76378400	9.47864200	-3.62574700
C	8.70609000	8.47512000	-3.65539900
H	8.42787100	8.28454100	-2.61587300
H	9.06515200	7.55626400	-4.11704400
H	6.96843900	10.93486400	-1.28643200
H	7.83197900	8.84852400	-4.19793500
H	6.76377600	9.91923800	2.76056700

(^{Me}PDP^{tBu})FeH$_2$ S= 0

Fe	8.97953800	11.04508300	-0.71077300
N	10.30769500	12.33806500	-0.69562500
C	10.33245100	13.27806800	0.29917700
C	11.27164500	14.30823100	0.29179300
H	11.28265600	15.03888300	1.09460500
C	12.18710700	14.38353500	-0.76307400
H	12.92880400	15.17621300	-0.78370700
C	9.27400900	13.00762400	1.24804700
C	8.81747800	13.56252500	2.45801400
H	9.22517700	14.41583100	2.97667900
C	7.73637000	12.79019800	2.85759900
C	6.86415900	12.95447400	4.09545400
C	7.45975400	14.07322900	4.97712800
H	6.84645100	14.19833800	5.87620200
H	7.47942300	15.03349800	4.45066100
H	8.48009500	13.83292500	5.29483500
C	5.42743100	13.37791600	3.70177200
H	4.82628400	13.54464400	4.60375500
H	4.91469500	12.62132800	3.10037400
H	5.44265100	14.30875600	3.12465600
C	6.82793800	11.65827900	4.94004700
H	6.26195100	11.83379900	5.86256200
H	7.84058200	11.34558600	5.21796100
H	6.34963200	10.82668200	4.41615400
N	8.49991600	11.94869900	0.90767700
N	7.56995600	11.82355300	1.88755200
C	6.66364000	10.69036000	1.79740500
H	6.61747300	10.42075000	0.73749400
H	5.67259600	10.96182300	2.16129600
H	9.92950200	10.13826000	0.05475000
C	11.17686200	12.43467000	-1.74872600
C	12.13426300	13.44664000	-1.80034200
H	12.82193400	13.50145000	-2.63854700
C	10.90272300	11.38086800	-2.70169800
C	11.44764200	10.93565900	-3.92038000
H	12.28738000	11.35749800	-4.44976300
C	10.69143600	9.83887400	-4.30788900
C	10.84527500	8.97864600	-5.55543800
C	12.11574800	9.42383800	-6.31134500
H	12.24425900	8.80842800	-7.20849900
H	13.01171400	9.30921500	-5.69176100
H	12.04866600	10.46931400	-6.63095300
C	11.01122400	7.48267900	-5.19581400
H	11.20181300	6.90239700	-6.10639100
H	10.12153400	7.06196700	-4.72015300
H	11.85888200	7.33660900	-4.51713900
C	9.63832600	9.17047700	-6.50673700

H	9.78864700	8.58785500	-7.42362700
H	9.52885900	10.22401700	-6.78571000
H	8.69400400	8.84388900	-6.06109900
N	9.84730000	10.60291200	-2.35928300
N	9.72507300	9.67112100	-3.33777600
C	8.70640100	8.65018700	-3.15441900
H	7.94982600	9.08917900	-2.49630600
H	9.12481200	7.75968800	-2.67317300
H	7.46892600	10.57505300	-1.14029500
H	8.26145400	8.37620900	-4.11107800
H	7.04493400	9.83601400	2.36691600

H-BBN(CH_3)$^-$

C	8.41526900	7.78697000	22.72002700
H	7.61810900	7.02353900	22.76244300
H	9.08560500	7.56645600	23.57048800
B	9.14063200	7.83219900	21.23829500
H	8.26387100	8.08758400	20.39056400
C	10.34600800	8.96242400	21.11495900
H	9.97621700	9.96850700	21.38958100
C	11.49648000	8.64538100	22.09956600
H	12.33062800	9.36971000	22.01138100
H	11.10261900	8.77029500	23.11938100
C	12.08980500	7.22086600	21.98606300
H	12.69433200	7.00775200	22.88442400
H	12.80344100	7.19235700	21.15318000
C	11.04424700	6.09572100	21.79924800
H	10.59087300	5.88540200	22.77955300
H	11.58582800	5.17097800	21.51676500
C	9.89476300	6.41847700	20.81532500
H	9.19484600	5.56323300	20.87047100
C	10.34698300	6.50930200	19.33978400
H	10.87363400	5.59287300	19.00481800
H	9.43453500	6.57743300	18.72893600
C	11.24279500	7.72335100	18.99739500
H	11.28224900	7.84548300	17.90129600
H	12.27697200	7.50505300	19.29272000
C	10.79944100	9.05893100	19.64019800
H	11.61905400	9.79241800	19.49999800
H	9.94348700	9.44442700	19.06657400
H	7.92711100	8.74686400	22.96586500

BBN(CH_3)

C	7.78218300	7.82034800	21.80863900
H	7.12795500	8.00232100	20.93756600
H	7.40306400	6.90647900	22.28253100
B	9.24825200	7.69856900	21.25221300
C	10.25064100	8.91010800	21.09821500
H	9.80145100	9.87524000	21.37354800
C	11.40301100	8.63819400	22.11647500
H	12.16900400	9.42306700	22.02963600
H	10.98623500	8.74035800	23.12987200
C	12.07244900	7.25190800	21.99841600
H	12.67433800	7.07110900	22.89937000
H	12.78595500	7.25627400	21.16953400
C	11.07668600	6.08522100	21.82190700
H	10.61809200	5.86571300	22.79794000
H	11.62610700	5.17470600	21.54014200
C	9.92366600	6.34337900	20.80098500
H	9.24168600	5.48316200	20.86430900
C	10.38674300	6.46290100	19.32128900
H	10.93701100	5.55753500	19.02417100
H	9.48429300	6.48121000	18.69177800
C	11.23870300	7.70703100	18.99250200
H	11.28485300	7.82722300	17.90157700
H	12.27274900	7.53967600	19.30799200
C	10.71030100	9.01589100	19.61638500
H	11.47430900	9.80106800	19.51372500
H	9.84864300	9.36166500	19.02557500
H	7.62557500	8.67030000	22.48426400

2-NH_2

Fe	4.63141900	4.63142800	0.00001400
N	3.09609700	3.09611100	0.00002000
N	4.96423100	3.34470900	1.93704200
N	5.82586000	3.19141500	2.95998000
N	6.21760100	3.79343500	-1.03601100
H	6.06158500	2.78218300	-0.97085100
H	6.05267600	3.99496700	-2.02334200
B	7.84238800	3.94738000	-0.75665900
C	1.13967300	1.13970000	0.00002500
H	0.37161600	0.37164900	0.00002600
C	2.07306000	1.19220700	1.03254500
H	2.04640800	0.47655200	1.84645400
C	3.05218100	2.19254400	1.00125200
C	4.09316000	2.32721000	2.02407000
C	4.39884300	1.51860800	3.13162200
H	3.88667400	0.62774500	3.45843200
C	5.52011300	2.09107800	3.72311100
C	6.27590500	1.60709300	4.95713200
C	5.50250300	0.42031600	5.57387600
H	4.48871300	0.70994600	5.87156600
H	6.02754600	0.06940400	6.46848500
H	5.43335800	-0.42332400	4.87858800
C	6.36679400	2.71365600	6.03568500
H	6.95632500	3.57552400	5.71457700
H	6.84184000	2.30789700	6.93615100
H	5.36888200	3.07142700	6.31302000
C	7.68719700	1.09575600	4.57417000
H	7.61915500	0.28480100	3.84113600
H	8.19205300	0.70731900	5.46629900
H	8.32450000	1.87414000	4.14638900
C	6.90158100	4.19426200	3.12362400
H	7.70305800	3.70955100	3.67919900
H	6.50671700	5.01275400	3.73799700
C	7.42746000	4.70888900	1.78202000
H	8.18073100	5.47099200	2.01794200
H	6.61762700	5.26295600	1.29500800
C	8.01093900	3.63177100	0.85023100
H	7.52021800	2.66494300	1.05874200
H	9.06189900	3.47558700	1.12772200
C	8.65213700	2.86707500	-1.70141100
H	8.35451600	1.82667700	-1.46711300
C	10.17041500	2.96031500	-1.40266900
H	10.34064600	2.57454700	-0.38831600
H	10.74262000	2.29391100	-2.06986100
C	10.77749800	4.38126500	-1.49631300
H	11.74951300	4.38874600	-0.98132000
H	11.01137100	4.60668900	-2.54231500

C	9.89466100	5.51305500	-0.91890300
H	10.30620000	6.47895400	-1.25558900
H	9.99994800	5.51369200	0.17561000
C	8.38356800	5.41261600	-1.25117300
H	7.89470000	6.24426100	-0.71325200
C	8.08148800	5.63892900	-2.75521900
H	8.49831500	6.59969000	-3.09988600
H	6.99073700	5.74629200	-2.87131500
C	8.56284600	4.52459500	-3.71388700
H	8.06713500	4.64767500	-4.68900900
H	9.62901000	4.66223000	-3.91879400
C	8.32752000	3.08563500	-3.20040400
H	7.27148300	2.81894700	-3.37375900
H	8.90205400	2.39041900	-3.83453800
N	3.34472600	4.96422000	-1.93701100
N	3.19145400	5.82583800	-2.95996200
N	3.79343400	6.21762200	1.03603000
H	2.78218200	6.06160600	0.97087600
H	3.99497100	6.05270700	2.02336200
B	3.94737700	7.84240600	0.75665900
C	1.19218500	2.07308300	-1.03250000
H	0.47653000	2.04643100	-1.84640900
C	2.19252900	3.05219600	-1.00121100
C	2.32721300	4.09316300	-2.02403800
C	1.51862500	4.39884500	-3.13160000
H	0.62775700	3.88668600	-3.45841200
C	2.09111900	5.52009700	-3.72309900
C	1.60715700	6.27588100	-4.95713400
C	0.42036700	5.50249500	-5.57387400
H	0.70997700	4.48869400	-5.87154700
H	0.06947200	6.02753200	-6.46849200
H	-0.42327900	5.43337800	-4.87858900
C	2.71372700	6.36673000	-6.03568400
H	3.57560600	6.95624900	-5.71458000
H	2.30798300	6.84177100	-6.93615800
H	3.07147900	5.36880800	-6.31300100
C	1.09584800	7.68719000	-4.57419600
H	0.28488800	7.61917500	-3.84116600
H	0.70742700	8.19204100	-5.46633400
H	1.87424400	8.32448200	-4.14642000
C	4.19431700	6.90154300	-3.12360700
H	3.70962600	7.70301700	-3.67920100
H	5.01281500	6.50666000	-3.73796100
C	4.70892800	7.42743400	-1.78200200
H	5.47104100	8.18069600	-2.01792100
H	5.26297900	6.61760200	-1.29497000
C	3.63179700	8.01093400	-0.85023900
H	2.66497100	7.52021400	-1.05876000

H	3.47562300	9.06188900	-1.12774900
C	2.86705100	8.65216600	1.70137700
H	1.82665800	8.35453500	1.46706700
C	2.96028900	10.17043900	1.40261000
H	2.57453700	10.34064900	0.38824700
H	2.29387000	10.74265200	2.06977900
C	4.38123300	10.77753100	1.49626800
H	4.38871800	11.74953700	0.98125700
H	4.60663800	11.01142500	2.54226900
C	5.51303800	9.89468900	0.91889300
H	6.47893000	10.30624000	1.25558900
H	5.51369400	9.99995600	-0.17562100
C	5.41260100	8.38360200	1.25119000
H	6.24425900	7.89472800	0.71329400
C	5.63888900	8.08155200	2.75524700
H	6.59964200	8.49839100	3.09992300
H	5.74625400	6.99080500	2.87136500
C	4.52453500	8.56292300	3.71388500
H	4.64760100	8.06723300	4.68901900
H	4.66216100	9.62909200	3.91877300
C	3.08558600	8.32757800	3.20038000
H	2.81890100	7.27154300	3.37375100
H	2.39035500	8.90212000	3.83449100

2-NHMe

Fe	3.64652600	3.64864700	-0.00162200
N	5.19660900	5.20342100	-0.00548700
N	3.30520500	4.98788400	1.91680800
N	2.43120600	5.16631700	2.92605200
C	5.22636500	6.12439100	0.97866900
C	6.20311700	7.12716200	1.00839800
C	7.15169100	7.16528200	-0.01029000
C	4.17482400	6.00766600	1.99158600
C	3.85684500	6.84138200	3.07666000
C	2.72834700	6.28334200	3.66738800
C	1.95704300	6.79662400	4.87984500
C	2.72459200	7.99597000	5.47941000
C	0.55212900	7.30134500	4.46595500
C	1.84883000	5.71574000	5.98254000
C	1.35665400	4.16669700	3.10575500
C	0.86448300	3.59769700	1.77516300
C	0.27599700	4.62476500	0.79284700
B	0.43833900	4.21664900	-0.79770600
N	2.05496400	4.44810200	-1.15648500
H	2.18266500	3.99907900	-2.06465800
C	2.38748400	5.87919900	-1.38040700
C	0.01617500	2.66401600	-1.14717900
C	-1.45422200	2.43839000	-0.70828100
C	-2.48487600	3.41603700	-1.31814800
C	-2.02012800	4.88963600	-1.39717200
C	-0.53543700	5.11227100	-1.79224000
C	-0.27337300	4.78411200	-3.28454100
C	-0.41124100	3.29251900	-3.65691800
C	0.24103500	2.32610600	-2.64417200
N	4.98270400	3.30676800	-1.92272900
N	5.16168500	2.43091700	-2.93026700
C	6.11504500	5.23394800	-0.99196200
C	7.11435600	6.21409500	-1.02655100
C	5.99945300	4.17953900	-2.00200000
C	6.83178400	3.86159300	-3.08815800
C	6.27610400	2.72981900	-3.67481400
C	6.78923900	1.95712700	-4.88643200
C	7.98458400	2.72722600	-5.49067300
C	7.29961500	0.55500800	-4.47002600
C	5.70622500	1.84234600	-5.98639100
C	4.16524600	1.35259000	-3.10505000
C	3.60082300	0.86191300	-1.77196900
C	4.63200600	0.27923900	-0.79051300
B	4.22634200	0.44361000	0.80044500
N	4.45277100	2.06185900	1.15514000
C	5.88309800	2.39985300	1.37587000
C	2.67584200	0.01668700	1.15362000

C	2.45472300	-1.45547100	0.71835700
C	3.43710400	-2.48129300	1.32874800
C	4.90916000	-2.01112800	1.40408700
C	5.12718100	-0.52478700	1.79553800
C	4.80067000	-0.26069200	3.28785700
C	3.31023300	-0.40301600	3.66316200
C	2.33975000	0.24363000	2.65070300
H	0.61381400	1.92952500	-0.58091700
H	1.32565500	2.31062900	-2.83934100
H	-0.09688300	1.30059400	-2.86684500
H	-1.47080200	3.04317600	-3.76707200
H	0.02710800	3.12398500	-4.65246900
H	-0.94033500	5.37066900	-3.93785000
H	0.74553100	5.11127000	-3.54898700
H	-0.36969600	6.19770400	-1.67768100
H	-2.68659400	5.42615700	-2.09319900
H	-2.18394400	5.35995500	-0.41837700
H	-2.76188500	3.06806600	-2.31885400
H	-3.41573900	3.36549300	-0.73410900
H	-1.77392500	1.40851900	-0.93753900
H	-1.50007100	2.52222000	0.38650200
H	-0.77631300	4.78234200	1.06375800
H	0.75361700	5.60370500	0.96143600
H	1.69144900	3.04142000	1.32205700
H	0.12402300	2.82820100	2.02524000
H	1.74068500	3.37479100	3.76096400
H	0.54040000	4.66807800	3.62405300
H	2.84184700	5.36070900	6.28025400
H	1.36471100	6.14426000	6.86748000
H	1.25936200	4.84911500	5.67451800
H	0.63170500	8.09514100	3.71549500
H	-0.08078900	6.51418600	4.04776400
H	0.03588800	7.71101100	5.34191400
H	3.73379800	7.71158400	5.79700500
H	2.80456700	8.82334700	4.76601000
H	2.18844500	8.36812200	6.35869400
H	4.36527100	7.73979600	3.38817700
H	6.21604900	7.85572900	1.81107000
H	7.91840100	7.93466700	-0.01218000
H	7.84088200	6.22758900	-1.83106200
H	7.72786500	4.37213400	-3.40293000
H	8.35661200	2.19015700	-6.36945400
H	7.69597500	3.73464900	-5.81015200
H	8.81326000	2.81187600	-4.77931900
H	8.09501600	0.63924600	-3.72178400
H	6.51560200	-0.07934300	-4.04810800
H	7.70879100	0.03773800	-5.34560800
H	6.13439200	1.35740100	-6.87104800

H	4.84235000	1.25067700	-5.67487500
H	5.34708100	2.83334800	-6.28587900
H	4.66822800	0.53668500	-3.62236000
H	3.37063700	1.73230300	-3.75949200
H	3.04291300	1.68820600	-1.31965300
H	2.83318700	0.11831200	-2.01842100
H	4.79283800	-0.77308200	-1.05948800
H	5.60885900	0.76006300	-0.96208500
H	1.93823500	0.61045500	0.58734000
H	2.32077100	1.32860900	2.84352500
H	1.31582800	-0.09741800	2.87591200
H	3.06482500	-1.46320400	3.77607800
H	3.14190500	0.03691600	4.65805200
H	5.39072100	-0.92418200	3.94155400
H	5.12469000	0.75991800	3.54957100
H	6.21181600	-0.35542400	1.67873800
H	5.44932000	-2.67415600	2.10058100
H	5.37829700	-2.17537400	0.42479500
H	3.09191000	-2.75732600	2.33068300
H	3.38881800	-3.41361800	0.74685400
H	1.42640300	-1.77834300	0.95012100
H	2.53681500	-1.50343500	-0.37646400
H	6.42744300	2.32192500	0.43082800
H	6.00266800	3.42082300	1.75672400
H	6.36053200	1.72046600	2.08748600
H	3.40714600	6.00163800	-1.76384000
H	1.70477500	6.35305100	-2.09123700
H	2.30988400	6.42488900	-0.43611500
H	4.00484800	2.19004600	2.06378800

2-NHPh

Fe	5.57854700	7.73066400	5.70169500
N	5.57761200	9.87407300	5.70254100
N	3.65985200	8.36233400	6.81868500
N	2.55413600	7.84263900	7.39106200
C	4.55665100	10.53981600	6.27297000
C	4.52536900	11.93773400	6.29391300
C	5.57642000	12.63546100	5.70366400
C	3.50837400	9.69552400	6.85134800
C	2.28931600	10.03134800	7.46012600
C	1.68769200	8.82463100	7.80324500
C	0.33836400	8.61214600	8.48335500
C	-0.24147000	9.99162100	8.86770100
C	0.48277200	7.78914500	9.78655000
C	-0.66558000	7.93661400	7.51622800
C	2.47621300	6.37624100	7.55795500
C	3.12888000	5.62234000	6.39989900
C	2.50318000	5.88922000	5.02103100
B	3.53830600	5.74572400	3.74895500
C	2.77994800	5.72763000	2.28826600
C	1.76693200	4.55051200	2.27076700
C	2.35095700	3.16355600	2.63617600
C	3.39480700	3.16411100	3.77937300
C	4.40256300	4.34590700	3.76804400
C	5.39928000	4.24830400	2.58483500
C	4.79220200	4.47288900	1.18333200
C	3.78196300	5.63850400	1.10851200
C	4.33127500	8.25645000	3.14676900
N	4.65186100	7.04868100	3.85684300
C	3.14171200	8.96353600	3.39322700
C	2.86084500	10.15020000	2.71538100
C	3.75253500	10.66802800	1.77419100
C	4.93393600	9.97151800	1.51368800
C	5.21650400	8.78399800	2.18770600
N	7.49671800	8.36490300	4.58522400
N	8.60287600	7.84662700	4.01241200
C	6.59799700	10.54115800	5.13265200
C	6.62807000	11.93912100	5.11284800
C	7.64700500	9.69825200	4.55357800
C	8.86572900	10.03562700	3.94498400
C	9.46841200	8.82970700	3.60093700
C	10.81785000	8.61900400	2.92051100
C	11.39642900	9.99941900	2.53753500
C	10.67399800	7.79719700	1.61656000
C	11.82248200	7.94333500	3.88676000
C	8.03000400	5.62502000	5.00170500
C	8.65551200	5.89122400	6.38078900
B	7.62052400	5.74590100	7.65277200

C	8.37895200	5.72724800	9.11342000
C	9.39291700	4.55093000	9.12993800
C	8.80998300	3.16379800	8.76345700
C	7.76609400	3.16442400	7.62029500
C	6.75739200	4.34540100	7.63260000
C	5.76079600	4.24606400	8.81576700
C	6.36774700	4.47001700	10.21742700
C	7.37706200	5.63637600	10.29314200
C	6.82557000	8.25550000	8.25695100
N	6.50591600	7.04801400	7.54596900
C	8.01455800	8.96372100	8.01098500
C	8.29451000	10.15008900	8.68972700
C	7.40245000	10.66648400	9.63135300
C	6.22161700	9.96883200	9.89137500
C	5.93996500	8.78160500	9.21645700
C	8.68202000	6.38043400	3.84427200
H	5.68250200	6.67218100	8.01577900
H	5.47561400	6.67388200	3.38680300
H	6.13521600	8.24714400	1.96293400
H	5.63861500	10.34593100	0.77507600
H	3.52618900	11.59004300	1.24595300
H	1.92792500	10.66915600	2.92257700
H	2.43123600	8.57638100	4.11166300
H	8.72530900	8.57768000	7.29222300
H	9.22700600	10.66994700	8.48288700
H	7.62808400	11.58827400	10.16028900
H	5.51667200	10.34211600	10.63030400
H	5.02169000	8.24384800	9.44085600
H	5.00671300	4.23378800	4.68511300
H	6.20327100	4.98966600	2.73303700
H	5.91860900	3.27622100	2.59616600
H	5.60428300	4.64916700	0.46159300
H	4.31128900	3.54884000	0.84849300
H	3.24058600	5.56675200	0.15090400
H	4.34049200	6.58231300	1.05143500
H	2.18503400	6.63999400	2.11796900
H	0.95115400	4.78518000	2.96729600
H	1.29026900	4.47334900	1.27964100
H	1.52700700	2.48735000	2.90772800
H	2.79923800	2.71571600	1.74318200
H	2.86172400	3.18044000	4.73984900
H	3.93165300	2.20172900	3.75951300
H	1.65485800	5.20267400	4.90562300
H	2.04446300	6.88816800	5.02328900
H	4.19986600	5.85024100	6.40246400
H	3.07728900	4.55693700	6.65475700
H	2.94393600	6.12103300	8.51744800
H	1.42000700	6.11781100	7.62062900

H	1.19042800	8.26671800	10.47352900
H	-0.48843300	7.73010600	10.29088700
H	0.82212500	6.76572000	9.61031000
H	-0.35339800	6.93688400	7.20266800
H	-1.64097000	7.84001000	8.00697700
H	-0.79804000	8.54048200	6.61209400
H	0.41750900	10.52841800	9.55888600
H	-0.40753100	10.62073800	7.98653700
H	-1.20800400	9.85462700	9.36383500
H	1.88674700	11.01804500	7.62437000
H	3.69979500	12.46183100	6.76202600
H	5.57595300	13.72159700	5.70410800
H	7.45319400	12.46431200	4.64516800
H	9.26745500	11.02279200	3.78147700
H	12.36266500	9.86379500	2.04044600
H	10.73652400	10.53658800	1.84749200
H	11.56270000	10.62753600	3.41935800
H	11.64534000	7.73906300	1.11236500
H	10.33509500	6.77345300	1.79182000
H	9.96624900	8.27511800	0.92991700
H	12.79795000	7.84840900	3.39581900
H	11.95433700	8.54620800	4.79163900
H	11.51138700	6.94285600	4.19903300
H	8.21448800	6.12566400	2.88457000
H	9.73844100	6.12292800	3.78135400
H	6.95883400	5.85205400	4.99935500
H	8.08245000	4.55987400	4.74595000
H	9.50433700	5.20520600	6.49562400
H	9.11351200	6.89050500	6.37934800
H	6.15329600	4.23352800	6.71546600
H	8.29913000	3.18194900	6.65981400
H	7.23002400	2.20159400	7.63940500
H	9.63445800	2.48845700	8.49134900
H	8.36208100	2.71490600	9.65611400
H	10.20847500	4.78680600	8.43356000
H	9.86968600	4.47336300	10.12098200
H	8.97313900	6.63995500	9.28441700
H	7.91853600	5.56428600	11.25066800
H	6.81778400	6.57969400	10.35100100
H	5.55555400	4.64506900	10.93933900
H	6.84941200	3.54608500	10.55150500
H	4.95620600	4.98690000	8.66818300
H	5.24224500	3.27357500	8.80368300

2-PHPh

C	-5.82495900	5.00001100	6.89121700
C	-7.22328000	4.99411500	6.86956000
C	-7.88062500	5.75382200	5.90587300
C	-7.14207200	6.49830000	4.99035600
C	-5.74603000	6.46175700	5.06493600
C	-5.03604100	4.24768900	7.86475600
C	-5.42670300	3.36447500	8.88456300
C	-4.25120000	2.94727000	9.49699400
C	-4.10311400	1.97725800	10.66636500
C	-3.41063800	2.65043200	11.87706400
C	-3.34325900	0.69799000	10.23531000
C	-5.51343600	1.54405700	11.12590000
C	-1.78360300	3.60383200	9.12322600
C	-0.90544400	3.56432500	7.87194900
C	-1.09140300	2.33809500	6.96564200
C	-0.56212700	1.18446600	4.50171600
C	0.41905100	0.17132600	5.15336200
C	1.84537800	0.70735400	5.42359000
C	1.90934900	2.15483800	5.96458800
C	0.94594200	3.16390300	5.27909400
C	1.33597500	3.45062200	3.80755200
C	1.10389000	2.28769300	2.81434100
C	-0.20670300	1.49600300	3.02735200
C	-3.43894600	3.11138200	3.94869000
C	-4.20452800	2.19331500	4.69128400
C	-5.33169500	1.58343400	4.13808000
C	-5.72522100	1.87741400	2.83108500
C	-4.97721600	2.78730300	2.08138500
C	-3.84912700	3.39608800	2.63338400
C	-4.87593400	7.19643200	4.14878900
C	-5.17679000	8.08909700	3.10701200
C	-3.95351300	8.48043900	2.57663100
C	-3.70524400	9.44886200	1.42307000
C	-5.07135900	9.91437700	0.87088300
C	-2.94792200	10.70999600	1.90860500
C	-2.94784700	8.76258500	0.25951700
C	-1.53231200	7.76741100	3.11412200
C	-0.73965300	7.78346100	4.42168400
C	-0.95435000	9.01318000	5.31685400
C	0.94378000	8.12780000	7.13034200
C	1.22796700	7.82624200	8.62300600
C	0.96354700	8.99260000	9.60408100
C	-0.30637000	9.82335400	9.30820200
C	-0.55537000	10.14787500	7.81481900
C	0.49492500	11.13375900	7.23302300
C	1.92029000	10.55775900	7.05694800
C	1.97865800	9.11067700	6.51449800

C	-3.51749100	8.30057200	8.16722300
C	-4.02097100	8.02749800	9.45225200
C	-5.16707500	8.66544300	9.92904100
C	-5.84028400	9.59364700	9.13238200
C	-5.35371100	9.87649800	7.85459300
C	-4.20842800	9.23751700	7.37655900
B	-0.56540100	2.54136400	5.41336000
B	-0.53740000	8.79336200	6.89985800
Fe	-2.96239000	5.69870000	6.07426600
N	-5.11353900	5.72343500	6.00114000
N	-3.70172100	4.37320000	7.84084900
N	-3.23102400	3.58342900	8.82799400
N	-3.54943800	7.04092700	4.26273600
N	-2.99545300	7.82090200	3.31160600
P	-1.95885900	3.92366500	4.68900400
P	-2.01290300	7.44977200	7.52630200
H	-1.49598300	4.54579400	3.50658200
H	-1.64739900	6.81537000	8.73600700
H	1.06784000	4.11699700	5.82145800
H	0.76140600	4.32294700	3.46459700
H	2.39266900	3.75747400	3.74469700
H	1.12026900	2.68516900	1.78856300
H	1.95238200	1.59731500	2.86336000
H	-0.14792400	0.56506400	2.43991200
H	-1.03909100	2.06514900	2.58964400
H	-1.54805400	0.69154900	4.48831600
H	-0.01646200	-0.16336500	6.10517100
H	0.49961300	-0.73584100	4.53233000
H	2.43597100	0.64309900	4.50401500
H	2.35107300	0.03772000	6.13478700
H	1.68303800	2.13781500	7.04053000
H	2.94969000	2.51013800	5.88838300
H	-0.56440000	1.49134400	7.42963200
H	-2.15157100	2.03991700	6.97376400
H	-1.06576000	4.49504600	7.31377400
H	0.13238700	3.62760000	8.22276100
H	-1.58157000	4.50429100	9.71642300
H	-1.57967600	2.73682400	9.74782900
H	-2.31974800	0.89319700	9.90518800
H	-3.29219200	-0.00029600	11.07867800
H	-3.86465800	0.19839900	9.41173800
H	-2.37766500	2.94253500	11.67358700
H	-3.95865900	3.54645000	12.18928800
H	-3.39399700	1.95335800	12.72262400
H	-5.42374600	0.84724300	11.96580600
H	-6.10951000	2.39920100	11.46292300
H	-6.05989600	1.03206700	10.32649400
H	-6.42802900	3.05884500	9.14197000

H	-7.77726800	4.41011600	7.59548700
H	-8.96597900	5.76565200	5.86843800
H	-7.63188300	7.09366600	4.22842000
H	-6.15130400	8.41752800	2.78332800
H	-4.90969800	10.61068200	0.04139000
H	-5.66211500	9.07344000	0.49140200
H	-5.65911600	10.43681000	1.63337200
H	-1.93739800	8.44781900	0.53083100
H	-3.49291900	7.87914500	-0.09130500
H	-2.85947000	9.46036500	-0.58098900
H	-1.95320400	10.49135000	2.30535400
H	-2.82543900	11.40891300	1.07315000
H	-3.51194700	11.21917600	2.69748400
H	-3.27224700	4.09355300	2.03153300
H	-5.26714400	3.02017500	1.05951000
H	-6.60030800	1.39853100	2.39976900
H	-5.89973100	0.86950100	4.72983100
H	-3.91208400	1.94440600	5.70681400
H	-3.84322900	9.47828100	6.38287900
H	-5.86286500	10.60433000	7.22725400
H	-6.72945000	10.09509600	9.50530100
H	-5.52983600	8.44081000	10.92927000
H	-3.50327900	7.31590200	10.09028400
H	-1.26665100	8.63083000	2.50800100
H	-1.31169500	6.86378700	2.53243700
H	-0.96110100	6.85669300	4.96534200
H	0.31750200	7.69364600	4.14145500
H	-0.37619900	9.84669600	4.89134600
H	-2.00369800	9.33850000	5.23903300
H	1.07396200	7.17303800	6.59290100
H	0.60846900	6.96915500	8.92350000
H	2.26937500	7.48993000	8.75370300
H	1.83313900	9.65787600	9.61520700
H	0.89975600	8.59190400	10.62674700
H	-1.18212600	9.27865700	9.68853300
H	-0.25865400	10.75119200	9.90151300
H	-1.52575100	10.66862100	7.76554500
H	0.13353700	11.48162800	6.25525500
H	0.55935200	12.03756600	7.86079300
H	2.49176600	11.21449600	6.38460600
H	2.44909100	10.60214100	8.01454600
H	3.00111700	8.72533500	6.65746400
H	1.82454900	9.13735200	5.42608900

2-OH

Fe	2.16008200	11.25459600	7.72756400
O	3.72658200	12.19139700	8.47910300
H	3.75130300	12.13687700	9.44472100
O	0.46753800	11.86406200	6.91485100
H	0.45748600	11.72881100	5.95695100
N	2.33418900	9.12955200	7.81263300
N	2.94696300	10.61788200	5.66451400
N	3.43892000	11.14070300	4.52385500
N	1.47341000	10.66337100	9.84042600
N	0.89563600	11.18740700	10.93953300
C	2.77945900	8.45571300	6.73422900
C	2.89821800	7.06158400	6.75365600
C	2.56105300	6.38182200	7.92262100
C	2.10961600	7.08786000	9.03613900
C	1.99845200	8.47971100	8.94409500
C	3.14105700	9.29112500	5.58491000
C	3.74764500	8.96202900	4.36316900
C	3.93548600	10.16744200	3.69327900
C	4.56652100	10.38379100	2.32078400
C	5.93104000	11.10657400	2.44706300
C	3.61658600	11.16190200	1.37838500
C	4.82990200	9.00375500	1.67769600
C	1.49821000	9.33325300	10.02611700
C	0.94638500	9.00725900	11.27438600
C	0.56011400	10.21498800	11.84816100
C	-0.10604600	10.43333200	13.20365400
C	0.69752200	11.42926100	14.07447100
C	-1.56984700	10.91001800	13.02993600
C	-0.14298700	9.08431600	13.95615000
C	3.39984500	12.60975500	4.35254800
C	3.64885700	13.36029900	5.66556300
C	4.95796300	12.99373700	6.39141100
B	4.91418300	13.18681600	8.01353000
C	6.28631000	12.73466300	8.78123200
C	6.08137300	12.72554400	10.31765700
C	5.52666900	14.03955800	10.91517900
C	4.38727700	14.68894800	10.09526500
C	4.59079100	14.69481400	8.55863600
C	5.73419100	15.63543900	8.09761300
C	7.16165800	15.18546600	8.49087400
C	7.43762200	13.67087700	8.33156300
C	0.33642300	13.24683200	9.62799600
C	-0.89094300	12.61810900	8.94005100
B	-0.86596800	12.69228700	7.30778700
C	-2.14313400	11.97309600	6.58113400
C	-1.92635800	11.88137800	5.04897800
C	-1.57992200	13.21771900	4.35213000

C	-0.56427100	14.09830300	5.11706400
C	-0.77946400	14.18726100	6.64941800
C	-2.06053100	14.96779300	7.04203600
C	-3.39584300	14.27002100	6.68887900
C	-3.43120400	12.74715700	6.96293900
C	0.69397500	12.65209600	10.99456700
H	4.06635900	11.22976100	0.38130300
H	2.65510900	10.64560400	1.28014100
H	3.41802500	12.18117900	1.71798000
H	5.53407000	8.40873500	2.26924700
H	3.90399400	8.43045500	1.55851500
H	5.26864600	9.14350500	0.68417800
H	6.38979200	11.20038000	1.45592200
H	5.84812600	12.11169700	2.86882200
H	6.61341600	10.53590400	3.08592700
H	4.03128500	7.98272200	4.01225100
H	3.24786700	6.52721800	5.87746000
H	2.65032900	5.30020900	7.96592300
H	1.84666000	6.57475500	9.95433700
H	0.82453600	8.02566400	11.70363800
H	0.86379100	8.68211300	14.11368900
H	-0.60451400	9.22857000	14.93863800
H	-0.73636500	8.33666100	13.41879000
H	1.73063000	11.08821000	14.20495900
H	0.72643900	12.43747100	13.65454700
H	0.23781400	11.49997200	15.06680900
H	-1.65024500	11.87780400	12.52800300
H	-2.14560200	10.18562400	12.44408600
H	-2.04361600	11.00688700	14.01369900
H	1.60758700	13.10607200	11.39850600
H	-0.11226200	12.82888400	11.70437600
H	0.18224500	14.32083500	9.79310500
H	1.22673100	13.18793300	8.99529300
H	-0.96832400	11.55649300	9.22283600
H	-1.79577100	13.08957000	9.34718900
H	0.07391500	14.76323500	7.04733700
H	-2.03196300	15.13484000	8.12865100
H	-2.06290400	15.97301700	6.58895100
H	-4.21019400	14.75232800	7.24931600
H	-3.63138600	14.45401400	5.63513400
H	-4.31076400	12.32171000	6.45137900
H	-3.61066100	12.59035100	8.03586300
H	-2.27813000	10.93796300	6.94164200
H	-1.11334000	11.15872100	4.85332200
H	-2.80634300	11.44313600	4.55058700
H	-1.19340700	13.01104800	3.34240300
H	-2.50067500	13.78688000	4.19236500
H	0.44830900	13.69693600	4.94274000

H	-0.55517900	15.10040700	4.65842400
H	4.17037100	12.85881400	3.62503000
H	2.42673900	12.87602600	3.92115900
H	3.62838900	14.42870100	5.41533300
H	2.77631300	13.20842600	6.30743000
H	5.77659500	13.57298100	5.94304500
H	5.20806500	11.94025600	6.18992400
H	6.58391500	11.70950600	8.49805600
H	5.39135300	11.90103300	10.57357600
H	7.01758100	12.46985400	10.84013100
H	5.17455800	13.85175700	11.94103600
H	6.34575800	14.75692900	11.02313500
H	3.44996800	14.14757100	10.30832000
H	4.21878100	15.70884300	10.47745300
H	3.65869900	15.09781800	8.12601000
H	5.68338600	15.71325900	7.00180700
H	5.57642600	16.65979800	8.47384700
H	7.89167400	15.74635100	7.88891400
H	7.36152800	15.48319500	9.52579700
H	8.37147100	13.42901800	8.86613100
H	7.64335700	13.46385300	7.27194700

2-SPh

C	6.87062500	1.64428200	13.35966000
C	6.11801200	2.33681200	12.41322200
C	6.13996400	3.73499600	12.43709600
C	5.41214000	4.58462400	11.49100200
C	4.55952800	4.26492600	10.42276800
C	4.18227200	5.47983800	9.85890000
C	3.25981700	5.70694000	8.66453500
C	3.99560300	6.43823100	7.51463900
C	2.80880000	4.33207600	8.12278300
C	1.98565100	6.48076400	9.08500000
C	4.88000100	7.91257400	10.39221100
C	4.79504100	8.71092400	11.69408500
C	3.52707400	8.49245400	12.53070200
C	2.33896100	8.80631300	15.01401600
C	1.31494000	9.84044400	14.45475500
C	1.83791800	11.29245000	14.33579000
C	3.28386100	11.42485900	13.80189200
C	4.30288100	10.40061100	14.38743500
C	4.59660100	10.63182900	15.88979000
C	3.43280200	10.30903400	16.85421700
C	2.64792800	9.02149200	16.51578400
C	4.41361200	5.98840400	15.47440600
C	3.43542800	5.30372000	14.73497200
C	2.83557700	4.15224000	15.24920100
C	3.20382900	3.66063700	16.50317600
C	4.17614700	4.33513800	17.24451500
C	4.77333000	5.49068400	16.73788700
B	3.65202300	8.95001400	14.08617000
N	6.86806300	4.40136800	13.35347800
N	5.55257700	5.91592100	11.58962400
N	4.80876900	6.45112000	10.60219300
S	5.20635400	7.48089000	14.86835600
Fe	6.86625300	6.51919200	13.34853700
C	7.62192400	2.34244400	14.30299800
C	7.59736600	3.74046200	14.27286200
C	8.32347500	4.59567800	15.21522700
C	9.17613500	4.28237900	16.28531900
C	9.55106700	5.50052900	16.84373200
C	10.47246900	5.73473700	18.03753300
C	9.73483200	6.47026700	19.18353500
C	10.92540100	4.36316100	18.58600600
C	11.74565500	6.50864100	17.61421900
C	8.84965300	7.92960400	16.29860400
C	8.93385600	8.72177800	14.99290700
C	10.20232500	8.50090400	14.15769400
C	11.39093200	8.80442900	11.67338200
C	12.41382000	9.84203200	12.22828100

C	11.88946800	11.29408800	12.34043100
C	10.44316100	11.42766000	12.87308300
C	9.42529100	10.39975600	12.29193200
C	9.13185300	10.62369100	10.78842600
C	10.29636300	10.29769900	9.82594500
C	11.08234700	9.01247800	10.17053700
C	9.31888600	5.98270000	11.22427400
C	10.29807100	5.30229700	11.96633300
C	10.89922000	4.14942200	11.45677100
C	10.53130300	3.65216300	10.20492800
C	9.55801500	4.32239600	9.46099400
C	8.95952500	5.47930500	9.96294300
B	10.07747100	8.95125100	12.60014300
N	8.18084200	5.92626300	15.11037000
N	8.92327100	6.46728300	16.09565300
S	8.52449600	7.47671400	11.82435600
H	8.21541400	6.00898300	9.37571600
H	9.26874400	3.95068500	8.48094000
H	11.00281600	2.75596300	9.81045800
H	11.66175100	3.64091900	12.04195000
H	10.59222700	5.68190700	12.93843000
H	11.87108300	7.81790500	11.76985100
H	12.01700600	9.00701900	9.58652700
H	10.50810100	8.14549600	9.81951700
H	9.89872200	10.20812900	8.80440600
H	10.98697300	11.14681600	9.78782300
H	8.27383800	9.99431200	10.51905500
H	8.81169700	11.66362900	10.61352800
H	8.47764900	10.57013800	12.82842100
H	10.45896600	11.31675300	13.96700000
H	10.09199900	12.45429600	12.68428200
H	12.56414600	11.86780000	12.99233700
H	11.95700400	11.77895500	11.36174100
H	12.73764900	9.50615500	13.22326900
H	13.32270700	9.84391400	11.60580800
H	11.02732900	9.05709000	14.63090200
H	10.50406900	7.44565500	14.21656500
H	8.04126000	8.48710700	14.40553900
H	8.82816200	9.77941900	15.26523000
H	9.67144600	8.19874800	16.95898900
H	7.90465400	8.13919200	16.81321200
H	12.28851400	5.96274700	16.83503500
H	11.53385200	7.50897600	17.22806300
H	12.41157300	6.62046600	18.47769800
H	11.58871700	4.51562000	19.44386200
H	10.07441500	3.76181600	18.92417700
H	11.47957500	3.79018200	17.83469700
H	10.39878000	6.55504500	20.05147300

H	9.41959600	7.48048600	18.91175200
H	8.84412700	5.91222400	19.49310100
H	9.48678600	3.30344900	16.61368600
H	8.21084800	1.81891800	15.04766500
H	6.87164200	0.55810600	13.36208700
H	5.53005600	1.80886000	11.67092000
H	4.25031100	3.28396700	10.09913500
H	3.66059300	3.73048900	7.78708500
H	2.25586700	3.76179900	8.87705900
H	2.14487200	4.47942700	7.26450700
H	2.19611500	7.48318600	9.46645000
H	1.31907600	6.58759000	8.22139100
H	1.44408700	5.93760200	9.86698700
H	4.88687800	5.88001700	7.20702500
H	3.33092900	6.51806300	6.64678800
H	4.30961100	7.45013400	7.78153800
H	5.82447100	8.12118000	9.87623500
H	4.05754900	8.17723500	9.73083800
H	5.68809100	8.48027600	12.28234000
H	4.89928900	9.76737600	11.41663100
H	2.70129400	9.04556200	12.05524800
H	3.22646800	7.43662000	12.47674800
H	5.25019800	10.56941200	13.84986000
H	5.45541400	10.00466800	16.16178400
H	4.91567800	11.67291900	16.05974500
H	3.83094800	10.22448500	17.87598700
H	2.74136000	11.15762700	16.88878500
H	1.71351500	9.01778200	17.10019900
H	3.22318100	8.15668400	16.87050900
H	1.85965300	7.81892900	14.92224900
H	0.99109400	9.49974500	13.46141200
H	0.40625600	9.84433300	15.07751600
H	1.16243600	11.86258800	13.68158600
H	1.77040100	11.78170400	15.31230200
H	3.26769300	11.30882000	12.70851200
H	3.63416800	12.45268600	13.98574200
H	5.51669300	6.02368500	17.32305400
H	4.46567700	3.96784900	18.22615900
H	2.73332600	2.76550800	16.90126900
H	2.07380300	3.64037100	14.66597400
H	3.14103900	5.67887400	13.76122000

(^{BBN}PDP^{tBu})Zn(SPh)$_2$

C	-1.65893100	-4.17543000	4.47284700
C	-0.91091700	-3.47384000	5.41369000
C	-0.93509600	-2.07559200	5.38474800
C	-0.20153400	-1.24665400	6.34043900
C	0.65153400	-1.59372200	7.40185500
C	1.03963400	-0.39241400	7.98333600
C	1.96697000	-0.19189300	9.17881500
C	1.24308800	0.53147500	10.34116800
C	2.40310500	-1.57933900	9.70052200
C	3.24974600	0.57220200	8.76661900
C	0.36382100	2.05250400	7.49643100
C	0.42572200	2.88563700	6.21576300
C	1.65748700	2.65802600	5.32830500
C	0.82645000	4.61677200	3.55009900
C	1.86425100	5.62358300	4.13326900
C	3.29308800	5.50590400	3.55174400
C	3.81038400	4.05764600	3.37525000
C	2.76827300	3.03982800	2.81928000
C	2.41420500	3.29830600	1.33430600
C	1.62174600	4.59555600	1.05644200
C	0.48812000	4.89154600	2.06450900
C	0.71082200	0.23589000	2.35324100
C	1.66374900	-0.48896400	3.08637000
C	2.27262900	-1.61823100	2.53510100
C	1.93935200	-2.04595200	1.24834700
C	0.99263000	-1.33061100	0.51266700
C	0.38571700	-0.19777800	1.05798200
B	1.48602200	3.15975300	3.79259000
N	-1.66076600	-1.40705700	4.46661000
N	-0.33135100	0.08220500	6.26294900
N	0.41813900	0.59583500	7.25496000
S	-0.08878400	1.70913600	3.00169100
Zn	-1.66212800	0.70221600	4.46195400
C	-2.40788300	-3.47907500	3.52886700
C	-2.38557000	-2.08067600	3.55151100
C	-3.12033500	-1.25702900	2.59217600
C	-3.97310900	-1.61002500	1.53247600
C	-4.36298900	-0.41186900	0.94571300
C	-5.29084600	-0.21794800	-0.25045500
C	-4.56829900	0.50143500	-1.41610500
C	-5.72498600	-1.60832300	-0.76600800
C	-6.57465800	0.54601900	0.15870800
C	-3.69054400	2.03614400	1.42156800
C	-3.75326700	2.87492600	2.69850500
C	-4.98457300	2.64967600	3.58720100
C	-4.15600100	4.61722000	5.35690300
C	-5.19517800	5.62007000	4.76939000

C	-6.62381200	5.50298500	5.35153300
C	-7.13913800	4.05480300	5.53430100
C	-6.09563800	3.04077900	6.09457700
C	-5.74185200	3.30603800	7.57841100
C	-4.95122400	4.60557900	7.85068700
C	-3.81806800	4.89890800	6.84129800
C	-4.03471500	0.24185700	6.57249500
C	-4.98649000	-0.48755900	5.84239600
C	-5.59387600	-1.61524100	6.39854200
C	-5.26023200	-2.03681300	7.68723000
C	-4.31465500	-1.31690200	8.41991700
C	-3.70924100	-0.18563200	7.86971400
B	-4.81353700	3.15822400	5.12073500
N	-2.99234300	0.07234200	2.66370000
N	-3.74273300	0.58048800	1.66955000
S	-3.23697300	1.71332700	5.91773600
H	-3.22558200	4.76919400	4.78617500
H	-4.84194300	6.65383600	4.90879300
H	-5.24450800	5.46825400	3.68143700
H	-6.66274800	6.02438400	6.31286300
H	-7.32053200	6.04991400	4.69980700
H	-8.02760100	4.07755800	6.18517500
H	-7.49328300	3.68152100	4.56339200
H	-6.57457000	2.05001400	6.04942100
H	-6.65799400	3.31887200	8.19090600
H	-5.15345500	2.45477100	7.94417500
H	-5.64404900	5.45322500	7.87822100
H	-4.52233600	4.55563400	8.86226700
H	-2.94862400	4.28443700	7.10829500
H	-3.49778900	5.94583900	6.96664700
H	-5.84226200	3.16604600	3.12747000
H	-5.25931100	1.58597300	3.57749200
H	-2.83009200	2.70623600	3.25873800
H	-3.70042200	3.92282900	2.37595500
H	-2.76220000	2.24163700	0.87569700
H	-4.53119500	2.27340000	0.77275900
H	-3.67013800	-0.05027100	-1.71539800
H	-5.23611600	0.55533500	-2.28357000
H	-4.26792500	1.52254300	-1.16948400
H	-4.86590900	-2.20492700	-1.09186200
H	-6.26933200	-2.17163300	-0.00035300
H	-6.39212200	-1.48552300	-1.62569400
H	-6.37730900	1.55824000	0.52089500
H	-7.24475400	0.62782000	-0.70494900
H	-7.10674000	0.00994300	0.95201300
H	-4.27325900	-2.60040700	1.22993100
H	-2.99616200	-4.00243600	2.78394800
H	-1.65821100	-5.26155500	4.47529200

H	-0.32196800	-3.99305800	6.16097600
H	0.95299900	-2.58232400	7.70887900
H	3.06990500	-1.45174600	10.55977400
H	1.54487200	-2.17579800	10.02885700
H	2.94843300	-2.14518500	8.93744400
H	1.91064000	0.59023400	11.20852200
H	0.94117200	1.55101600	10.08999100
H	0.34572200	-0.02030100	10.64270300
H	3.78269800	0.03359800	7.97561400
H	3.05103100	1.58264200	8.40023000
H	3.91960800	0.65852400	9.63001700
H	1.20394000	2.29385200	8.14441700
H	-0.56498700	2.25913900	8.04109000
H	-0.49711900	2.71323300	5.65610200
H	0.37142700	3.93490800	6.53359500
H	2.51444100	3.17748600	5.78592300
H	1.93355400	1.59471900	5.34272400
H	-0.10416600	4.76993600	4.12017900
H	-0.38039100	4.27461500	1.80016100
H	0.16627800	5.93744600	1.93463600
H	2.31335200	5.44407300	1.02534500
H	1.19299800	4.54068100	0.04505900
H	3.33037800	3.30983600	0.72183300
H	1.82704800	2.44466500	0.97211500
H	3.24852700	2.04990700	2.86867300
H	4.69884300	4.07879700	2.72431700
H	4.16499200	3.68901600	4.34776800
H	3.33143400	6.02321300	2.58818600
H	3.98901300	6.05656600	4.20117300
H	1.50962100	6.65625000	3.98934100
H	1.91372800	5.47658300	5.22187600
H	1.93117800	-0.16344400	4.08534300
H	3.01422700	-2.16253700	3.11490400
H	2.41719600	-2.92361900	0.82115600
H	0.72962000	-1.64856300	-0.49330000
H	-0.33990100	0.36524400	0.47873500
H	-5.25421500	-0.16684900	4.84194300
H	-6.33460200	-2.16314600	5.82101800
H	-5.73691700	-2.91326000	8.11820200
H	-4.05138300	-1.63004000	9.42732400
H	-2.98452000	0.38096700	8.44659600

2’

Fe	8.64158900	10.84114500	-0.79699200
N	10.33638600	12.19412800	-0.68763500
C	10.42011300	13.03030900	0.36856800
C	11.46495400	13.95315600	0.48151400
H	11.52202300	14.61606500	1.33805700
C	12.43126000	13.98690200	-0.52298800
H	13.25739100	14.68922500	-0.45780200
C	9.34249500	12.85838700	1.34290500
C	8.94420200	13.56714900	2.48873300
H	9.38953700	14.46012300	2.89817900
C	7.81901700	12.90392000	2.97659000
C	6.92269400	13.31529100	4.14014600
C	7.54786200	14.54405000	4.83595600
H	6.91229400	14.85222000	5.67293200
H	7.63427500	15.39606700	4.15300500
H	8.54249900	14.31740200	5.23574600
C	5.52701200	13.72612700	3.60884300
H	4.89892800	14.06843200	4.43977700
H	5.00659900	12.89765500	3.11921900
H	5.61058100	14.54347900	2.88440100
C	6.77920500	12.19835500	5.19968900
H	6.21119300	12.57956600	6.05632300
H	7.75939300	11.86985900	5.56189700
H	6.25006600	11.32231400	4.81831300
N	8.51812700	11.82205400	1.14011000
N	7.60839500	11.84562800	2.12441600
C	6.70149800	10.68497800	2.16504200
H	6.47124100	10.46687200	1.11899100
H	5.77770900	10.99507200	2.65661800
C	7.31950900	9.45978000	2.85820600
H	6.55389000	8.67408900	2.79757300
H	7.43007500	9.69337000	3.92687300
C	8.65070900	8.93356200	2.28317900
H	8.98540600	8.17217900	3.00375400
H	9.41194100	9.72529500	2.36483600
B	8.67252600	8.24282600	0.79404600
H	8.63032900	9.17407400	-0.14400500
C	7.43884500	7.22083800	0.46843600
H	6.45086500	7.69017800	0.61996000
C	7.51331800	6.03610300	1.46854600
H	7.31074400	6.42839200	2.47595100
H	6.71198200	5.30462000	1.26960300
C	8.86327000	5.28154100	1.50253500
H	8.89832400	4.57058400	0.67005400
H	8.90147700	4.65919600	2.40901100
C	10.11923400	6.18472500	1.45881500
H	10.99294600	5.55354500	1.22413300

H	10.30378600	6.57353900	2.46987600
C	10.03770800	7.39123100	0.48604700
H	10.94668300	7.99317400	0.66424200
C	10.07676700	6.96550300	-1.00013600
H	10.96736700	6.35023800	-1.21528000
H	10.19296600	7.87987100	-1.60032800
C	8.82821500	6.19985400	-1.49608700
H	8.83436000	6.16991500	-2.59752700
H	8.90341500	5.15131000	-1.19051500
C	7.47674200	6.77455400	-1.01116500
H	7.22681200	7.65842000	-1.61909300
H	6.68794300	6.03346300	-1.22614700
C	11.26237500	12.22722900	-1.66348000
C	12.33959800	13.11944300	-1.61052300
H	13.08088100	13.13483500	-2.40185600
C	11.01858700	11.29261400	-2.76422400
C	11.73212800	11.04564900	-3.94949800
H	12.65994700	11.49668500	-4.26364400
C	11.00258600	10.08491300	-4.64172200
C	11.35383600	9.41668200	-5.96747500
C	12.65319600	10.05175800	-6.50989500
H	12.92082600	9.57919400	-7.46090700
H	13.49142700	9.90851000	-5.81967500
H	12.53222700	11.12544400	-6.69146800
C	11.62032000	7.90557700	-5.75613300
H	11.92618900	7.44780200	-6.70417000
H	10.73978700	7.36543000	-5.39703400
H	12.42356400	7.75127100	-5.02787400
C	10.25236800	9.62783000	-7.03371300
H	10.58601200	9.21157000	-7.99127000
H	10.04940500	10.69436800	-7.18127700
H	9.31065500	9.13777300	-6.77505500
N	9.91819900	10.52658800	-2.71455800
N	9.91197400	9.80550000	-3.85357800
C	8.71214300	8.99657000	-4.11169400
H	8.48726800	8.47592400	-3.17907200
H	8.96466300	8.24215000	-4.85680100
C	7.50825700	9.84164900	-4.54924300
H	7.75515300	10.38411000	-5.47116700
H	7.32268400	10.59326500	-3.77408000
C	6.25236800	8.98192300	-4.75241200
H	6.06137800	8.38246600	-3.84487100
H	6.42248300	8.21806300	-5.53280200
B	4.89950000	9.71995100	-5.09656100
H	7.20294500	11.35310500	-1.48628600
C	4.68454400	11.27512000	-5.25448500
H	5.61550200	11.85416900	-5.18769600
C	3.79861300	11.70726800	-4.04201400

H	4.40539800	11.60017600	-3.13136300
H	3.56517700	12.77954100	-4.12137900
C	2.48825000	10.90955000	-3.86629000
H	1.73288600	11.27943000	-4.56609600
H	2.08270100	11.11270400	-2.86585200
C	2.65124900	9.38329700	-4.03502500
H	1.65857100	8.91438900	-4.10773700
H	3.10690100	8.97689100	-3.11995900
C	3.53501500	8.93711900	-5.24222800
H	3.65667800	7.84661000	-5.16466500
C	2.92134600	9.23788900	-6.63930200
H	1.93146900	8.76520400	-6.72559300
H	3.55231400	8.74451300	-7.39456100
C	2.80496800	10.73400600	-6.99916800
H	2.60618200	10.82654800	-8.07578300
H	1.92894200	11.16411700	-6.50510800
C	4.05820000	11.56422300	-6.64954900
H	4.82989500	11.36759100	-7.40971500
H	3.82070500	12.63498900	-6.73839700

2-OH'

Fe	2.22530800	11.29223400	7.69641200
O	3.73591700	12.26872700	8.22866400
H	3.90128000	12.38661900	9.17380000
O	0.51612500	11.90277100	6.83732700
H	0.46516700	11.68582700	5.89665800
N	2.33432000	9.13569700	7.87333400
N	3.02722600	10.53669600	5.69896400
N	3.49641000	11.01417100	4.52931400
N	1.43454900	10.72940400	9.84532500
N	0.85065000	11.28398700	10.92240500
C	2.81411500	8.41962500	6.83704500
C	2.94514700	7.02854600	6.91307900
C	2.58165000	6.39045400	8.09741700
C	2.09687400	7.13722700	9.16874000
C	1.97902800	8.52478100	9.02024200
C	3.19820400	9.20752700	5.66122700
C	3.77791400	8.82905800	4.43742200
C	3.96723400	10.00717400	3.72160400
C	4.52070700	10.16805800	2.30932500
C	5.75704700	11.09764600	2.27564300
C	3.42091700	10.69749700	1.35584200
C	4.96482700	8.78209400	1.79232300
C	1.45460400	9.40772800	10.06656000
C	0.88609200	9.11519700	11.31885700
C	0.49968800	10.33831000	11.85591900
C	-0.18600600	10.59902900	13.19351400
C	0.61187700	11.60949500	14.05246700
C	-1.64011500	11.08913100	12.98117200
C	-0.25238700	9.27149600	13.98085100
C	3.53839800	12.47943900	4.39591400
C	4.67778800	13.12314300	5.19715300
C	4.60497800	14.65670000	5.14446000
B	5.60958400	15.46362100	6.05815600
C	5.44892100	17.01534300	6.30449800
C	6.79218600	17.74967600	6.04608500
C	8.01857200	17.15104600	6.76582000
C	8.10014800	15.61164200	6.69393000
C	6.76482300	14.85881100	6.94397300
C	6.21194700	14.96664100	8.40511200
C	5.76194400	16.38097100	8.83307600
C	4.91913400	17.12342200	7.77223100
C	0.42887700	13.33329200	9.55159700
C	-0.80942200	12.76131300	8.83571700
B	-0.74004100	12.82531400	7.20194200
C	-2.06866700	12.21779400	6.45760800
C	-1.84672500	12.12048200	4.92684700
C	-1.39964800	13.43360000	4.24433900

C	-0.32642200	14.22890500	5.02336600
C	-0.53902100	14.31823800	6.55511100
C	-1.75516400	15.19366600	6.95069000
C	-3.13860000	14.60690500	6.58048600
C	-3.29631400	13.08737000	6.83211200
C	0.69322300	12.75417000	10.94536300
H	3.81401600	10.75812300	0.33430800
H	2.55628700	10.02501900	1.34825700
H	3.06545900	11.69439300	1.63206900
H	5.75137400	8.35062900	2.42113900
H	4.12685000	8.07784500	1.75243900
H	5.36395700	8.88179300	0.77736900
H	6.17362000	11.11552900	1.26190600
H	5.52069100	12.12825300	2.55079600
H	6.53658200	10.73699700	2.95565800
H	4.02851600	7.83296100	4.10885600
H	3.32475900	6.46489000	6.06802300
H	2.67712000	5.31195800	8.18539600
H	1.81275200	6.65905100	10.09959400
H	0.75425200	8.14550900	11.77208100
H	0.74687800	8.86305100	14.16780300
H	-0.73146200	9.44577600	14.95022400
H	-0.84248600	8.51613600	13.45082900
H	1.63934600	11.26209200	14.20927400
H	0.65720900	12.60544400	13.60540700
H	0.13648700	11.71150000	15.03487200
H	-1.69706300	12.04227200	12.44876000
H	-2.21476900	10.35539500	12.40599100
H	-2.13067300	11.22169900	13.95270600
H	1.60066000	13.18350100	11.39023800
H	-0.14229000	12.97241300	11.60969400
H	0.33417300	14.41938700	9.68285700
H	1.33499600	13.19334100	8.95545500
H	-0.93704900	11.70417600	9.11627800
H	-1.70058300	13.27322000	9.22482900
H	0.35748300	14.82001100	6.96065000
H	-1.72124300	15.34457600	8.03948900
H	-1.67746600	16.20193600	6.50981200
H	-3.91723100	15.14416200	7.14219000
H	-3.35081200	14.82355500	5.52782600
H	-4.20015300	12.74040900	6.30310500
H	-3.50326600	12.93128200	7.89997200
H	-2.28925200	11.19382900	6.80799400
H	-1.08585400	11.34300600	4.72960700
H	-2.75160100	11.75000100	4.41744900
H	-1.02311300	13.20880300	3.23454800
H	-2.27585000	14.06976900	4.08541500
H	0.65131100	13.75124000	4.84877200

H	-0.23960000	15.23165300	4.57267500
H	3.59707700	12.72340000	3.33464700
H	2.57604700	12.84404500	4.76587300
H	4.59934900	12.78830100	6.23767900
H	5.64288200	12.77056200	4.81044500
H	3.58681800	14.99019000	5.40888300
H	4.73888500	15.02451000	4.10993900
H	4.68762100	17.47661000	5.65816500
H	6.97936700	17.73038100	4.96137000
H	6.69967000	18.81358900	6.31192500
H	8.93174000	17.57704400	6.32755600
H	8.02299300	17.47152400	7.81185100
H	8.45993900	15.32872400	5.69259800
H	8.86983000	15.25730900	7.39631500
H	6.94515700	13.79145600	6.75882000
H	5.36115000	14.27559600	8.48336600
H	6.97296700	14.59767200	9.10959900
H	5.17177100	16.29987400	9.75637000
H	6.63515600	16.98438500	9.09894000
H	4.82339000	18.18285700	8.05357400
H	3.89801800	16.71526800	7.78918500

2-SPh'

C	6.82461900	1.65706800	13.61271200
C	6.10614700	2.26638600	12.58644600
C	6.11064600	3.66258400	12.50537000
C	5.43230000	4.41759400	11.44915200
C	4.76902600	3.98852500	10.28760600
C	4.40621800	5.14464100	9.60487500
C	3.71894600	5.24643600	8.24575400
C	4.70276400	5.79688300	7.18305700
C	3.29446700	3.82876400	7.80204700
C	2.44227400	6.11817500	8.29971200
C	4.75190800	7.64798300	10.18664700
C	3.62853300	8.30003400	11.00171700
C	3.61815100	9.82598300	10.82864800
C	2.54907400	12.23578300	11.64690200
C	2.88145800	12.64823900	13.11533900
C	1.97725400	12.01743200	14.19619400
C	1.70842100	10.51046200	13.99277600
C	1.37459200	10.08347700	12.52711800
C	0.01463800	10.61910700	11.99130500
C	-0.06317300	12.14790900	11.79604500
C	1.18229100	12.76000900	11.12078200
C	4.11201400	6.20612900	15.14694200
C	3.04930500	5.65355600	14.40954500
C	2.33376400	4.55806200	14.89621200
C	2.65938000	3.99026800	16.13009400
C	3.70901300	4.53361200	16.87422100
C	4.42659900	5.62888900	16.39036100
B	2.53813500	10.65630800	11.62901900
N	6.78339700	4.41121700	13.40152000
N	5.46927400	5.75682700	11.49460600
N	4.85337400	6.19136000	10.37637400
S	5.00805500	7.64292800	14.55631600
Fe	6.67107700	6.53693300	13.28325900
C	7.52792900	2.43662800	14.52791500
C	7.48457800	3.82856500	14.39369800
C	8.17156000	4.75426700	15.29621600
C	8.98696800	4.52075500	16.41599800
C	9.34011500	5.77664000	16.89727300
C	10.22086700	6.10156100	18.10033300
C	9.44855100	6.92174100	19.16280300
C	10.65343800	4.77607600	18.76599700
C	11.50833100	6.84218800	17.66094200
C	8.64010300	8.15483000	16.16961200
C	8.68846600	8.86419900	14.81694200
C	9.95775800	8.64114700	13.98437500
C	11.11446800	8.89765800	11.47863300
C	12.12256200	9.96041400	12.00857800

C	11.57523300	11.40567200	12.09807200
C	10.12809800	11.52637000	12.63215200
C	9.12628500	10.47004600	12.07828200
C	8.81958500	10.66043100	10.57301400
C	9.98536200	10.33989300	9.61053500
C	10.79597200	9.07521800	9.97378900
C	9.11684800	6.07142800	11.10214000
C	10.09761000	5.40073700	11.85132600
C	10.71884600	4.25760400	11.34430200
C	10.36916500	3.75917100	10.08760800
C	9.39371800	4.41864000	9.33709400
C	8.77553200	5.56617000	9.83679000
B	9.79722100	9.02877700	12.40967400
N	8.03198100	6.07192300	15.08883200
N	8.73902300	6.68442500	16.05752800
S	8.29417000	7.54648400	11.70897200
H	8.02947300	6.08709500	9.24414800
H	9.11788400	4.04546800	8.35359900
H	10.85569900	2.87008100	9.69514900
H	11.48196200	3.75699100	11.93554500
H	10.37544900	5.78077800	12.82824600
H	11.61274500	7.92122400	11.58700700
H	11.72804300	9.07721100	9.38522200
H	10.23621600	8.19259400	9.63908000
H	9.58528200	10.22622100	8.59213200
H	10.65982000	11.20107700	9.55557500
H	7.97341200	10.00831800	10.31988700
H	8.47752100	11.69048200	10.37954000
H	8.17798200	10.63588100	12.61603100
H	10.14947600	11.43919400	13.72803300
H	9.76099500	12.54389900	12.42282800
H	12.24249600	12.00148300	12.73796500
H	11.63278200	11.87479300	11.11094500
H	12.45752200	9.64770700	13.00725500
H	13.02832300	9.96768900	11.38115000
H	10.77275700	9.23201400	14.43209400
H	10.28184800	7.59480200	14.08041100
H	7.80330600	8.55492200	14.25522400
H	8.54482600	9.93230200	15.02378000
H	9.46536400	8.48074200	16.80019000
H	7.69728200	8.37760400	16.68328700
H	12.07593100	6.23809500	16.94488400
H	11.30958600	7.80886300	17.19100200
H	12.14567400	7.02248400	18.53448600
H	11.28842800	4.99343500	19.63138600
H	9.79062300	4.20128700	19.12006500
H	11.23095200	4.14826000	18.07881600
H	10.08368500	7.07044700	20.04374300

H	9.14663800	7.90891300	18.80513300
H	8.54577500	6.38973900	19.48312600
H	9.28688500	3.56902900	16.82467700
H	8.09680400	1.98062000	15.33037000
H	6.83821600	0.57427300	13.69774000
H	5.55488000	1.67664600	11.86278500
H	4.59373000	2.97350000	9.96890000
H	4.15750300	3.16385900	7.68989400
H	2.59737500	3.37543000	8.51528800
H	2.79199900	3.88595200	6.83067800
H	2.65361900	7.16842900	8.51314600
H	1.93165900	6.07754100	7.33071000
H	1.74771500	5.75030300	9.06296400
H	5.59325600	5.16275000	7.11379800
H	4.21724700	5.81047400	6.20023400
H	5.03497100	6.81614900	7.40042800
H	5.72623400	8.05426000	10.47410900
H	4.62263500	7.83463600	9.12000600
H	2.66200400	7.87458700	10.70277800
H	3.77625700	8.05242600	12.05833500
H	4.60915100	10.23839200	11.08458800
H	3.49553300	10.09572400	9.76277400
H	1.31776200	8.98630300	12.52353200
H	-0.18028800	10.13293300	11.02274100
H	-0.80136700	10.29601500	12.65499600
H	-0.94874500	12.38464900	11.19019400
H	-0.23433500	12.63307400	12.76124100
H	1.14095800	13.85618000	11.20721500
H	1.13573200	12.54576800	10.04189300
H	3.33374500	12.66574000	11.00695200
H	3.92286400	12.35664400	13.31661600
H	2.85507400	13.74429700	13.20810300
H	2.44843500	12.16105900	15.17784800
H	1.02916600	12.56150000	14.24653400
H	2.59577500	9.94513400	14.31032800
H	0.89485700	10.19169200	14.66133000
H	5.23280400	6.05616500	16.97928100
H	3.96862900	4.10753700	17.84082100
H	2.09804300	3.14052800	16.50983700
H	1.51298900	4.15127900	14.30960500
H	2.78182900	6.09679100	13.45514400

2-SPh''

C	6.89800700	1.48672100	13.36066300
C	6.27371200	2.09387100	12.27226900
C	6.22460300	3.49119100	12.22306500
C	5.60148300	4.25438600	11.14170500
C	5.05817200	3.85583800	9.90932900
C	4.66249000	5.02623200	9.26979000
C	4.08159600	5.17002600	7.86590600
C	5.09380000	5.88660200	6.93847600
C	3.83225800	3.75817400	7.29071500
C	2.72824300	5.91882600	7.86401100
C	4.72355500	7.49636200	10.05985000
C	3.45854000	7.93217300	10.81101200
C	3.30561500	9.45977800	10.82291400
C	0.93020700	9.28704600	12.34380900
C	-0.43301200	9.71966200	11.72784100
C	-0.67810100	11.24227700	11.66728000
C	0.53827000	12.05628500	11.17746700
C	1.90729200	11.63653300	11.78615000
C	2.05765000	11.92969400	13.31104600
C	1.14593700	11.09343800	14.23459900
C	1.08236400	9.59513100	13.86718200
C	4.77356000	7.19455700	15.89239300
C	4.60360300	5.87398800	16.34779700
C	4.41063700	5.60061500	17.70269500
C	4.37186800	6.63789300	18.63838400
C	4.53382200	7.95465500	18.19903700
C	4.73549000	8.22990600	16.84592300
B	2.08408900	10.07555200	11.61133800
N	6.76977900	4.24459600	13.20086300
N	5.53983500	5.58867300	11.26566900
N	4.97311200	6.04856900	10.13393600
S	4.94788400	7.59144900	14.16358500
Fe	6.66678900	6.37367800	13.07902500
C	7.45751500	2.27032100	14.36847300
C	7.37687000	3.66261200	14.25611100
C	7.92089500	4.59972600	15.23886200
C	8.49763800	4.39757800	16.50353600
C	8.77827000	5.66542000	17.00272500
C	9.34247600	6.02226900	18.37511000
C	8.26720900	6.74130200	19.22642300
C	9.72448900	4.71478200	19.10380600
C	10.61865500	6.89065700	18.27765200
C	8.48258300	8.01244800	15.93741900
C	9.70195200	8.47615700	15.12969500
C	9.70099300	9.99770300	14.92501400
C	10.87497800	12.15965700	13.67193000
C	10.72049400	12.21852700	12.12047000

C	11.73359300	11.36652600	11.32589000
C	11.95217900	9.95023100	11.90074600
C	12.10993600	9.87680200	13.45268600
C	13.40732100	10.53790700	14.00453200
C	13.48532500	12.07162000	13.85073000
C	12.17958500	12.80771400	14.21843100
C	8.49889900	7.02978900	10.18857500
C	8.80740000	5.68471500	9.91320500
C	9.04735900	5.25559500	8.60709600
C	8.99680600	6.15872700	7.54185800
C	8.69783300	7.49891900	7.80197900
C	8.44850200	7.92871500	9.10597000
B	10.86366100	10.62827900	14.06271200
N	7.85425800	5.91111100	14.96414300
N	8.37192600	6.54859600	16.03144700
S	8.25640900	7.63191500	11.84846900
H	8.22189700	8.97296100	9.30211600
H	8.66193900	8.21685300	6.98542700
H	9.19872500	5.82604200	6.52692900
H	9.29037200	4.21112500	8.42360300
H	8.87924900	4.97912500	10.73611700
H	10.02859000	12.71637600	14.10113900
H	12.24721200	13.85517000	13.88778400
H	12.09828500	12.84782000	15.31568700
H	14.29870300	12.45206700	14.48411300
H	13.77365600	12.32365500	12.82616500
H	13.48199800	10.29015300	15.07481800
H	14.28970500	10.08066100	13.53202400
H	12.14940200	8.81121800	13.71665200
H	11.09449300	9.32127400	11.62484100
H	12.82999100	9.49324600	11.41966500
H	11.38091600	11.27452200	10.28972300
H	12.68982100	11.89478900	11.26147100
H	9.70582300	11.87332300	11.87365700
H	10.77359600	13.26390900	11.78055900
H	8.74951200	10.30816900	14.46074500
H	9.70074600	10.52317000	15.89839000
H	10.62295300	8.15707000	15.63329000
H	9.68382500	7.97771100	14.15495300
H	8.49722600	8.41457300	16.95100400
H	7.55753800	8.35016600	15.46121800
H	11.37911000	6.40731300	17.65424000
H	10.42339900	7.88319500	17.86528000
H	11.04135100	7.03017900	19.27938000
H	10.13560000	4.95432600	20.09023200
H	8.85389800	4.06787600	19.25560000
H	10.48437500	4.15132600	18.55085700
H	8.66003400	6.93059000	20.23267000

H	7.96451300	7.70212300	18.80117400
H	7.36452400	6.12899300	19.31512300
H	8.66737200	3.45834200	17.00535900
H	7.95266700	1.81728000	15.22028100
H	6.94833000	0.40346900	13.42343600
H	5.82685500	1.50187200	11.48116300
H	4.98426600	2.85396200	9.51742100
H	4.76150100	3.18378500	7.21307400
H	3.12317700	3.19139600	7.90441900
H	3.41064900	3.84445500	6.28362300
H	2.82419100	6.96551500	8.16157600
H	2.30538600	5.90389100	6.85278700
H	2.00998300	5.43856100	8.53781200
H	6.05068100	5.35582400	6.91950200
H	4.69563800	5.92357700	5.91731300
H	5.30089500	6.91335800	7.25237800
H	5.60845000	7.97278700	10.49203100
H	4.67929400	7.77619400	9.00674500
H	2.57756100	7.46213900	10.35631500
H	3.51914600	7.56317700	11.84014800
H	4.21881100	9.92010700	11.23740000
H	3.25890500	9.85623700	9.79146600
H	2.68657400	12.21552500	11.26841400
H	3.10470000	11.73485500	13.58582600
H	1.89096000	13.00054700	13.50253300
H	1.50896500	11.18698600	15.26708000
H	0.13783300	11.51910600	14.24175400
H	0.26102700	9.11829800	14.42289000
H	2.00414600	9.10716200	14.21291100
H	1.00735400	8.19704500	12.23201700
H	-0.48259000	9.31708500	10.70415300
H	-1.25891100	9.24084400	12.27513100
H	-1.52965200	11.43965800	11.00139700
H	-0.99005600	11.60332400	12.65149900
H	0.61228000	11.95014800	10.08410400
H	0.35705100	13.12633300	11.35974100
H	4.85485000	9.25613600	16.50994700
H	4.49892200	8.77473800	18.91298100
H	4.20659600	6.42464400	19.69135400
H	4.27457200	4.57083800	18.02627100
H	4.60235200	5.06151000	15.62669800

(^{Me}PDP^{tBu})Fe(NH$_2$)$_2$

Fe	4.40235100	4.40215800	-0.00004300
N	2.92701700	2.92703000	0.00001400
N	4.80776700	3.10262300	1.75323900
N	5.71472200	3.05436900	2.75540800
N	6.20351000	4.15934400	-0.65187100
H	6.67458000	3.26632000	-0.77450700
H	6.64317400	4.82839100	-1.28017000
C	0.93351200	0.93373400	0.00008800
H	0.16604400	0.16634200	0.00011200
C	1.92206800	0.95678600	0.99098300
H	1.93816400	0.20905000	1.77840700
C	2.89301400	1.95168100	0.96996400
C	3.95421800	2.08723700	1.94996800
C	4.32041900	1.37857300	3.11478600
H	3.83097000	0.51431600	3.53570200
C	5.44474900	2.01846800	3.61965000
C	6.25534000	1.67060400	4.86170800
C	5.53670000	0.53724200	5.62488700
H	4.52837700	0.83668400	5.93029500
H	6.10305900	0.28507400	6.52823800
H	5.45731300	-0.37020400	5.01673500
C	6.36903100	2.88399200	5.81505400
H	6.92438900	3.71608200	5.37405700
H	6.89288800	2.58772300	6.73160300
H	5.37620300	3.25242900	6.09613900
C	7.66410400	1.15855400	4.47267400
H	7.59040000	0.28633200	3.81418800
H	8.21569300	0.86140600	5.37274600
H	8.26141800	1.91610400	3.95651400
C	6.73681700	4.09248000	2.75408900
H	7.66536500	3.71277000	3.17938500
H	6.40557700	4.96750600	3.32552000
N	3.10268500	4.80775800	-1.75324200
N	3.05443300	5.71472400	-2.75540000
N	4.16021200	6.20348500	0.65158500
H	3.26735000	6.67476900	0.77458600
H	4.82968500	6.64314800	1.27942800
C	0.95662600	1.92226700	-0.99084000
H	0.20886300	1.93841400	-1.77823800
C	1.95161800	2.89310400	-0.96988200
C	2.08723400	3.95428100	-1.94991700
C	1.37859100	4.32047000	-3.11474900
H	0.51432400	3.83103500	-3.53565900
C	2.01849500	5.44479800	-3.61961100
C	1.67061700	6.25540100	-4.86165700
C	0.53728800	5.53673200	-5.62485400
H	0.83677000	4.52842400	-5.93027500

H	0.28510400	6.10309500	-6.52819800
H	-0.37015900	5.45730000	-5.01670900
C	2.88400500	6.36915200	-5.81499500
H	3.71606200	6.92455600	-5.37399500
H	2.58771300	6.89299200	-6.73154700
H	3.25249600	5.37634300	-6.09607800
C	1.15850900	7.66414100	-4.47260600
H	0.28629100	7.59039300	-3.81412000
H	0.86133500	8.21572800	-5.37267100
H	1.91603600	8.26147900	-3.95644200
C	4.09258300	6.73678400	-2.75411000
H	3.71284500	7.66541000	-3.17921500
H	4.96750400	6.40559300	-3.32572900
H	6.89326100	4.37259200	1.70608300
H	4.37286600	6.89306100	-1.70612200

(^{Me}PDP^{tBu})Fe(NHMe)$_2$

Fe	4.30792000	4.31141700	-0.00283200
N	5.58742200	5.60060100	-0.00989400
N	3.73747600	5.31774400	1.56221800
N	2.73451700	5.26414200	2.47441000
C	5.60530800	6.58051500	0.96851900
C	6.57843500	7.57211200	0.97656700
C	7.56136900	7.58927800	-0.02063300
C	4.50542800	6.38101800	1.87997500
C	3.98045600	7.01127500	3.02892500
C	2.85789200	6.28493500	3.39630700
C	1.90468400	6.53880600	4.55684000
C	2.46576000	7.69053200	5.41821800
C	0.51162900	6.97200200	4.03709100
C	1.77287300	5.29207400	5.46386700
C	1.80251500	4.14966300	2.36943300
N	2.78020300	4.67769400	-1.01831500
H	2.90013200	4.49978100	-2.01500200
C	1.80820800	5.75150700	-0.88846000
N	5.30997700	3.73992600	-1.57029500
N	5.25905200	2.73157300	-2.47668700
C	6.56189600	5.62039700	-0.99366300
C	7.54616500	6.60080200	-1.01236000
C	6.36576700	4.51403400	-1.89796700
C	6.99386300	3.98740300	-3.04734200
C	6.27401400	2.85744700	-3.40466900
C	6.52897000	1.89967000	-4.56119200
C	7.67218300	2.46431100	-5.43153600
C	6.97499100	0.51274500	-4.03593000
C	5.27866300	1.75372400	-5.46110400
C	4.15182400	1.79222700	-2.36101500
N	4.69030200	2.79181200	1.01886200
C	5.76967800	1.82606100	0.88862300
H	2.09910700	3.31951300	3.01941000
H	0.79362700	4.47088800	2.62844800
H	2.75406900	4.97146700	5.83144600
H	1.14730700	5.53020700	6.33226300
H	1.31043700	4.44443300	4.95106900
H	0.59326000	7.86708400	3.41118600
H	0.02192300	6.19382100	3.44390300
H	-0.14739100	7.20452900	4.88227600
H	3.45474500	7.44525700	5.82002800
H	2.54770600	8.61948800	4.84396400
H	1.79430900	7.87861700	6.26319900
H	4.36796900	7.88815800	3.52313800
H	6.56516200	8.32686200	1.75759700
H	8.32580700	8.35943200	-0.02480100
H	8.29679400	6.58885500	-1.79737200

H	7.86522100	4.37867400	-3.54832100
H	7.86090900	1.78953200	-6.27371800
H	7.41763100	3.44921200	-5.83758500
H	8.60340400	2.55625600	-4.86248800
H	7.87256700	0.60443300	-3.41500800
H	6.20342000	0.02065600	-3.43611700
H	7.20813600	-0.14925500	-4.87861400
H	5.51690300	1.12490100	-6.32711300
H	4.43696300	1.28820400	-4.94136400
H	4.94917300	2.73047800	-5.83264100
H	4.47893800	0.78424700	-2.61617500
H	3.31633300	2.07934100	-3.00840800
H	5.96273100	1.59636900	-0.16507500
H	6.73132500	2.16751500	1.31687300
H	5.52334600	0.87000600	1.38322800
H	2.14106200	6.71305900	-1.32365300
H	0.85105600	5.49639400	-1.37645200
H	1.58310700	5.94868300	0.16546500
H	4.51710400	2.91609200	2.01584300
H	3.81995300	1.81767400	-1.32119000
H	1.82469400	3.81273100	1.33116500

(^{Me}PDP^{tBu})Fe(NHPh)$_2$

Fe	5.63977700	8.63906300	5.91898400
N	5.50007800	10.83564100	5.84500200
N	3.47704300	9.30674500	6.64304600
N	2.30756200	8.75299100	7.00501300
C	4.42769000	11.49045400	6.33294100
C	4.40340200	12.88746900	6.41451500
C	5.51661900	13.60117700	5.97280800
C	3.31161800	10.63038900	6.73744700
C	2.00824700	10.92764200	7.18282800
C	1.37375600	9.70230300	7.34971700
C	-0.05921500	9.42588900	7.78708200
C	-0.70496200	10.75425600	8.23683000
C	-0.10573600	8.44724500	8.98433400
C	-0.89027100	8.86850400	6.60523300
C	2.24604300	7.29396500	6.98571600
C	4.20641900	7.27453600	3.55186400
N	4.99964700	7.22785800	4.67738200
C	3.67295500	8.50626000	3.09102800
C	2.86845600	8.57034300	1.95820700
C	2.55043800	7.41886600	1.22936000
C	3.06278200	6.19445500	1.66896200
C	3.86975000	6.11870900	2.80077900
N	7.47695400	9.35684500	4.93230300
N	8.57114900	8.80464100	4.37926000
C	6.57529400	11.52327100	5.40745500
C	6.61841800	12.92145100	5.45850300
C	7.65350400	10.68511900	4.88206000
C	8.89719600	10.98367200	4.29508400
C	9.47611800	9.75862600	3.97991300
C	10.81976400	9.48711700	3.31550900
C	11.55502000	10.83031100	3.11748800
C	10.62250500	8.84604400	1.91975800
C	11.71068800	8.58741800	4.20584800
C	7.34236300	7.67214900	8.36958900
N	6.17847900	7.95072800	7.68997100
C	8.59161900	8.22253500	7.97617400
C	9.76839200	7.91825600	8.65554200
C	9.76954400	7.06297700	9.76204400
C	8.54761900	6.52439900	10.17918000
C	7.36688900	6.81843300	9.50573000
C	8.63044300	7.34512400	4.39488000
H	5.39228400	7.57145900	8.21599900
H	5.26876600	6.26884700	4.88995800
H	4.25911200	5.15355600	3.12376200
H	2.83165900	5.28194600	1.12216800
H	1.92264000	7.47489900	0.34452700
H	2.48159300	9.53664300	1.63900000

H	3.89777600	9.41221300	3.64999800
H	8.61166000	8.92393200	7.14826200
H	10.70155700	8.37080400	8.32241600
H	10.69089000	6.83195000	10.28926800
H	8.51351900	5.86175800	11.04232800
H	6.42895900	6.38035000	9.84648800
H	2.41109500	6.88516500	7.98779900
H	1.28051000	6.95785100	6.60880900
H	0.49261800	8.82263000	9.82198600
H	-1.14016700	8.33777800	9.32982700
H	0.25879900	7.44921300	8.72730900
H	-0.51920200	7.90437100	6.24539000
H	-1.93114500	8.72468800	6.91827200
H	-0.88053900	9.56497000	5.76019100
H	-0.15780800	11.20446300	9.07231800
H	-0.74575300	11.48068700	7.41805700
H	-1.73264800	10.56887700	8.56725300
H	1.57440900	11.90122300	7.34892700
H	3.53531200	13.39838500	6.81647200
H	5.52408000	14.68600500	6.02849800
H	7.49336600	13.45700000	5.10639500
H	9.32050400	11.95831600	4.11018500
H	12.52826000	10.64898800	2.64900100
H	10.99208100	11.50641700	2.46479100
H	11.73105200	11.33684000	4.07267400
H	11.59607500	8.70656500	1.43550700
H	10.13602600	7.86741000	1.96609300
H	10.01199100	9.49095300	1.27859800
H	12.69516300	8.46689500	3.73905100
H	11.85632700	9.03802500	5.19366500
H	11.29243700	7.58838100	4.35295300
H	7.61121100	6.98369000	4.24059000
H	9.27356600	6.98453900	3.59523100
H	8.99814700	6.99967600	5.36673200
H	3.03759200	6.95794200	6.31170300

(^{Me}PDP^{tBu})Fe(PHPh)$_2$

Fe	-3.22893900	5.71963100	6.05932000
N	-5.35775900	5.74618500	5.97696000
N	-3.92238300	4.29407000	7.66040300
N	-3.40853700	3.48878000	8.61107100
N	-3.77733500	7.17691900	4.40672700
N	-3.18220300	7.96616000	3.49098600
P	-1.95920100	3.98470800	4.83442000
P	-1.98584100	7.43500000	7.34831400
C	-6.06837900	4.98468800	6.83508000
C	-7.46603000	4.97119400	6.80900100
C	-8.12324400	5.77186800	5.87637200
C	-7.38502900	6.55977500	4.99466100
C	-5.98971900	6.52057000	5.07042200
C	-5.25566400	4.20402600	7.76920500
C	-5.59791200	3.33045700	8.81734300
C	-4.39506600	2.88471000	9.35354000
C	-4.17665400	1.92301400	10.51553600
C	-3.31898300	2.57445800	11.62719700
C	-3.52536600	0.60569300	10.02643100
C	-5.54890500	1.56811500	11.12843500
C	-1.95324300	3.45721500	8.72935500
C	-3.28158100	2.94331800	4.08528500
C	-3.92106800	1.95866200	4.86828800
C	-4.90946000	1.13090100	4.33676100
C	-5.28770600	1.24785200	2.99672800
C	-4.66072500	2.20950700	2.20078700
C	-3.67955200	3.04460100	2.73606000
C	-5.09709200	7.28469200	4.19726500
C	-5.34719400	8.15447900	3.12018700
C	-4.10101500	8.57860700	2.67250400
C	-3.78167900	9.52851300	1.52420600
C	-5.09864100	9.89865600	0.80766000
C	-3.14952000	10.83980800	2.05289900
C	-2.85273800	8.85689900	0.48412400
C	-1.72171600	7.97556900	3.48170100
C	-3.34488400	8.43962000	8.08260000
C	-3.77859700	8.30481900	9.41773700
C	-4.78756200	9.11366400	9.94164300
C	-5.40738300	10.08147400	9.14762200
C	-4.99375700	10.23160800	7.82139100
C	-3.97777600	9.43023100	7.30156900
H	-1.59355200	4.67183500	3.63806200
H	-1.64514900	6.72332500	8.53767400
H	-1.60219500	4.30583500	9.32457800
H	-1.63629500	2.52479700	9.19057200
H	-2.52524500	0.75279900	9.60863500
H	-3.43088100	-0.09406400	10.86496400

H	-4.14163600	0.13137900	9.25510900
H	-2.30348600	2.80960500	11.29798100
H	-3.78111500	3.50209500	11.98242600
H	-3.23755700	1.88896200	12.47862100
H	-5.40670600	0.88427600	11.97204500
H	-6.06551500	2.45920800	11.50110100
H	-6.19875500	1.06909800	10.40144800
H	-6.58724700	3.05540000	9.14696900
H	-8.02180900	4.35003200	7.50285500
H	-9.20855500	5.78186400	5.83670100
H	-7.87729400	7.19053700	4.26253500
H	-6.30485900	8.44006300	2.71465200
H	-4.88350700	10.57496400	-0.02651500
H	-5.59863700	9.01253400	0.40189500
H	-5.79408600	10.41143500	1.48090300
H	-1.86833400	8.60971900	0.89003300
H	-3.30053600	7.93336200	0.10094800
H	-2.69774700	9.53497100	-0.36303200
H	-2.18657800	10.68107800	2.54681000
H	-2.98073700	11.53161800	1.21944100
H	-3.81541900	11.32908700	2.77185800
H	-3.20723800	3.78664100	2.09663800
H	-4.93791300	2.31284100	1.15354800
H	-6.05198500	0.59751100	2.57919300
H	-5.37969000	0.38182000	4.97080800
H	-3.62598400	1.83169600	5.90779300
H	-3.65545000	9.58302700	6.27368300
H	-5.45797300	10.98613600	7.18940100
H	-6.19333100	10.71128500	9.55629600
H	-5.09201200	8.98496800	10.97845300
H	-3.31217200	7.55771700	10.05560700
H	-1.35717700	8.89855800	3.03699500
H	-1.34079600	7.11606200	2.92142400
H	-1.53395400	3.52288000	7.72307400
H	-1.37989400	7.91385900	4.51715600

(^{Me}PDP^{tBu})Fe(OH)$_2$

Fe	1.88528500	10.95376400	7.61283300
O	2.69136100	12.62839100	7.95361900
H	3.58139800	12.61148300	8.33647600
O	0.18789500	11.15091200	6.88353200
H	-0.35828900	10.38772100	6.65072800
N	2.26139200	8.90948300	7.78040500
N	3.16149700	10.41854100	5.91399000
N	3.56662600	11.05880000	4.79362900
N	1.53306000	10.43018700	9.71121800
N	1.00159200	11.07709600	10.77344300
C	2.89147900	8.22916800	6.77008400
C	3.13050700	6.86054600	6.84623200
C	2.75127200	6.16190000	7.99877600
C	2.17974900	6.86736100	9.06459900
C	1.96270900	8.23581200	8.93693400
C	3.29305200	9.10056900	5.68031400
C	3.80818700	8.89923800	4.38340300
C	3.96938300	10.16351400	3.83018100
C	4.51336800	10.53134800	2.45530400
C	5.87993100	11.24721100	2.58705100
C	3.52003700	11.42072000	1.67078500
C	4.73190200	9.23662500	1.64351000
C	1.45193800	9.11371600	9.97455600
C	0.86678500	8.92022700	11.24264400
C	0.57931500	10.18767300	11.73395400
C	-0.04102700	10.56386700	13.07376000
C	0.99821600	11.28189200	13.96914900
C	-1.29206100	11.45526400	12.89045100
C	-0.48163500	9.27394000	13.79834500
C	3.42791000	12.51258600	4.78248100
C	0.89882800	12.53035400	10.67188200
H	3.89833100	11.58878300	0.65556100
H	2.53981900	10.93776800	1.59171600
H	3.37816700	12.40079400	2.13314900
H	5.45975600	8.57577900	2.12646200
H	3.79608400	8.68252600	1.51291300
H	5.11743600	9.48721700	0.64918900
H	6.28731900	11.46021000	1.59148000
H	5.80433900	12.19885000	3.12164400
H	6.59882100	10.61733700	3.12219400
H	4.02404900	7.95666600	3.90526700
H	3.62096900	6.35143800	6.02203400
H	2.92821600	5.09389400	8.07789700
H	1.92005800	6.36360100	9.99078800
H	0.66739400	7.98064900	11.73366200
H	0.36832200	8.61194100	13.99599100
H	-0.93542900	9.53066400	14.76181500

H	-1.22280500	8.71871200	13.21334600
H	1.87951100	10.65026900	14.12500200
H	1.33641200	12.22995900	13.54030700
H	0.55817700	11.50204700	14.94914700
H	-1.05263400	12.43317600	12.46523200
H	-2.02567600	10.97126600	12.23633000
H	-1.76700300	11.62827900	13.86334500
H	1.20642700	13.00401500	11.60587100
H	-0.12545500	12.82852900	10.42725300
H	4.31981000	12.98087800	4.36223400
H	2.54769100	12.81195800	4.20505100
H	3.28916200	12.82532800	5.82280200
H	1.55928900	12.83814700	9.85433300

(^{Me}PDP^{tBu})Fe(SPh)$_2$

Fe	7.00928300	5.92557200	13.66261500
N	7.35287100	3.78784900	13.54571300
N	5.67908500	5.16003500	12.04149400
N	4.75846700	5.64590800	11.19181100
S	5.51483200	6.73304000	15.27499000
S	8.21029400	7.59436200	12.46421800
C	7.79317100	1.06912800	13.37160900
C	6.86113900	1.67783100	12.53293600
C	6.66403300	3.05875000	12.64695600
C	5.72022800	3.83460600	11.83979100
C	4.79528600	3.46848200	10.84674200
C	4.18088700	4.65033000	10.44373300
C	3.09509700	4.84134900	9.39162700
C	3.65192300	5.59807200	8.16053100
C	2.62040200	3.45120100	8.91516500
C	1.87024000	5.58435800	9.97729800
C	4.51021500	7.08682900	11.23996600
C	3.80706100	6.60903200	14.78425800
C	3.01274800	7.76817300	14.68459000
C	1.66449500	7.68937600	14.33116500
C	1.07101200	6.45169500	14.06668400
C	1.84567200	5.29269700	14.16829700
C	3.19321400	5.36895400	14.52482600
C	8.50181300	1.83084400	14.30020100
C	8.25226900	3.20567300	14.36224600
C	8.89993600	4.12958600	15.29704600
C	9.82527400	3.94027500	16.33872300
C	10.04137200	5.19984400	16.89055900
C	10.94796000	5.58016400	18.05483300
C	10.14177100	6.25848100	19.18906000
C	11.57878300	4.29400600	18.63145000
C	12.10179700	6.49754200	17.58023200
C	9.00694500	7.49990400	16.29129300
C	9.28571400	6.52375200	11.51265300
C	10.54436600	6.13488700	12.00791900
C	11.39549700	5.32634400	11.25287500
C	11.01411300	4.88729800	9.98290000
C	9.76984000	5.27006000	9.47656600
C	8.91677200	6.07829300	10.22968500
N	8.56820700	5.42416100	15.20729900
N	9.25928900	6.06428100	16.16381200
H	7.95618600	6.38210800	9.82391400
H	9.46151900	4.94249200	8.48600700
H	11.67929000	4.26106600	9.39396800
H	12.36468700	5.04331900	11.65805100
H	10.85352800	6.48390300	12.98891300
H	9.81489700	7.97302200	16.84328900

H	8.05173400	7.66361800	16.79850800
H	12.68837100	6.00836300	16.79498800
H	11.75101300	7.45517000	17.18522800
H	12.77168900	6.71424800	18.42048300
H	12.22777300	4.55163500	19.47523300
H	10.81416700	3.59951400	18.99602000
H	12.19154400	3.77540100	17.88601700
H	10.80259200	6.46249300	20.03955700
H	9.69521100	7.20843000	18.88421800
H	9.33377000	5.60518600	19.53589300
H	10.27906400	3.01492300	16.65662900
H	9.22854600	1.37302800	14.96234800
H	7.96737100	-0.00085400	13.30237900
H	6.30036900	1.10038500	11.80613100
H	4.59389500	2.47915900	10.46732100
H	3.43434800	2.88124900	8.45378500
H	2.20973100	2.86202300	9.74232700
H	1.83246000	3.57166700	8.16406500
H	2.09307700	6.61815800	10.25171800
H	1.06584900	5.60706200	9.23285100
H	1.49540400	5.07939500	10.87365200
H	4.49964300	5.05934700	7.72324300
H	2.87191700	5.68517300	7.39508700
H	3.98902300	6.61037400	8.40208200
H	5.45519500	7.56989200	11.49850600
H	4.18022100	7.43829900	10.26442800
H	3.78179600	4.46085200	14.61911100
H	1.39581300	4.31956400	13.98145500
H	0.01974700	6.39085500	13.79712800
H	1.07429200	8.60087300	14.26451200
H	3.46788200	8.73268800	14.89117000
H	8.95340000	7.91672000	15.28232600
H	3.75911600	7.31486500	12.00061600

(^{BBN}PDP^{tBu})Fe(NH$_2$)$_2^-$

Fe	-2.29031000	4.87538400	5.31056600
N	-0.51064300	3.86114600	5.30437700
N	-2.08356500	4.01100200	3.18251600
N	-2.78500700	3.86530800	2.02494000
C	1.95432400	2.45667300	5.29541100
C	1.13770400	2.49475100	4.15136900
C	-0.06475300	3.18388500	4.17564700
C	-0.97170500	3.26264200	3.04870000
C	-0.95737500	2.64919700	1.77534900
C	-2.12127500	3.04761700	1.13818000
C	-2.60359300	2.65773700	-0.25533400
C	-1.51291500	1.80219200	-0.93696700

C	-2.83517200	3.90200100	-1.14705000
C	-3.88782100	1.79509600	-0.18053700
C	-4.02580500	4.63362400	1.86064900
C	-4.84343400	4.73315100	3.15243900
C	-5.25421000	3.39251000	3.78327700
B	-5.43599800	3.45471400	5.42103200
N	-3.92792900	3.69167100	5.99007900
H	-3.47816700	2.77423300	5.90973400
H	-3.97248100	3.83750200	6.99904100
C	-6.46603500	4.61766600	5.96467800
C	-7.86014200	4.38805600	5.33172100
C	-8.47160800	2.98682000	5.57160300
C	-7.47811800	1.80681600	5.43659000
C	-6.06877000	2.05142900	6.03162600
C	-6.06938100	2.07947700	7.57956200
C	-6.79351800	3.29274000	8.20746100
C	-6.51025800	4.64684700	7.51384500
N	-1.42985100	5.13141200	7.43580800
N	-1.65061200	5.81491700	8.59206700
C	1.51169500	3.13690400	6.44378000
C	0.30580000	3.82006100	6.42831900
C	-0.21610900	4.56029100	7.55919500
C	0.33153300	4.86784000	8.82537900
C	-0.59908900	5.66832300	9.46806200
C	-0.49213100	6.29479600	10.85457900
C	0.80581700	5.79483300	11.52638000
C	-1.67189500	5.87424200	11.76481000
C	-0.39917900	7.83821000	10.76159500
C	-2.94097700	6.49497800	8.76238400
C	-3.44098000	7.15874400	7.47505900
C	-2.48871500	8.18925100	6.84697300
B	-2.63523600	8.31808700	5.20983700
N	-2.09876200	6.88908200	4.63758900
H	-1.07870600	6.95559400	4.71224500
H	-2.25330600	6.86011900	3.62938100
C	-4.15446700	8.64731500	4.66637900
C	-4.63224500	9.97938600	5.29654800
C	-3.70888700	11.19589200	5.05091400
C	-2.19437300	10.90587700	5.18755700
C	-1.72102000	9.55476100	4.59562400
C	-1.74724900	9.53977800	3.04781700
C	-3.16025600	9.57493300	2.42096600
C	-4.20174300	8.66591200	3.11709900
H	2.89751000	1.91925100	5.29216500
H	-1.52326200	6.27371500	12.77605000
H	-2.63655400	6.23920000	11.40429800
H	-1.73297200	4.78236100	11.83667500
H	0.46422400	8.13220600	10.15495600

H	-1.28485400	8.29205100	10.30949100
H	-0.27677300	8.26820000	11.76417000
H	1.69204300	6.08753700	10.95332400
H	0.89441700	6.23146900	12.52818900
H	0.80863800	4.70428600	11.62979900
H	1.29288300	4.56277500	9.20815700
H	2.10806100	3.13248800	7.35260700
H	1.44120100	1.98755300	3.23905700
H	-0.20340600	1.98430300	1.38394000
H	-1.31806200	0.88090400	-0.37770500
H	-1.84136400	1.52066100	-1.94443600
H	-0.57091300	2.35366800	-1.02871100
H	-3.70660300	0.89092400	0.41064300
H	-4.72844400	2.32200300	0.27825100
H	-4.19389100	1.49016800	-1.18965000
H	-1.92269600	4.50570400	-1.21118900
H	-3.10632100	3.58752900	-2.16293900
H	-3.63563700	4.54676200	-0.77616300
H	-3.77125300	5.63578100	1.48501500
H	-4.61505200	4.13312400	1.09176800
H	-4.28278200	5.34766600	3.86436900
H	-5.73078800	5.33412100	2.91011500
H	-4.47814900	2.64049200	3.56347500
H	-6.15547100	3.03167600	3.26564600
H	-5.45413700	1.17886600	5.73726100
H	-7.94692100	0.90938100	5.87953600
H	-7.35736900	1.57733300	4.36892000
H	-8.93102100	2.96115600	6.56655500
H	-9.30695800	2.83385300	4.87003200
H	-8.58468400	5.14383100	5.68312900
H	-7.77013000	4.54662200	4.24742500
H	-6.14720800	5.62681900	5.65071700
H	-5.54090600	5.02329400	7.87464000
H	-7.25071400	5.38201100	7.87490600
H	-7.87296000	3.10554000	8.20658200
H	-6.51879500	3.36817800	9.27168200
H	-6.51058300	1.15731400	7.99773600
H	-5.02329800	2.08032400	7.92396900
H	-3.67582900	5.76551100	9.13383100
H	-2.80733200	7.25131900	9.53624200
H	-3.69094100	6.36939400	6.75877900
H	-4.40573600	7.62259700	7.72243300
H	-1.44825600	7.89355800	7.06198500
H	-2.62533400	9.14835700	7.36864000
H	-4.88132800	7.87905800	4.98242000
H	-5.64678700	10.24198900	4.94815500
H	-4.72271900	9.82571400	6.38156500
H	-3.91097600	11.60385800	4.05385400

H	-3.98381300	12.00305100	5.74834900
H	-1.63963600	11.75154200	4.74218300
H	-1.93554200	10.91480100	6.25530100
H	-0.65908300	9.44470200	4.88889000
H	-1.16076200	10.37647200	2.62836500
H	-1.23429200	8.62800700	2.70330000
H	-3.52620500	10.60762600	2.41970400
H	-3.09194000	9.29625600	1.35728200
H	-4.05421300	7.63527200	2.75968300
H	-5.20533200	8.94940400	2.75454700

(^{BBN}PDP^{tBu})Fe(OH)$_2^-$

Fe	2.17120000	11.11730000	7.73660000
O	3.58620000	12.38650000	8.48700000
H	3.57880000	12.31030000	9.44990000
O	0.57040000	12.06340000	6.88450000
H	0.59340000	11.89770000	5.93320000
N	2.35150000	9.10300000	7.82730000
N	2.94960000	10.52600000	5.68640000
N	3.45510000	11.06990000	4.54350000
N	1.49030000	10.57770000	9.84150000
N	0.87700000	11.11730000	10.93270000
C	2.81440000	8.37520000	6.74160000
C	2.94380000	6.99580000	6.78260000
C	2.61230000	6.29170000	7.95410000
C	2.14800000	7.02470000	9.06090000
C	2.02190000	8.40250000	8.97750000
C	3.16310000	9.19660000	5.60020000
C	3.78150000	8.89100000	4.36820000
C	3.96060000	10.09730000	3.71090000
C	4.59780000	10.32630000	2.34390000
C	5.94710000	11.07590000	2.47400000
C	3.64250000	11.08330000	1.38950000
C	4.89530000	8.95390000	1.69940000
C	1.51790000	9.24400000	10.04380000
C	0.94580000	8.93890000	11.29810000
C	0.54160000	10.14490000	11.84730000
C	-0.15500000	10.37120000	13.18550000
C	0.62820000	11.36510000	14.07730000
C	-1.61300000	10.85400000	12.98120000
C	-0.21850000	9.02750000	13.94510000
C	3.38140000	12.52630000	4.36180000
C	3.61570000	13.31490000	5.65800000
C	4.91480000	12.98190000	6.41550000
B	4.82910000	13.24810000	8.03110000
C	6.16820000	12.75350000	8.84860000
C	5.93750000	12.83730000	10.37820000
C	5.45600000	14.21220000	10.89940000

C	4.38310000	14.89830000	10.02040000
C	4.62060000	14.81360000	8.49190000
C	5.83620000	15.64770000	8.01620000
C	7.21940000	15.11800000	8.46500000
C	7.38870000	13.58210000	8.37580000
C	0.34800000	13.19880000	9.63320000
C	-0.85960000	12.58340000	8.90160000
B	-0.79440000	12.75630000	7.27310000
C	-2.02950000	12.01920000	6.47530000
C	-1.78970000	12.05100000	4.94450000
C	-1.50950000	13.45000000	4.34650000
C	-0.56650000	14.33750000	5.19300000
C	-0.81540000	14.30570000	6.72110000
C	-2.14990000	14.97240000	7.13880000
C	-3.43030000	14.21490000	6.71210000
C	-3.36810000	12.67870000	6.89000000
C	0.69250000	12.57380000	10.99150000
H	4.09870000	11.16700000	0.39490000
H	2.69510000	10.54250000	1.28400000
H	3.41220000	12.09440000	1.73340000
H	5.60320000	8.37320000	2.30020000
H	3.98150000	8.36210000	1.57820000
H	5.33900000	9.10110000	0.70770000
H	6.41360000	11.18210000	1.48620000
H	5.84030000	12.07650000	2.90100000
H	6.63320000	10.51680000	3.11930000
H	4.07850000	7.91520000	4.01720000
H	3.30510000	6.46750000	5.90400000
H	2.71250000	5.21190000	8.00280000
H	1.88320000	6.51980000	9.98640000
H	0.82160000	7.95900000	11.73170000
H	0.78300000	8.62280000	14.12690000
H	-0.70680000	9.17570000	14.91550000
H	-0.79540000	8.28000000	13.39030000
H	1.65360000	11.01320000	14.23810000
H	0.68340000	12.36830000	13.64830000
H	0.14050000	11.45000000	15.05670000
H	-1.67590000	11.81440000	12.46300000
H	-2.17650000	10.12550000	12.38830000
H	-2.11080000	10.96550000	13.95310000
H	1.60520000	13.03040000	11.40340000
H	-0.11520000	12.76170000	11.69890000
H	0.17840000	14.26770000	9.82560000
H	1.24560000	13.16970000	9.01000000
H	-0.89770000	11.50430000	9.11400000
H	-1.78230000	12.99960000	9.33310000
H	-0.00800000	14.90520000	7.17560000
H	-2.15130000	15.06150000	8.23500000

H	-2.21710000	16.00670000	6.75660000
H	-4.28740000	14.60780000	7.28160000
H	-3.65560000	14.44850000	5.66510000
H	-4.21850000	12.23280000	6.34350000
H	-3.54240000	12.44470000	7.94970000
H	-2.10100000	10.95420000	6.75850000
H	-0.93390000	11.39300000	4.71500000
H	-2.63680000	11.60070000	4.39800000
H	-1.08710000	13.33320000	3.33570000
H	-2.46020000	13.97320000	4.19710000
H	0.47060000	14.01040000	5.01930000
H	-0.61400000	15.36760000	4.79870000
H	4.14060000	12.79150000	3.62600000
H	2.40100000	12.78030000	3.93170000
H	3.59400000	14.37680000	5.37480000
H	2.73900000	13.18130000	6.29650000
H	5.74610000	13.52930000	5.94620000
H	5.14990000	11.91620000	6.27350000
H	6.39810000	11.69700000	8.62450000
H	5.19170000	12.07360000	10.65750000
H	6.84650000	12.55210000	10.93620000
H	5.06510000	14.09490000	11.92280000
H	6.31950000	14.87850000	11.00060000
H	3.40740000	14.43330000	10.23290000
H	4.28060000	15.94590000	10.35350000
H	3.72910000	15.25880000	8.01760000
H	5.81560000	15.67310000	6.91700000
H	5.74860000	16.70060000	8.33900000
H	8.00320000	15.60160000	7.86070000
H	7.41340000	15.44380000	9.49330000
H	8.30070000	13.30190000	8.93310000
H	7.58850000	13.31550000	7.32830000

(^{BBN}PDP^{tBu})Fe(PHPh)$_2^-$

C	-5.92820000	5.00840000	6.90090000
C	-7.31610000	5.02540000	6.87490000
C	-7.99190000	5.82200000	5.94030000
C	-7.22490000	6.58140000	5.04570000
C	-5.83860000	6.53180000	5.10030000
C	-5.16200000	4.22590000	7.85130000
C	-5.56350000	3.32260000	8.86140000
C	-4.40130000	2.86520000	9.45920000
C	-4.27350000	1.86260000	10.60210000
C	-3.59120000	2.49100000	11.84250000
C	-3.51330000	0.59280000	10.14500000
C	-5.68870000	1.42150000	11.03590000
C	-1.93290000	3.53170000	9.14430000
C	-1.00850000	3.56760000	7.92590000

C	-1.08790000	2.34750000	6.99390000
C	-0.39170000	1.28750000	4.52680000
C	0.65000000	0.34950000	5.19350000
C	2.01780000	1.00000000	5.51180000
C	1.93860000	2.43650000	6.07940000
C	0.91290000	3.37130000	5.38210000
C	1.32190000	3.72170000	3.93090000
C	1.22300000	2.56450000	2.90910000
C	-0.01540000	1.65120000	3.06980000
C	-3.39650000	2.90640000	3.97340000
C	-4.19920000	2.06470000	4.76640000
C	-5.22800000	1.30810000	4.20450000
C	-5.49120000	1.37620000	2.83460000
C	-4.71140000	2.21300000	2.03420000
C	-3.67890000	2.96520000	2.59610000
C	-4.98170000	7.26490000	4.18880000
C	-5.27710000	8.19530000	3.16680000
C	-4.06170000	8.56430000	2.61400000
C	-3.81530000	9.55020000	1.47620000
C	-5.17780000	10.07600000	0.97210000
C	-2.99970000	10.77420000	1.96180000
C	-3.11550000	8.86930000	0.27420000
C	-1.65310000	7.75490000	3.06630000
C	-0.82780000	7.72760000	4.35520000
C	-0.95080000	8.96930000	5.25340000
C	0.91190000	7.94890000	7.02540000
C	1.21610000	7.62470000	8.50830000
C	1.06260000	8.80500000	9.49590000
C	-0.15280000	9.72490000	9.23320000
C	-0.42280000	10.06520000	7.74700000
C	0.67550000	10.97900000	7.13930000
C	2.05310000	10.30560000	6.92530000
C	1.99520000	8.85830000	6.38270000
C	-3.47030000	8.46070000	8.17580000
C	-3.83480000	8.38090000	9.53220000
C	-4.89050000	9.13710000	10.04380000
C	-5.60940000	9.99790000	9.21260000
C	-5.26270000	10.08740000	7.86270000
C	-4.21100000	9.32730000	7.35040000
B	-0.55460000	2.63070000	5.45570000
B	-0.53410000	8.70930000	6.83090000
Fe	-3.15590000	5.66260000	6.07230000
N	-5.16090000	5.75470000	6.02320000
N	-3.81960000	4.31520000	7.82450000
N	-3.35980000	3.47830000	8.79730000
N	-3.65250000	7.07010000	4.26110000
N	-3.09750000	7.86640000	3.30690000
P	-2.04070000	3.90460000	4.72710000

P	-2.08640000	7.46340000	7.47960000
H	-1.58810000	4.48330000	3.51530000
H	-1.69390000	6.85020000	8.69460000
H	0.93660000	4.32030000	5.94290000
H	0.68170000	4.54590000	3.58820000
H	2.35030000	4.12100000	3.90450000
H	1.22900000	2.98420000	1.89100000
H	2.13070000	1.95280000	2.96730000
H	0.15020000	0.73860000	2.47100000
H	-0.88100000	2.14880000	2.61300000
H	-1.33100000	0.71290000	4.47090000
H	0.21820000	-0.03020000	6.12990000
H	0.82710000	-0.54220000	4.56690000
H	2.63510000	1.00570000	4.60670000
H	2.56280000	0.36170000	6.22500000
H	1.67860000	2.37540000	7.14580000
H	2.94890000	2.87920000	6.04570000
H	-0.51510000	1.52950000	7.45890000
H	-2.12530000	1.97880000	6.97460000
H	-1.21540000	4.49040000	7.37460000
H	0.01220000	3.68860000	8.31300000
H	-1.76830000	4.41640000	9.77600000
H	-1.71500000	2.64880000	9.74480000
H	-2.49110000	0.80060000	9.81850000
H	-3.46190000	-0.12990000	10.96940000
H	-4.03320000	0.11720000	9.30620000
H	-2.55630000	2.78710000	11.65530000
H	-4.13930000	3.38040000	12.17320000
H	-3.58480000	1.76880000	12.66870000
H	-5.61270000	0.69470000	11.85320000
H	-6.28130000	2.27090000	11.39290000
H	-6.23120000	0.94590000	10.21200000
H	-6.57250000	3.03330000	9.10970000
H	-7.86890000	4.42070000	7.58850000
H	-9.07670000	5.84710000	5.90770000
H	-7.70550000	7.20510000	4.29710000
H	-6.25130000	8.56080000	2.88250000
H	-5.01820000	10.78580000	0.15200000
H	-5.80740000	9.26200000	0.59650000
H	-5.72540000	10.59600000	1.76530000
H	-2.11350000	8.50590000	0.51470000
H	-3.70440000	8.01580000	-0.08030000
H	-3.01900000	9.58350000	-0.55320000
H	-2.00720000	10.50720000	2.33370000
H	-2.86830000	11.48710000	1.13780000
H	-3.52560000	11.28590000	2.77530000
H	-3.08050000	3.60910000	1.95650000
H	-4.90510000	2.28130000	0.96550000

H	-6.29590000	0.78920000	2.39820000
H	-5.83080000	0.66640000	4.84350000
H	-4.02420000	2.00890000	5.83630000
H	-3.96880000	9.39930000	6.29440000
H	-5.81750000	10.74850000	7.20040000
H	-6.43210000	10.58770000	9.61020000
H	-5.14980000	9.05290000	11.09730000
H	-3.28420000	7.71810000	10.19500000
H	-1.36050000	8.60910000	2.45660000
H	-1.47360000	6.84410000	2.47820000
H	-1.10310000	6.82210000	4.90550000
H	0.21740000	7.57410000	4.05520000
H	-0.33020000	9.76730000	4.81570000
H	-1.98030000	9.35610000	5.19270000
H	0.96180000	6.98940000	6.48490000
H	0.54420000	6.81550000	8.82530000
H	2.23510000	7.21450000	8.61280000
H	1.97820000	9.40730000	9.48500000
H	0.99670000	8.40820000	10.52100000
H	-1.05300000	9.24390000	9.63820000
H	-0.02070000	10.64760000	9.82480000
H	-1.35700000	10.65040000	7.72600000
H	0.31370000	11.35160000	6.17100000
H	0.82160000	11.87670000	7.76490000
H	2.65230000	10.92270000	6.23750000
H	2.60860000	10.31200000	7.86970000
H	2.99480000	8.40500000	6.49590000
H	1.81060000	8.89940000	5.30020000

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