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. ($^{1}$BNPDP$^{tBu}$)$_2$FeBr$_2$, ($^{1}$BNPDP$^{tBu}$)$_2$FeBr$_2$, LiBDEt$_3$, and potassium graphite$^3$ were synthesized according to literature procedures.

NMR spectra were recorded on Varian Vnmrs 700 or Varian MR400 spectrometers.$^{1}$H, $^{13}$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 $^{1}$H 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 ($^{1}$BNPDP$^{tBu}$)$_2$FeH$_2$, [K(18-crown-6)$_2$][($^{1}$BNPDP$^{tBu}$)$_2$Fe(OPh)$_2$], ($^{1}$BNPDP$^{tBu}$)$_2$Fe(SPh)$_2$(NH$_3$)$_2$, ($^{1}$BuPDP$^{tBu}$)$_2$Fe(SPh)$_2$, and ($^{1}$BNPDP$^{tBu}$)$_2$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)][($^{1}$BNPDP$^{tBu}$)$_2$FeH$_2$], ($^{1}$BNPDP$^{tBu}$)$_2$Fe(SPh)$_2$, [($^{1}$BNPDP$^{tBu}$)$_2$Fe(NC)$_2$)$_2$, ($^{1}$BNPDP$^{tBu}$)$_2$Fe(PhPh)$_2$, (BBNPDP$^{tBu}$)$_2$Fe(NHMe)$_2$, (BBNPDP$^{tBu}$)$_2$Fe(NHPh)$_2$, and (BBNPDP$^{tBu}$)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, CH2, and CH3 moieties, respectively. Methyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density. Ueq(H) values were set to a multiple of Ueq(C) with 1.5 for CH3, and 1.2 for CH2, 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 \((^{BBN}PDP^{Bu})\)FeH2.** A 20 mL scintillation vial was charged with \((^{BBN}PDP^{Bu})\)FeBr2 (0.200 g, 0.232 mmol), 6 mL THF, and stir bar and frozen. On thawing, KBHEt3 (1.0 M in THF, 0.505 mL, 0.505 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 (0.164 g, 0.229 mmol, 89%) assigned as \((^{BBN}PDP^{Bu})\)FeH2. Single, X-ray quality crystals were obtained by layering a concentrated toluene solution of \((^{BBN}PDP^{Bu})\)FeH2 with n-pentane at -35 °C. 1H NMR (THF, 25 °C) δ = -16.9 (155, 2H), -11.6 (228, 2H), -8.5 (688, 2H), -7.2 (190, 2H), 8.7 (11, 18H, C(CH3)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). μeff = 4.6 +/- 0.2 μB (THF, 25 °C). MALDI-TOF of C41H63N5B2Fe1: Calc. 705.48; Found 705.81. UV-Vis (THF, ambient temperature): λmax = 327 nm (7,900 M⁻¹cm⁻¹). IR (KBr, ambient temperature): 1839 cm⁻¹ (Fe-H-B, broad).

**Synthesis of \((^{BBN}PDP^{Bu})\)ZnI2.** A 20 mL scintillation vial was charged with zinc(II) iodide (0.282 g, 0.883 mmol), \((^{BBN}PDP^{Bu})\) (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 \((^{BBN}PDP^{Bu})\)ZnI2. This sample was subjected to elemental analysis: Calc. for C41H65N5B2Zn1 C, 50.94; H, 6.57; N, 7.24. Found C, 49.97; H, 6.32; N, 7.01. 1H NMR (CDCl3, 25 °C) δ = 1.20-1.28 (m, 4H, 9-BBN-CH), 1.46 (s, 18H, C(CH3)3), 1.54 (t, J = 8.0, 4H, B-CH2), 1.72-1.87 (m, 24H, 9-BBN-CH), 4.63 (t, J = 8.4, 4H, N-CH2), 6.50 (s, 2H, pyrazole-CH), 7.61 (d, J = 8.0, 2H, m-pyridine-CH), 7.95 (t, J = 8.0, 1H, p-pyridine-CH). 13C NMR (CDCl3, 25 °C) δ = 23.41 (9-BBN-CH2), 24.71 (9-BBN-CH), 27.04 (CH2CH2CH2), 30.39 (C(CH3)3), 31.32 (B-CH3), 32.10 (C(CH3)3), 33.34 (9-BBN-CH2), 54.52 (N-CH2), 101.58 (pyrazole-CH), 119.06 (m-pyridine-CH), 141.00 (p-pyridine-CH), 143.29 (Ar-C), 148.53 (Ar-C), 155.06 (Ar-C). 11B NMR (CDCl3, 25 °C) δ = 86.63 (9-BBN). MALDI-TOF of C41H65N5B2Zn1 - I: Calc. 838.360; Found 838.090.

**Synthesis of \((^{BBN}PDP^{Bu})\)ZnH2.** A 20 mL scintillation vial was charged with \((^{BBN}PDP^{Bu})\)ZnI (0.250 g, 0.259 mmol), 10 mL THF, a stir bar and frozen. On thawing, KBHEt3 (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 \((^{BBN}PDP^{Bu})\)ZnH2. Single, X-ray quality crystals were obtained by slow diffusion of n-pentane into a toluene solution of \((^{BBN}PDP^{Bu})\)ZnH2 at room temperature. 1H NMR (THF-d8, 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, CH3), 1.75-2.05 (m, 14H), 4.55-4.71 (m, 4H, N-CH2 x 2), 6.78 (s, 2H, pyrazole-CH), 7.76 (d, J = 7.6, 2H, m-pyr-CH), 8.07 (t, J = 7.6, 1H, p-pyr-CH). 13C NMR (THF-d8, 25 °C) δ = 18.62 (broad), 25.80, 26.24 (broad), 26.37, 26.94 (broad), 28.93, 30.37 (C(CH3)3), 30.86, 32.91, 34.00-36.00 (broad, 3 resonances), 54.03 (N-CH2), 102.74 (pyrazole-CH), 119.80 (m-pyr-CH), 143.07 (Ar-C), 143.81 (Ar-C), 148.40 (Ar-C), 157.21 (Ar-C). 11B NMR (THF-d8, 25 °C) δ = 5.43 (B-H). MALDI-TOF of C41H65N5B2Zn1: Calc. 713.472; Found 713.855. IR (KBr, ambient temperature): 1775 cm⁻¹ (Zn-H-B, broad).
Synthesis of [K(2,2,2-cryptand)][(BBPDPBu)FeH2]. A 20 mL scintillation vial was charged with (BBPDPBu)FeH2 (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)][(BBPDPBu)FeH2]. Single, X-ray quality crystals were obtained by layering a THF solution of [K(2,2,2-cryptand)][(BBPDPBu)FeH2] with n-pentane at -35 °C. 1H 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(CH3)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): λmax = 344 nm (7,200 M⁻¹cm⁻¹), 475 nm (3,500 M⁻¹cm⁻¹), 646 nm (1700 M⁻¹cm⁻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 (BBPDPBu)Fe(NH2). A 20 mL scintillation vial was charged with (BBPDPBu)FeH2 (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 (BBPDPBu)Fe(NH2) by 1H NMR spectroscopy.¹

Synthesis of (BBPDPBu)Fe(NHMe). A 20 mL scintillation vial was charged with (BBPDPBu)FeH2 (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 (BBPDPBu)Fe(NHMe)2. Single, X-ray quality crystals were obtained by layering a DCM solution of (BBPDPBu)Fe(NHMe)2 with hexamethyldisiloxane at room temperature. 1H NMR (THF, 25 °C) δ = -23.1 (35, 1H, p-pyridine-C), -21.2 (390, 2H), -2.3 (55, 2H), -0.8 (29, 2H), -0.5 (23, 2H), -0.3 (50, 2H), 0.4 (54, 2H × 2), 4.2 (38, 2H), 4.5 (11, 18H, C(CH3)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). μeff = 5.2+/−0.1 μB (THF, 25 °C). MALDI-TOF of C43H71N7B2Fe1: Calc. 763.53; Found 763.36. UV-Vis (THF, ambient temperature): λmax = 339 nm (10,000 M⁻¹cm⁻¹). IR (KBr, ambient temperature): 3321, 3288, 3220, 3144 cm⁻¹ (NH).

Synthesis of (BBPDPBu)Fe(NHPh). A 20 mL scintillation vial was charged with (BBPDPBu)FeH2 (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 (BBPDPBu)FeH2, 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 to afford light yellow powder (0.045 g, 0.051 mmol, 73%) assigned as (BBPDPBu)Fe(NHPh)2. Single, X-ray quality crystals were obtained by layering a THF solution of (BBPDPBu)Fe(NHPh)2 with 2,2,4-trimethylpentane at room temperature. 1H 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-CH), -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(CH3)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). μeff = 4.5+/−0.1 μB (THF, 25 °C). UV-Vis (THF, ambient temperature): λmax = 330 nm (8,600 M⁻¹cm⁻¹). IR (KBr, ambient temperature): 3372, 3293, 3135, 3067 cm⁻¹ (NH).
Synthesis of (BBNPDPBu)Fe(OH)2. A 20 mL scintillation vial was charged with (BBNPDPBu)FeH2 (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 (BBNPDPBu)Fe(OH)2. This sample was subjected to elemental analysis: Calc. for C41H65N5O2B2Fe1 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 (BBNPDPBu)Fe(OH)2 at room temperature. 1H NMR (CDCl3, 24 °C) δ = -28.9 (29, 1H, p-pyridine-C6H4), -23.0 (316, 2H), -6.3 (201, 2H), -3.9 (179, 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). μeff = 5.3 +/− 0.1 μB (THF, 25 °C). MALDI-TOF of C41H65N5O2B2Fe1: Calc. 737.47; Found 737.53. UV-Vis (THF, ambient temperature): λmax = 333 nm (10,200 M−1cm−1). IR (KBr, ambient temperature): 3630 cm−1 (OH).

Synthesis of (BBNPDPBu)Fe(PHPh)2. Caution! This compound is extremely malodorous even in trace quantities! A 20 mL scintillation vial was charged with (BBNPDPBu)FeH2 (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 (BBNPDPBu)Fe(PHPh)2. Single, X-ray quality crystals were obtained by slow diffusion of n-pentane into a THF solution of (BBNPDPBu)Fe(PHPh)2 at -35 °C. 1H NMR (CDCl3, 24 °C) δ = -29.5 (45, 1H, p-pyridine-C6H4), -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(CH3)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). μeff = 5.2 +/− 0.1 μB (THF, 25 °C). UV-Vis (THF, ambient temperature): λmax = 336 nm (11,500 M−1cm−1), 405 nm (3,800 M−1cm−1). IR (KBr, ambient temperature): 2340 cm−1 (PH).

Synthesis of (BBNPDPBu)Fe(SPh)2. A 20 mL scintillation vial was charged with (BBNPDPBu)FeH2 (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 orange powder (0.088 g, 0.095 mmol, 72%) assigned as (BBNPDPBu)Fe(SPh)2. This sample was subjected to elemental analysis: Calc. for C53H73N5S2B2Fe1 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 (BBNPDPBu)Fe(SPh)2 at room temperature. 1H NMR (CD6D6, 24 °C) δ = -32.6 (214, 4H), -28.7 (21, 2H, p-phenyl-CH), -18.8 (39, 1H, p-pyridine-CH), -0.3 (44, 4H), 1.8 (58, 16H (3 overlapping resonances: 4H, 4H, 8H), BBN-CH2 (for 8H)), 4.0 (18, 8H, BBN-CH2), 7.0 (12, 18H, C(CH3)3), 18.2 (26, 4H), 25.2 (172, 4H), 29.4 (760, 4H), 31.9 (285, 4H), 45.5 (43, 2H, IM-CH or m-pyridine-CH), 57.5 (46, 2H, IM-CH or m-pyridine-CH). μeff = 5.5 +/− 0.1 μB (THF, 25 °C). MALDI-TOF of C53H73N5S2B2Fe1 - SPh: Calc. 812.47; Found 812.55. UV-Vis (THF, ambient temperature): λmax = 330 nm (5,200 M−1cm−1).
Alternative synthesis of \((\text{BBNPDP}^{\text{Bu}})\text{Fe(SPh)}_2\). A 20 mL scintillation vial was charged with \((\text{BBNPDP}^{\text{Bu}})\text{FeH}_2\) (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 change 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 \((\text{BBNPDP}^{\text{Bu}})\text{Fe(SPh)}_2\). Repeating the reaction in a sealed J-Young NMR tube revealed the formation of H$_2$ by $^1$H NMR spectroscopy.

Synthesis of \((\text{BBNPDP}^{\text{Bu}})\text{Zn(SPh)}_2\). A 20 mL scintillation vial was charged with \((\text{BBNPDP}^{\text{Bu}})\text{ZnH}_2\) (0.080 g, 0.112 mmol) 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 \((\text{BBNPDP}^{\text{Bu}})\text{ZnH}_2\) 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 \((\text{BBNPDP}^{\text{Bu}})\text{Zn(SPh)}_2\). Single, X-ray quality crystals were obtained by diffusing n-pentane into a C$_6$H$_6$ solution of \((\text{BBNPDP}^{\text{Bu}})\text{Zn(SPh)}_2\) at room temperature. Repeating the reaction in a sealed J-Young NMR tube revealed the formation of H$_2$. $^1$H NMR (C$_6$D$_6$, 23 °C) $\delta = 1.13$ (s, 18H, C(C$_3$H$_3$)$_3$), 1.40 (t, $J = 8.4$, 4H, B-C$_2$H$_2$), 1.58-1.66 (m, 4H, BBN-C$_3$H), 1.76 (s, 4H, BBN-C$_3$H), 2.07-2.23 (m, 12H (4H and 8H), BBN-CH and phenyl-CH), 2.74 (p, $J = 7.6$, 4H, CH$_2$C$_2$CH$_2$), 4.27 (t, $J = 7.2$, 4H, N-C$_2$H), 6.08 (s, 2H, IM-C$_3$H), 6.60-6.66 (m, 8H, m-pyridine-C$_3$H and phenyl-C$_3$H), 6.85 (t, $J = 8.0$, 1H, p-pyridine-CH), 7.22-7.27 (m, 4H, phenyl-CH). $^{13}$C NMR (C$_6$D$_6$, 23 °C) $\delta = 22.38$ (B-C$_2$H$_2$), 24.79 (9-BBN-C$_3$H), 26.40 (CH$_2$C$_2$CH$_2$), 29.01 (9-BBN-C$_3$H), 31.63 (C(C$_3$H$_3$)$_3$), 33.54 (9-BBN-C$_3$H), 33.84 (9-BBN-C$_3$H), 54.51 (N-C$_2$H), 100.84 (pyrazole-C$_3$H), 118.35 (m-pyridine-CH), 123.23, 127.27 (SPh-CH), 134.17 (SPh-CH), 139.49, 141.72 (p-pyridine-CH), 143.99, 148.63, 155.03. The $^{11}$B resonance was not observed. MALDI-TOF of C$_{53}$H$_{73}$N$_5$B$_2$S$_2$Zn$_1$-SPh: Calc. 820.467; Found 820.454.

Synthesis of \((\text{BBNPDP}^{\text{Bu}})\text{Fe(SPh)}_2(NH}_3)_2\). A 20 mL scintillation vial was charged with \((\text{BBNPDP}^{\text{Bu}})\text{Fe(SPh)}_2\) (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 \((\text{BBNPDP}^{\text{Bu}})\text{Fe(SPh)}_2(NH}_3)_2\). This sample was subjected to elemental analysis: Calc. for C$_{53}$H$_{79}$N$_7$S$_2$B$_2$Fe$_1$ 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 n-pentane into a toluene solution of \((\text{BBNPDP}^{\text{Bu}})\text{Fe(SPh)}_2(NH}_3)_2\) at room temperature. $^1$H NMR (CD$_2$Cl$_2$, 23 °C) $\delta = -30.8$ (317, 4H), -28.6 (72, 1H, p-pyr-CH), -26.8 (57, 2H), -8.2 (96, 6H, NH$_3$), -0.9 (56, 4H, BBN-CH), -0.7 (58, 4H, BBN-CH), 0.3 (56, 2H, BBN-CH), 0.6 (55, 2H, BBN-CH), 1.2 (65, 2H, BBN-CH), 1.6 (53, 4H, BBN-CH), 1.9 (55, 2H, BBN-CH), 2.4 (55, 4H, BBN-CH), 3.2 (78, 4H, BBN-CH), 7.7 (34, 18H, C(C$_3$H$_3$)$_3$), 7.8 (31, 4H), 9.8 (326, 4H, CH$_3$CH$_2$CH$_2$), 22.1 (58, 4H), 27.2 (424, 4H, N-CH$_2$), 44.8 (72, 2H, IM-CH or m-pyridine-CH), 57.1 (72, 2H, IM-CH or m-pyridine-CH). $\mu_{\text{eff}} = 5.16 \pm 0.05 \mu_B$ (THF, 25 °C). MALDI-TOF of C$_{53}$H$_{73}$N$_5$B$_2$S$_2$Fe$_1$-(SPh + 2(NH$_3$)): Calc. 812.473; Found 812.667. UV-Vis (THF, ambient temperature): $\lambda_{\text{max}} = 336$ nm (10,500 M$^{-1}$cm$^{-1}$). IR (KBr, ambient temperature): 3353, 3306, 3135, 3062 cm$^{-1}$ (N-H).
Synthesis of \((BBNPDP)Fe(NC)2\). A 20 mL scintillation vial was charged with \((BBNPDP)Fe(H)2\) (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 Me3SiCN was added to the solution containing \((BBNPDP)Fe(H)2\) 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 \((BBNPDP)Fe(NC)2\). Single, X-ray quality crystals were obtained by diffusing n-pentane into a dichloromethane solution of \((BBNPDP)Fe(NC)2\) at room temperature (note: crystals rapidly desolvate when removed from mother liquor). 1H NMR (CDCl3, 23 °C) δ = -35.0 (25, 1H, p-pyridine-CH), -8.8 (69, 4H), -6.7 (265, 4H), -3.8 (40, 2H), -0.6 (52, 4H, BBN-CH), -0.4 (28, 2H, BBN-CH), 0.3 (36, 4H, BBN-CH), 1.4 (22, 4H, BBN-CH), 2.8 (33, 4H), 7.8 (264, 2H), 10.0 (13, 18H, C(CH3)3), 13.1 (67, 4H, CH2CH2), 13.3 (280, 2H), 25.4 (339, 4H, N-CH2), 44.7 (53, 2H, IM-C or m-pyridine-CH), 53.1 (39, 2H, IM-CH or m-pyridine-CH). MALDI-TOF of C86H126N14B4Fe2: Calc. 1510.94; Found 1511.59. UV-Vis (THF, ambient temperature): λmax = 330 nm (7,600 M⁻¹cm⁻¹). IR (KBr, ambient temperature): 2170 cm⁻¹ (CN).

Synthesis of \([K(2,2,2-cryptand)]2(BBNPDP)Fe(OPh)4\). A 20 mL scintillation vial was charged with \([K(2,2,2-crypt)](BBNPDP)Fe(H)2\) (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 \([K(2,2,2-cryptand)]2(BBNPDP)Fe(OPh)4\). This species is unstable and attempts at purification resulted in further degradation of the compound. A representative 1H 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 \((BBNPDP)Fe(H)2\) and 2,4,6-tri-tert-butylphenylisocyanide. A 20 mL scintillation vial was charged with \((BBNPDP)Fe(H)2\) (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 \((BBNPDP)Fe(CNAr)2\). 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 \((BBNPDP)Fe(CNAr)2\) is made on the basis of 1H NMR and infrared spectroscopies, MALDI-TOF mass spectrometry, and the production of H2 (see details below). Characterization associated with complex: 1H NMR (tol-d8, 25 °C) δ = 1.09 (s, broad, C(CH3)3), 1.13 (s, broad), 1.22 (s, broad, C(CH3)3), further broad resonances spanning 1.25-1.80, 4.77 (broad, N-CH2), 6.65 (s, 2H, pyrazole-CH), 7.26 (t, J = 7.5, 1H, p-pyridine-CH), 7.30 (s, 4H, ArNC-CH), 7.73 (d, J = 7.0, 2H, m-pyr-CH). MALDI-TOF of C79H126N14B2Fe2 – (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*Bu* ligand, (*butyl*PDP*Bu*)Fe(E)₂ (E = H, NH₂, OH, PHPh, NHPh, SPh).

A) Reaction between (*butyl*PDP*Bu*)FeBr₂ and KBHEt₃. A 20 mL scintillation vial was charged with (*butyl*PDP*Bu*)FeBr₂ (0.020 g, 0.031 mmol) and 2 mL THF and the yellow slurry frozen. On thawing, KBHEt₃ (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 C₆D₆, insoluble black material gradually precipitates. After 20 min of reaction time, volatiles were removed in vacuo. Addition of C₆D₆ (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 ¹H NMR spectrum was obtained (see below).

B) Reaction between (*butyl*PDP*Bu*)FeBr₂ and NaOH/NaNH₂. These reactions provided analogous results. A 20 mL scintillation vial was charged with (*butyl*PDP*Bu*)FeBr₂ (0.020 g, 0.031 mmol) and 6 mL THF. While stirring, NaOH or NaNH₂ (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 ¹H NMR (the precipitate was black and the filtrate was faint yellow). ¹H NMR spectroscopy revealed only starting material (*butyl*PDP*Bu*)FeBr₂ and uncoordinated (*butyl*PDP*Bu*). No other paramagnetic resonances were observed. The reaction was allowed to stir an additional 14 hr at room temperature. Filtration of the black precipitate afforded a colorless solution which was identified to only contain uncoordinated (*butyl*PDP*Bu*) by ¹H NMR spectroscopy.

C) Reaction between (*butyl*PDP*Bu*)FeBr₂ and LiPHPh/LiNHPh. These reactions provided analogous results. A 20 mL scintillation vial was charged with (*butyl*PDP*Bu*)FeBr₂ (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. ¹H NMR spectroscopy of each (THF) revealed primarily uncoordinated (*butyl*PDP*Bu*) ligand as well a trace paramagnetic species that is identical between the two reactions.

D) Synthesis of (*butyl*PDP*Bu*)Fe(SPh)₂. A 20 mL scintillation vial was charged with (*butyl*PDP*Bu*)FeBr₂ (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 (*butyl*PDP*Bu*)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 C₃₉H₅₁N₅S₂Fe₂ – SPh: Calc. 600.282; Found 600.511. ¹H NMR (THF, 23 °C) δ = -33.7 (236, 4H, SPh‐C₆H₄), -31.3 (20, 2H, p-SPh‐CH), -24.3 (27, 1H, p-pyr‐CH), 0.5 (24, 6H, C₆H₁₃), 3.3 (55, 4H, C₆H₂), 6.1 (10, 18H, C(CH₃)₃), 7.6 (214, 4H, CH₂), 22.1 (19, 4H, SPh‐CH), 22.7 (284, 4H, N‐C₆H₂), 44.0 (42, 2H, pyridine or pyrazole‐CH), 57.0 (45, 2H, pyridine or pyrazole‐CH). μeff = 5.30 +/- 0.09 μB (THF, 25 °C). UV-Vis (THF, ambient temperature): λmax = 330 nm (13,600 M⁻¹cm⁻¹).
E) Validation of salt metathesis route for attempts to form \( (\text{butylPDP}^{\text{Bu}})\text{Fe(E)}^2 \) variants

The compounds \( (\text{butylPDP}^{\text{Bu}})\text{Fe(PHPh)}_2 \) and \( (\text{butylPDP}^{\text{Bu}})\text{Fe(OH)}_2 \) 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 \( (\text{BBLN}^{\text{Bu}})\text{Fe(PHPh)}_2 \). A 20 mL scintillation vial was charged with \( (\text{BBLN}^{\text{Bu}})\text{FeBr}_2 \) (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(SiMe3)2 was added to the vial containing \( (\text{BBLN}^{\text{Bu}})\text{FeBr}_2 \). 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 \( (\text{BBLN}^{\text{Bu}})\text{Fe(PHPh)}_2 \). The spectroscopic data and purity by this method were analogous to the protonation method.

2) Alternate synthesis of \( (\text{BBLN}^{\text{Bu}})\text{Fe(OH)}_2 \). A 20 mL scintillation vial was charged with \( (\text{BBLN}^{\text{Bu}})\text{FeBr}_2 \) (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(SiMe3)2 was added to the vial containing \( (\text{BBLN}^{\text{Bu}})\text{FeBr}_2 \) 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 \( (\text{BBLN}^{\text{Bu}})\text{Fe(OH)}_2 \). The spectroscopic data and purity by this method were analogous to the protonation method.
Figure S1. $^1$H NMR spectrum (THF, 24 °C) of (BNPDPBu)FeH$_2$.

Figure S2. Infrared spectrum (KBr) of (BNPDPBu)FeH$_2$.
Figure S3. MALDI-TOF spectrum of \((\text{BBN}^{\text{PDP}^{\text{Bu}}})\text{FeH}_2\) (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for \(\text{C}_{43}\text{H}_{65}\text{N}_{5}\text{B}_{2}\text{Fe}_1\).

Figure S4. \(^1\text{H}\) NMR spectrum (CDCl\(_3\), 25 °C) of \((\text{BBN}^{\text{PDP}^{\text{Bu}}})\text{ZnI}_2\).
Figure S5. $^1$H–$^1$H COSY spectrum (CDCl$_3$, 25 °C) of (BBNPDP$_{tBu}$)ZnI$_2$.

Figure S6. $^{13}$C NMR spectrum (CDCl$_3$, 25 °C) of (BBNPDP$_{tBu}$)ZnI$_2$. 
Figure S7. $^{11}$B NMR spectrum (CDCl$_3$, 25 °C) of (BBNPD$_4$Bu)ZnI$_2$.

Figure S8. Infrared spectrum (KBr) of (BBNPD$_4$Bu)ZnI$_2$. 
Figure S9. MALDI-TOF spectrum of (BBN-PDPBu)ZnI₂ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for C₄₁H₆₃N₅B₂I₂Zn₁ – I.

Figure S10. ¹H NMR spectrum (THF, 25 °C) of (BBN-PDPBu)ZnH₂.
Figure S11. $^1$H-$^1$H COSY spectrum (THF-\textit{d}_8, 25 °C) of (BBNpDP\textit{tBu})ZnH\textsubscript{2}.

Figure S12. $^2$H NMR spectrum (THF, 25 °C) of (BBNpDP\textit{tBu})ZnD\textsubscript{2}. 
**Figure S13.** $^{13}$C NMR spectrum (THF, 25 °C) of $^{(\text{BBN})}$PDP$^{(\text{tBu})}$ZnH$_2$.

**Figure S14.** $^{11}$B NMR spectrum (THF, 25 °C) of $^{(\text{BBN})}$PDP$^{(\text{tBu})}$ZnH$_2$. 
Figure S15. MALDI-TOF spectrum of \( \text{^{(BNNPDP}^{tBu})ZnH}_2 \) (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for \( \text{C}_{41}\text{H}_{65}\text{N}_5\text{B}_2\text{Zn}_3 \).

Figure S16. Infrared spectrum (KBr) of \( \text{^{(BNNPDP}^{tBu})ZnH}_2 \).
Figure S17. Difference infrared spectrum (KBr) of \(^{BBN}pDP^{iBu}\)ZnH\(_2\) minus \(^{BBN}pDP^{iBu}\)ZnD\(_2\).

Figure S18. \(^1\)H NMR spectrum (C\(_6\)D\(_6\), 25 °C) of reaction between \(^{Bu}pDP^{Bu}\)FeBr\(_2\) and two equiv. KBHEt\(_3\).
Figure S19. $^1$H NMR spectrum (THF, 25 °C) of [K(2,2,2-cryptand)][(B$^{BN}$PDP$^{Bu}$)FeH$_2$].

Figure S20. Infrared spectrum (KBr) of [K(18-crown-6)][(B$^{BN}$PDP$^{Bu}$)FeH$_2$].
Figure S21. X-band EPR spectrum (black) of [K(2,2,2-cryptand)][(88NpDPamb)FeH₂] (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 (88NpDPamb)Fe(NHMe)₂.
Figure S23. Infrared spectrum (KBr) of \((^{11}B^{11}N)PDP^{11}Bu\)Fe(NHMe)₂. Inset highlights N-H region.

Figure S24. MALDI-TOF spectrum of \((^{11}B^{11}N)PDP^{11}Bu\)Fe(NHMe)₂ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for \(C_{43}H_{71}N_{7}B_{2}Fe\).
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 (BBNPD$^\text{Bu}$)Fe(OH)$_2$.

Figure S28. Infrared spectrum (KBr) of (BBNPD$^\text{Bu}$)Fe(OH)$_2$. 
Figure S29. MALDI-TOF spectrum of (BBNPDBu)Fe(OH)₂ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for C₄₁H₆₅N₅O₂B₂Fe₁.

Figure S30. ¹H NMR spectrum (CDCl₃, 25 °C) of (BBNPDBu)Fe(PPh)₂.
Figure S31. Infrared spectrum (KBr) of \( \left( ^{8}B\text{NPDP}^{tBu}\right) \text{Fe(PHPh)}_{2} \).

Figure S32. \( ^{1}\text{H} \) NMR spectrum (C\(_{6}\)D\(_{6}\), 25 °C) of \( \left( ^{8}B\text{NPDP}^{tBu}\right) \text{Fe(SPh)}_{2} \).
**Figure S33.** Infrared spectrum (KBr) of (BBNPDlpBu)Fe(SPh)₂.

**Figure S34.** MALDI-TOF spectrum of (BBNPDlpBu)Fe(SPh)₂ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for C₅₃H₇₃N₅B₂S₂Fe₁ - SPh.
Figure S35. Crude $^1$H NMR spectrum (THF, 25 °C) of the reaction between (BBN-PDPBu)FeH$_2$ and PhSSPh to produce (BBN-PDPBu)Fe(SPh)$_2$ and H$_2$ in a sealed J-Young NMR tube.
Figure S36. Variable temperature $^1$H NMR spectra (CH$_2$Cl$_2$) of (BBNPDPhBu)Fe(SPh)$_2$. The residual CH$_2$Cl$_2$ resonance is omitted to increase clarity.
Figure S37. $^1$H NMR spectrum ($\text{C}_6\text{D}_6$, 25 °C) of (BBNPDP$^\text{Bu}$)Zn(SPh)$_2$.

Figure S38. $^1$H-$^1$H COSY spectrum ($\text{C}_6\text{D}_6$, 25 °C) of (BBNPDP$^\text{Bu}$)Zn(SPh)$_2$. 
Figure S39. $^{13}$C NMR spectrum (C$_6$D$_6$, 25 °C) of (BBNPDP$^t$Bu)Zn(SPh)$_2$.

Figure S40. Infrared spectrum (KBr) of (BBNPDP$^t$Bu)Zn(SPh)$_2$. 
**Figure S41.** MALDI-TOF spectrum of (BNPDPBu)Zn(SPh)₂ (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for C₅₃H₇₃N₅B₂S₂Zn₁ - SPh.

**Figure S42.** Crude ¹H NMR spectrum (THF, 25 °C) of the reaction between (BNPDPBu)ZnH₂ and PhSSPh to produce (BNPDPBu)Zn(SPh)₂ and H₂ in a sealed J-Young NMR tube.
Figure S43. Variable temperature $^1$H NMR spectra (CDCl$_3$) of (BBNPD)$_2$BuZn(SPh)$_2$. 
Figure S44. $^1$H NMR spectrum (CH$_2$Cl$_2$, 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 [(BBNPDpBu)Fe(SPh)2(NH3)] (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for C53H73N5B2S2Fe1 – (SPh + 2(NH3)).

Figure S47. 1H NMR spectrum (CDCl3, 25 °C) of [(BBNPDpBu)Fe(NC)]2.
Figure S48. Infrared spectrum (KBr) of [(BBNPDPBu)Fe(NC)2]2.

Figure S49. MALDI-TOF spectrum of [(BBNPDPBu)Fe(NC)2]2 (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for C86H126N14B4Fe2.
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^Bu)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^Bu)Fe(CNAr)_2. Monoisotopic mass calculated for C_{60}H_{92}N_{6}B_{2}Fe_{1}.

Figure S53. ^1H NMR spectrum (THF, 25 °C) of (butyl-PDP^Bu)Fe(SPh)_2.
Figure S54. Infrared spectrum (KBr) of \((\text{butylPDP}^\text{Bu})\text{Fe(SPh)}_2\).

Figure S55. MALDI-TOF spectrum of \((\text{butylPDP}^\text{Bu})\text{Fe(SPh)}_2\) (bottom, black) obtained in an anthracene matrix and the predicted isotopic pattern (top, red). Monoisotopic mass calculated for C$_{35}$H$_{51}$N$_5$S$_2$Fe$_1$ - SPh.
Quantification of H₂ produced by addition of 2,4,6-tri-tert-butylphenylisocyanide

Four samples for each (BBNpDP₁Bu)FeH₂ and (BBNpDP₁Bu)ZnH₂ were set up under analogous conditions:

A C₆H₆ slurry (approx. 1.0 mL) of a known quantity of (BBNpDP₁Bu)MH₂ was transferred to a J-Young NMR tube. Additional C₆H₆ (approx. 1.0 mL) was used to ensure all (BBNpDP₁Bu)MH₂ was transferred. The tube was then carefully layered with additional C₆H₆ 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 (BBNpDP₁Bu)MH₂. The tube was then slowly inverted repeatedly for 30 min and an ¹H 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 H₂ production.
### Table S1. Quantification of H₂ from reaction between (BBNPDPtrBu)FeH₂ and 2,4,6-tri-tert-butylphenylisocyanide.

|                  | (BBNPDPtrBu)FeH₂ (mass, mg) | ArNC (mass, mg) | Percent H₂ |
|------------------|-----------------------------|-----------------|------------|
| 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 H₂ from reaction between (BBNPDPtrBu)ZnH₂ and 2,4,6-tri-tert-butylphenylisocyanide.

|                  | (BBNPDPtrBu)ZnH₂ (mass, mg) | ArNC (mass, mg) | Percent H₂ |
|------------------|-----------------------------|-----------------|------------|
| 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$_6$H$_6$, 25 °C) of reaction between ($^{18}$BNPDP$^{8}$Bu)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$_6$H$_6$, 25 °C) of reaction between (BBNPD$_3$Bu)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$_6$H$_6$, 25 °C) of reaction between (BBN$_2$PDP$_2$Bu)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 (BBNPD^Bu)FeH_2 (0.47 mM) recorded in THF with 0.2 M [Bu4N][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 \((^{11}\text{BNPDP}^{11}\text{Bu})\text{Fe(NH}_2)_2\) (0.91 mM) recorded in THF with 0.2 M [Bu4N][PF6] 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 \textit{[^{11}BuPDP}^{3} \text{Bu})Fe(SPh)\textsubscript{2} (0.72 mM) recorded in THF with 0.2 M [Bu\textsubscript{4}N][PF\textsubscript{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)\textsuperscript{1/2} vs. current.

Figure S63. Electrochemical analysis of \textit{[^{11}BNPDP}^{3} \text{Bu})Fe(SPh)\textsubscript{2}(NH\textsubscript{3})\textsubscript{2} (0.70 mM) recorded in THF with 0.2 M [Bu\textsubscript{4}N][PF\textsubscript{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)\textsuperscript{1/2} vs. current.
Figure S64. Electrochemical analysis of \( \text{BBNPDp}^{\text{Bu}} \text{Fe(PHPh)}_2 \) (0.72 mM) recorded in THF with 0.2 M \([\text{Bu}_4\text{N}]\text{[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 (BBNPDpBu)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 $(\text{scan rate})^{1/2}$ vs. current.
Figure S66. Electrochemical analysis of (BBNPDPBu)Fe(NHPh)_2 (0.75 mM) recorded in THF with 0.2 M [Bu4N][PF6] 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 \((\text{BBNPD}^{\text{Bu}})\text{Fe(NHMe)}_2\) \((0.87 \text{ mM})\) recorded in THF with 0.2 M \([\text{Bu}_4\text{N}]\text{[PF}_6\text{]}\) 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 \((\text{scan rate})^{1/2}\) vs. current.
Figure S68. Electrochemical analysis of (butylPDPBu)Fe(SPh)2 (0.94 mM) recorded in THF with 0.2 M [Bu4N][PF6] 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') |
|----------|------------------------|
| (BBnPDPBu)FeBr2 | -2.14<sup>a</sup> |
| (BBnPDPBu)FeCl2 | -2.07<sup>a</sup> |
| (BBnPDPBu)FeH2 | -2.06 |
| (BBnPDPBu)Fe(NH2)2 | -2.12 |
| (BBnPDPBu)Fe(NHMe)2 | -2.30 |
| (BBnPDPBu)Fe(NPh)2 | -2.18 |
| (BBnPDPBu)Fe(OH)2 | -2.12 |
| (BBnPDPBu)Fe(PPh)2 | -1.96 |
| (BBnPDPBu)Fe(SPh)2 | -2.13 |
| (BBnPDPBu)Fe(SPh)2(NH3)2 | -2.21 |

<sup>a</sup>Values for (BBnPDPBu)FeX2 (X = Cl, Br) taken from ref. 1
Figure S69. Electronic absorption spectra of $\left(\text{BBN} \text{PDP}^{6\text{Bu}}\right)\text{FeH}_2$ (red) and $[\text{K}(18\text{-crown-6})][\left(\text{BBN} \text{PDP}^{6\text{Bu}}\right)\text{FeH}_2]$ (green) recorded in THF at ambient temperature.

Figure S70. Electronic absorption spectra of iron complexes recorded in THF at ambient temperature.
Compound: \((\text{BBNPDP}^\text{Bu})\text{FeH}_2\)

Local Name: jk3155

CCDC 1884221

**Table S4. Crystallographic parameters for \((\text{BBNPDP}^\text{Bu})\text{FeH}_2\)**

| Crystal data |  |
|--------------|---|
| Chemical formula | \(\text{C}_{41}\text{H}_{65}\text{B}_2\text{FeN}_5\cdot0.892(\text{C}_7\text{H}_8)\) |
| \(M_r\) | 787.61 |
| Crystal system, space group | Tetragonal, \(P\text{4}3\text{2}1\text{2}\) |
| Temperature (K) | 150 |
| \(a, c (\text{Å})\) | 16.0995 (5), 16.3816 (5) |
| \(V (\text{Å}^3)\) | 4246.0 (3) |
| \(Z\) | 4 |
| Radiation type | \(\text{Cu K}\alpha\) |
| \(\mu (\text{mm}^{-1})\) | 3.13 |
| Crystal size (mm) | 0.12 \(\times\) 0.11 \(\times\) 0.10 |

| Data collection |  |
|-----------------|---|
| Diffractometer | Bruker AXS D8 Quest CMOS diffractometer |
| Absorption correction | Multi-scan SADAB5 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10 |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.427, 0.526 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 30458, 4559, 3416 |
| \(R_{\text{int}}\) | 0.070 |
| \((\sin \theta/\lambda)_{\text{max}} (\text{Å}^{-1})\) | 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 |
| \(\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}} (\text{e Å}^{-3})\) | 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), SHELXL 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 $^{(BBN)PDP^{(Bu)}}$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: \([\text{K} (2,2,2\text{-cryptand})]\)\([(\text{BBNPDP}^{\text{Bu}})\text{FeH}_2]\)

Local Name: jk2200

CCDC 1884231

**Table S5. Crystallographic parameters for \([\text{K} (2,2,2\text{-cryptand})]\)\([(\text{BBNPDP}^{\text{Bu}})\text{FeH}_2]\)**

| Crystal data |  |
|--------------|--|
| Chemical formula | \( \text{C}_{18}\text{H}_{36}\text{KN}_2\text{O}_6 \cdot \text{C}_{41}\text{H}_{65}\text{B}_2\text{FeN}_5 \) |
| \( M_r \) | 1121.03 |
| Crystal system, space group | Triclinic, \( P\bar{1} \) |
| Temperature (K) | 150 |
| \( a, b, c \) (Å) | 19.503 (3), 21.623 (3), 22.147 (4) |
| \( \alpha, \beta, \gamma \) (°) | 67.321 (5), 71.202 (5), 89.815 (4) |
| \( V \) (Å³) | 8079 (2) |
| \( Z \) | 4 |
| Radiation type | Mo Kα |
| \( \mu \) (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. |
| \( T_{\text{min}}, T_{\text{max}} \) | 0.446, 0.563 |
| No. of measured, independent and observed \( I > 2\sigma(I) \) reflections | 70366, 70366, 41234 |
| \( R_{\text{int}} \) | 0.053 |
| \( \langle \sin \theta/\lambda \rangle_{\text{max}} \) (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 |
| \( w = 1/[\sigma^2(F_o^2) + (0.2025P)^2 + 20.270P] \) where \( P = (F_o^2 + 2F_c^2)/3 \) |  |
| \( \Delta \rho_{\text{max}}, \Delta \rho_{\text{min}} \) (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), SHELXL 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:

\[
\begin{bmatrix}
1.000 & 0.000 & 0.000 \\
0.007 & -1.000 & 0.000 \\
0.732 & 0.000 & -1.000 \\
\end{bmatrix}
\]

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\textsuperscript{i} 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 Shelx2017) 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)][(BNPDPBu)FeH2] 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)$_4$][($^{18}$BPDP$_{tBu}$)FeH$_2$]

Local Name: jk2177

CCDC 1884224

Table S6. Crystallographic parameters for [K(DME)$_4$][($^{18}$BPDP$_{tBu}$)FeH$_2$]

| Crystal data                              |                  |
|-------------------------------------------|------------------|
| Chemical formula                          | 4(C$_{41}$H$_{65}$B$_2$FeN$_5$)$_2$.2.808(C$_4$H$_9$O$_2$)$_3$.2(C$_4$H$_{10}$O$_2$)$_4$(K) |
| $M_r$                                     | 3498.78          |
| Crystal system, space group               | Tetragonal, $I4_2d$ |
| Temperature (K)                           | 150              |
| $a$, $c$ (Å)                              | 26.450 (2), 20.9410 (19) |
| $V$ (Å$^3$)                               | 14650 (3)        |
| $Z$                                       | 2                |
| Radiation type                            | Mo Kα            |
| $\mu$ (mm$^{-1}$)                         | 0.29             |
| Crystal size (mm)                         | 0.42 x 0.28 x 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 [$I > 2\sigma(I)$] 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: \(U_{ij}^{ji}\) components of ADPs for atoms closer to each other than 2.0 Å were restrained to be similar within an esd of 0.01 Å².

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. \(U_{ij}^{ji}\) 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 Å³. 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/Å³ 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 \([\text{K}(\text{DME})_2][\text{BBN}(\text{PDPBu})\text{FeH}_2]\) 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.
Table S7. Crystallographic parameters for (BBNPDPBu)ZnH₂

| Crystal data                                      |                     |
|--------------------------------------------------|----------------------|
| Chemical formula                                  | C₄₁H₆₅B₂N₅Zn·0.718(C₇H₈) |
| Molecular weight (M_r)                            | 781.14               |
| Crystal system, space group                       | Tetragonal, P₄₁2₁₂   |
| Temperature (K)                                   | 150                  |
| a, c (Å)                                          | 16.1630 (5), 16.4362 (6) |
| V (Å³)                                           | 4293.8 (3)           |
| Z                                                | 4                    |
| Radiation type                                   | Mo Kα                |
| 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 > 2σ(I)] reflections | 62259, 6563, 4926 |
| R_{int}                                           | 0.088                |
| (sin θ/λ)_{max} (Å⁻¹)                            | 0.716                |

| Refinement                                        |                     |
|--------------------------------------------------|----------------------|
| R(F² > 2σ(F²)), wR(F²), 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 |
| Δρ_{max}, Δρ_{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), SHELXL 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 \( \text{(BBN-PDP}^{\text{tBu}})\text{ZnH}_2 \) 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: \((^\text{BBNPdP}^\text{Bu})\text{Fe(NHMe)}_2\)

Local Name: jk2150

CCDC 1884223

Table S8. Crystallographic parameters for \((^\text{BBNPdP}^\text{Bu})\text{Fe(NHMe)}_2\)

| Crystal data |          |
|--------------|----------|
| Chemical formula | C\(_{43}\)H\(_{71}\)B\(_2\)FeN\(_7\)\(\cdot\)CH\(_2\)Cl\(_2\) |
| \(M_r\)      | 848.46   |
| Crystal system, space group | Tetragonal, \(P\4\3212\) |
| Temperature (K) | 150      |
| \(a, c\) (Å) | 16.4289 (8), 16.7181 (10) |
| \(V\) (Å\(^3\)) | 4512.4 (5) |
| \(Z\)        | 4        |
| Radiation type | Mo \(K\alpha\) |
| \(\mu\) (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 SADA8S 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10 |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.194, 0.263 |
| No. of measured, independent and observed \(|I| > 2\sigma(I)\) reflections | 47133, 5321, 4539 |
| \(R_{\text{int}}\) | 0.080 |
| (\(\sin \theta/\lambda\))\(_{\text{max}}\) (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 |
| \(\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}\) (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), SHELXL 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$_{12b}$)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: \((\text{BBNPDP}^\text{tBu})\text{Fe(OH)}_2\)

Local Name: jk238

CCDC 1884227

**Table S9. Crystallographic parameters for \((\text{BBNPDP}^\text{tBu})\text{Fe(OH)}_2\)**

| Crystal data                        |                              |
|-------------------------------------|------------------------------|
| Chemical formula                    | \(\text{C}_{41}\text{H}_{65}\text{B}_{2}\text{FeN}_{5}\text{O}_{2}\cdot\text{C}_{5}\text{H}_{12}\) |
| \(M_r\)                            | 809.59                       |
| Crystal system, space group         | Monoclinic, \(P2_1/n\)      |
| Temperature (K)                     | 150                          |
| \(a, b, c\) (\(\text{Å}\))        | 13.8891 (4), 17.2913 (6), 19.1228 (7) |
| \(\beta\) (°)                      | 94.835 (2)                   |
| \(V\) (\(\text{Å}^3\))           | 4576.2 (3)                   |
| \(Z\)                              | 4                            |
| Radiation type                      | \(\text{Cu } K\alpha\)      |
| \(\mu\) (\(\text{mm}^{-1}\))     | 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 |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.524, 0.754                 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 32363, 9656, 7951 |
| \(R_{\text{int}}\)                | 0.060                        |
| \((\sin \theta/\lambda)_{\text{max}}\) (\(\text{Å}^{-1}\)) | 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 |
| \(\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}}\) (e \(\text{Å}^{-3}\)) | 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), SHELXLX 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 $U_{ij}^{ij}$ 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 (BBNPD$^\text{Bu}$)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:** \((^\text{BBNPDP}^\text{Bu})\Fe(N\text{HPh})_2\)

**Local Name:** jk318

**CCDC 1884228**

**Table S10.** Crystallographic parameters for \((^\text{BBNPDP}^\text{Bu})\Fe(N\text{HPh})_2\)

| **Crystal data** |  |
|------------------|---|
| Chemical formula | \(\text{C}_{53}\text{H}_{75}\text{B}_{2}\text{FeN}_{7} \cdot 3(\text{C}_4\text{H}_8\text{O})\) |
| \(M_r\)        | 1103.98 |
| Crystal system, space group | Monoclinic, \(P2_1/c\) |
| Temperature (K) | 150 |
| \(a, b, c\) (Å) | 12.0303 (5), 11.0429 (4), 22.8724 (9) |
| \(\beta\) (°)   | 94.3767 (15) |
| \(V\) (Å\(^3\)) | 3029.7 (2) |
| \(Z\)          | 2 |
| Radiation type  | Mo \(K\alpha\) |
| \(\mu\) (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 |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.652, 0.746 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 22161, 8157, 6386 |
| \(R_{\text{int}}\) | 0.031 |
| \((\sin \theta/\lambda)_{\text{max}}\) (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 |
| \(\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}\) (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), SHELXL 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\textsuperscript{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\textsuperscript{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 (\textsuperscript{BBN}PDP\textsuperscript{Bu})Fe(NHPh\textsubscript{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: \((\text{BBNPDP}^\text{tBu})\text{Fe(PHPh)}_2\)

Local Name: jk319

CCDC 1884232

**Table S11.** Crystallographic parameters for \((\text{BBNPDP}^\text{tBu})\text{Fe(PHPh)}_2\)

| Crystal data          |                  |
|-----------------------|------------------|
| Chemical formula      | \(\text{C}_{53}\text{H}_{74}\text{B}_{2}\text{FeN}_{5}\text{P}_{2}\cdot3(\text{C}_4\text{H}_8\text{O})\) |
| \(M_r\)               | 1137.90          |
| Crystal system, space group | Triclinic, \(P\bar{1}\) |
| Temperature (K)       | 150              |
| \(a, b, c\) (Å)       | 10.989 (6), 12.928 (6), 24.431 (11) |
| \(\alpha, \beta, \gamma\) (°) | 92.678 (16), 91.124 (18), 114.185 (16) |
| \(V\) (Å\(^3\))       | 3160 (3)         |
| \(Z\)                 | 2                |
| Radiation type        | Mo Kα            |
| \(\mu\) (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 \textit{SADABS} 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10 |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.509, 0.745 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 33481, 11734, 4754 |
| \(R_{\text{int}}\)      | 0.142                                    |
| \((\sin \theta/\lambda)_{\text{max}}\) (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 |
| \(\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}\) (e Å\(^{-3}\)) | 0.73, -0.87 |

Computer programs: \textit{Apex3} v2017.3-0 (Bruker, 2016), \textit{SAINT} V8.38A (Bruker, 2016), \textit{SHELXS97} (Sheldrick, 2008), \textit{SHELXL2018}3 (Sheldrick, 2015, 2018), \textit{SHELXL} Rev915 (Hübschle \textit{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 (BBNPDPtBu)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: \((\text{BBNPD}^\text{tBu})\text{Fe(SPh)}_2\)

Local Name: jk3188  
CCDC 1884229

**Table S12.** Crystallographic parameters for \((\text{BBNPD}^\text{tBu})\text{Fe(SPh)}_2\)

| Crystal data |  |
|--------------|---|
| Chemical formula | \(\text{C}_{53}\text{H}_{73}\text{B}_{2}\text{FeN}_{5}\text{S}_{2}\) |
| \(M_r\) | 921.75 |
| Crystal system, space group | Monoclinic, \(C2/c\) |
| Temperature (K) | 150 |
| \(a\), \(b\), \(c\) (Å) | 23.8853 (10), 11.6376 (5), 19.0401 (8) |
| \(\beta\) (°) | 110.8255 (16) |
| \(V\) (Å\(^3\)) | 4946.8 (4) |
| \(Z\) | 4 |
| Radiation type | \(\text{Mo K}\alpha\) |
| \(\mu\) (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 |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.674, 0.747 |
| No. of measured, independent and observed \([I > 2s(I)]\) reflections | 35885, 9150, 6037 |
| \(R_{\text{int}}\) | 0.061 |
| \((\sin \theta/\lambda)_{\text{max}}\) (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 |
| \(\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}\) (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), SHELXL Rev900 (Hübschle et al., 2011).
Figure S79. Molecular structure of \((^{\text{BBN}}\text{PDP})_{\text{Bu}}\text{Fe(SPh)}\text{)}_2\) displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.
Compound: \((^{BBNPDP}t_{Bu})Fe(SPh)_{2}(NH_{3})_{2}\)

Local Name: jk4207

CCDC 1884230

**Table S13.** Crystallographic parameters for \((^{BBNPDP}t_{Bu})Fe(SPh)_{2}(NH_{3})_{2}\)

| Crystal data |  |
|--------------|---|
| Chemical formula | C\textsubscript{53}H\textsubscript{79}B\textsubscript{2}FeN\textsubscript{7}S\textsubscript{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) |
| \(\alpha, \beta, \gamma\) (°) | 92.316 (3), 99.766 (2), 99.769 (2) |
| \(V\) (Å\textsuperscript{3}) | 2618.6 (2) |
| \(Z\) | 2 |
| Radiation type | Cu K\(\alpha\) |
| \(\mu\) (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. |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.131, 0.330 |
| No. of measured, independent and observed \(|I > 2\sigma(I)|\) reflections | 34295, 10649, 8780 |
| \(R_{\text{int}}\) | 0.077 |
| \((\sin \theta/\lambda)_{\text{max}}\) (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 |
| \(\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}}\) (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 P\textbar 1) and application of the twin transformation matrix \(-1 \ 0 \ 0, \ 0 \ 0 \ -1, \ 0 \ -1 \ 0\) (180 degree rotation around (0 1\textbar 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:

\[
\begin{pmatrix}
1.00000 & -0.00008 & 0.00008 \\
-0.67226 & -1.00047 & -0.00735 \\
-0.66839 & 0.00736 & -0.99948
\end{pmatrix}
\]

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\textsubscript{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 \((\text{BNPDP}^{\text{Bu}})\text{Fe(SPh)}_2(\text{NH}_3)_2\) 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: \([\text{BNNPDP}^\text{tBu}]\text{Fe(NC)}\text{2}]_2\)

Local Name: jk217

CCDC 1884225

**Table S14.** Crystallographic parameters for \([\text{BNNPDP}^\text{tBu}]\text{Fe(NC)}\text{2}]_2\)

| Crystal data |  |
|--------------|---|
| Chemical formula | \(\text{C}_{86}\text{H}_{126}\text{B}_{4}\text{Fe}_{2}\text{N}_{14}\cdot3.272\text{(CH}_2\text{Cl}_2)\) |
| \(M_r\) | 1807.60 |
| Crystal system, space group | Monoclinic, \(Cc\) |
| Temperature (K) | 100 |
| \(a\), \(b\), \(c\) (Å) | 14.7395(8), 31.7053(18), 22.0966(13) |
| \(\beta\) (°) | 90.451(2) |
| \(V\) (Å\(^3\)) | 10325.9(10) |
| \(Z\) | 4 |
| Radiation type | Mo \(K\alpha\) |
| \(\mu\) (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 |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.630, 0.747 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 123502, 24774, 23021 |
| \(R_{\text{int}}\) | 0.043 |
| \((\sin \theta/\lambda)_{\text{max}}\) (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 |
| \(\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}\) (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. \(U^i\) 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 \([{(BBNPD\textsubscript{Bu})_2Fe(NC)}_2]_2\) displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The 9-BBN moieties are displayed in wireframe for clarity.
Compound: \((BBNPDP^\text{tBu})\text{Zn(SPh)}_2\)

Local Name: jk3257

CCDC 1884226

**Table S15.** Crystallographic parameters for \((BBNPDP^\text{tBu})\text{Zn(SPh)}_2\)

| Crystal data          |
|-----------------------|
| Chemical formula      | C\(_{53}\)H\(_{73}\)B\(_2\)N\(_5\)S\(_2\)Zn |
| \(M_r\)              | 931.27 |
| Crystal system, space group | Monoclinic, \(C2/c\) |
| Temperature (K)       | 150 |
| \(a\), \(b\), \(c\) (Å) | 23.8971 (10), 11.5743 (5), 19.0415 (7) |
| \(\beta\) (°)        | 110.4440 (14) |
| \(V\) (Å\(^3\))      | 4935.0 (4) |
| \(Z\)                | 4 |
| Radiation type        | Mo K\(\alpha\) |
| \(\mu\) (mm\(^{-1}\)) | 0.62 |
| Crystal size (mm)     | 0.21 \(\times\) 0.18 \(\times\) 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. |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.718, 0.747 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 146991, 9441, 7807 |
| \(R_{\text{int}}\)    | 0.041 |
| \((\sin \theta/\lambda)_{\text{max}}\) (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 |
| \(\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}}\) (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), SHELXL Rev882 (Hübschle et al., 2011).
Figure S82. Molecular structure of (BBNPDPBu)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-crown-6)(THF)]₂[(BNPDpBu)₂Fe(OPh)₄]
Local Name: jk337
CCDC 1884222

Table S16. Crystallographic parameters for [K(18-crown-6)(THF)]₂[(BNPDpBu)₂Fe(OPh)₄]

| Crystal data                  |                  |
|-------------------------------|------------------|
| Chemical formula              | $\text{C}_{106}\text{H}_{146}\text{B}_4\text{FeN}_{10}\text{O}_4\cdot 2\text{C}_{16}\text{H}_{32}\text{KO}_7\cdot 2\text{C}_4\text{H}_8\text{O}$ |
| $M_r$                         | 2618.64          |
| Crystal system, space group   | Monoclinic, C2/c |
| Temperature (K)               | 150              |
| $a$, $b$, $c$ (Å)             | 33.6410 (7), 16.3704 (3), 27.3584 (6) |
| $\beta$ (°)                  | 100.166 (1)      |
| $V$ (Å³)                     | 14830.2 (5)      |
| $Z$                           | 4                |
| Radiation type                | Cu Kα            |
| $\mu$ (mm⁻¹)                 | 1.84             |
| Crystal size (mm)             | $0.35 \times 0.28 \times 0.13$ |

| 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 |
| $T_{\text{min}}$, $T_{\text{max}}$ | 0.442, 0.754      |
| No. of measured, independent and observed $|I| > 2\sigma(|I|)$ reflections | 39390, 14541, 13474 |
| $R_{\text{int}}$              | 0.040            |
| $(\sin \theta/\lambda)_{\text{max}}$ (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 |
| $w = 1/[s^2(F_h^2) + (0.1402P)^2 + 15.7177P]$ where $P = (F_h^2 + 2F_g^2)/3$ |                  |
| $\Delta \rho_{\text{max}}$, $\Delta \rho_{\text{min}}$ (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), SHELXL 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. $U^\text{eq}$ 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 $[K(18\text{-crown-6})(\text{THF})]_2[[\text{9-BBN}][\text{DPBu}]_2\text{Fe(OPh)}_4]$ displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The 9-BBN and phenoxide moieties are displayed in wireframe for clarity.
**Compound:** \((\text{butylPDP}_\text{Bu})\text{Fe(SPh)}_2\)

**Local Name:** jk566

**CCDC 1903500**

**Table S17. Crystallographic parameters for \((\text{butylPDP}_\text{Bu})\text{Fe(SPh)}_2\)**

| Crystal data |
|--------------|
| **Chemical formula** | C_{39}H_{51}FeN_{5}S_{2} |
| **\(M_r\)** | 709.81 |
| **Crystal system, space group** | Monoclinic, \(P2_1/n\) |
| **Temperature (K)** | 150 |
| **\(a, b, c (\text{Å})\)** | 9.2208 (10), 15.9972 (18), 25.443 (3) |
| **\(\beta (\degree)\)** | 93.373 (6) |
| **\(V (\text{Å}^3)\)** | 3746.5 (7) |
| **\(Z\)** | 4 |
| **Radiation type** | Cu \(K\alpha\) |
| **\(\mu (\text{mm}^{-1})\)** | 4.52 |
| **Crystal size (mm)** | 0.21 \(\times\) 0.06 \(\times\) 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 |
| **\(T_{\text{min}}, T_{\text{max}}\)** | 0.496, 0.754 |
| **No. of measured, independent and observed \(|I > 2\sigma(I)|\) reflections** | 20041, 7782, 5293 |
| **\(R_{\text{int}}\)** | 0.058 |
| **\(\langle \sin \theta/\lambda \rangle_{\text{max}} (\text{Å}^{-1})\)** | 0.640 |

**Refinement**

| **\(R(R^2 > 2\sigma(R^2)), wR(F^2), S\)** | 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 |
| **\(\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}} (\text{e Å}^{-3})\)** | 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 \((\text{butylPDPBu})\text{Fe(SPh})\)\(_2\) displayed with 50% probability ellipsoids. Hydrogen atoms are omitted for clarity. The phenyl moieties are displayed in wireframe for clarity.
Figure S85. Comparison of intraligand bond distances in (BuPDP Bu)FeBr₂, (BBNPDP Bu)FeH₂, and [K(2,2,2-crypt)][(BBNPDP Bu)FeH₂]. The data for (BuPDP Bu)FeBr₂ is taken from reference 1.

Table S18. Metrical parameters for hydride containing compounds.

|                  | (BBNPDP Bu)FeH₂ | [K(2,2,2-crypt)][(BBNPDP Bu)FeH₂] | (BBNPDP Bu)ZnH₂ |
|------------------|-----------------|---------------------------------|-----------------|
| M-Npyrazole (Å)  | 2.174(17)       | 2.155(6)                        | 2.176(13)       |
| M-Npyrazole (Å)  | --              | 2.153(6)                        | --              |
| M-Npyridine (Å)  | 2.178(5)        | 2.021(6)                        | 2.153(4)        |
| M-B (°)          | 2.970           | 2.977                           | 2.977           |
| M-B (°)          | --              | 3.060                           | --              |
| τ₅               | 0.314           | 0.363                           | 0.374           |
| IR ν(M-H-B) (cm⁻¹) | 1839           | 1866                            | 1775            |
Table S19. Metrical parameters for complexes 2.

|            | 2-NH₂ | 2-NHMe | 2-NHPhe | 2-OH  | 2-PHPhe | 2-SPh  |
|------------|-------|--------|---------|-------|---------|--------|
| Fe-Npyrazole (Å) | 2.2950(18) | 2.327(4) | 2.2460(14) | 2.2604(16) | 2.248(11) | 2.2148(13) |
| Fe-Npyrazole (Å) | --     | --     | --      | 2.2812(16) | 2.304(12) | --     |
| Fe-Npyridine (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-B        | --     | --     | --      | 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) |
| Fe-B (Å)    | 3.349   | 3.329   | 3.418    | 3.343     | 3.907     | 3.848   |
| ΣB₁α °      | 325.6(2) | 326.4(6) | 326.54(18) | 321.69(16) | 323.9(9)  | 319.57(12) |
| ΣB₂α °      | --     | --     | --      | 322.34(16) | 320.9(9)  | --     |
| τ₅          | 0.02   | 0.04   | 0.14    | 0.35     | 0.26     | 0.27    |

Table S20. Metrical parameters for (BBNPDPBu)M(SPh)₂ species.

|            | 2-SPh | (BBNPDPBu)Fe(SPh)₂(NH₃)₂ | (BBNPDPBu)Zn(SPh)₂ | (butylPDPBu)Fe(SPh)₂ |
|------------|-------|--------------------------|-------------------|---------------------|
| M-Npyrazole (Å) | 2.2148(13) | 2.321(5) | 2.2508(9) | 2.162(5) |
| M-Npyrazole (Å) | --     | 2.346(6) | --       | 2.407(9) |
| M-Npyridine (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) |
| ΣB₁α (°)   | 319.57(12) | 322.8(6) | 319.14(8) | --     |
| ΣB₂α (°)   | --     | 319.4(6) | --       | --     |
| τ₅          | 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 |
|----------|----------|------------------|-----------|
| (BBNPDPBu)FeH₂ | 2.970 | 1839 | This work |
| [(BBNPDPBu)FeH₂]²⁻ | 2.977 / 3.060 | 1866 | This work |
| (BBNPDPBu)ZnH₂ | 2.977 | 1775 | This work |
| (P₂B-H)FeH(CO)₂ | 2.743 | 2080 | J. Am. Chem. Soc. 2013, 135, 12580. |
| (PNP)FeH(CO)(BH₄) | 2.702 | 2339 | Adv. Synth. Catal. 2016, 358, 820. |
| (PNP)FeH(CO)(BH₄) | 2.744 | 2051 | Angew. Chem. Int. Ed. 2013, 52, 14162. |
| (P₂B-H)FeH(CO)(BH₄) | 2.746 | 2030 | Inorg. Chim. Acta 1986, 114, C27. |
| (P₂B-H)FeH(CO)(BH₄) | 2.826 | 1866 | This work |
| (PNP)FeH(CO)(BH₄) | 2.721 | Not reported | Organometallics 2014, 33, 6905. |
| (PNP)FeH(CO)(BH₄) | 2.721 | 2130 / 2000 | Organometallics 2015, 34, 4560. |
| (PNP)FeH(CO)(BH₄) | 2.708 / 2.700 | 2360 | Catal. Sci. Technol. 2016, 6, 4768. |
| (PNP)FeH(CO)(BH₄) | 2.745 | 1896 | Inorg. Chem. 2014, 53, 2133. |
| (PNP)FeH(CO)(BH₄) | 2.749 | 2038 | J. Am. Chem. Soc. 2014, 136, 7869. |
| (P₂)FeH(H₂) | 2.760 | 2090 | Chem. Sci. 2018, 9, 6264. |
| (P₂)FeH(H₂) | 2.763 / 2.769 | 2483 | Chem. Sci. 2018, 9, 6264. |
| (P₂)FeH(H₂) | 2.763 / 2.769 | 2483 | Chem. Sci. 2018, 9, 6264. |
| (P₂)FeH(H₂) | 2.436 | Not reported | Organometallics 2017, 37, 729. |
| (P₂)FeH(H₂) | 2.649 | 2360 / 2340 | Chem. Eur. J. 2018, 24, 12346. |
DFT Calculations

Calculations were performed using Gaussian 09 revision D.01. 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. Natural bonding orbital analysis and Wiberg bond index analysis were performed using NBO version 3.1. Becke orbital composition analysis was performed using Multiwfn version 3.5. Solvation corrections were determined for thermodynamic profiles by the integral-equation-formalism polarizable continuum model (IEFPCM) using a SMD solvation model of THF.

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), (BBNPDpBu)ZnH₂, and (BBNPDpBu)ZnH₂
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-NH₂ d) 2-NHMe, e) 2-NHPh, f) 2-PPhPh g) 2-OH h) 2-SPh
Table S23. Summary of thermodynamics for E-BBN binding

| Compound | | | |
|----------|--------|--------|--------|
| | 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 |
| 2-NH₂ | 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%   |
| (BBNpDPBu)ZnH2              | 0.22 | 0.65 | 0.18    | 0.92            | 3.48            | 71%   | 24%   |
| (MePDPBu)FeH2               | 0.65 | 0.23 | 0.73    | 3.53            | 81%             | 14%   | 89%   |
| H-BBN(CH3)                  | 0.95 |      | 0.99    | 3.59            |                 |       |       |
| BBN(CH3)                    |      |      |         | 2.83            |                 |       |       |
| 2-NH2                       | 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    | 0.76            | 3.51            |       |       |
| 2-OH'                       | 0.66 | 0.00 |         | 1.31            | 2.82            |       |       |
| 2-SPh'                      | 0.36 | 0.64 | 0.17    | 1.34            | 2.81            |       |       |
| (MePDPBu)Fe(NH2)2           | 0.55 | 0.35 |         | 2.34            |                 |       |       |
| (MePDPBu)Fe(NHMe)2          | 0.54 | 0.41 |         | 2.62            |                 |       |       |
| (MePDPBu)Fe(NHPh)2          | 0.40 | 0.18 |         | 2.66            |                 |       |       |
| (MePDPBu)Fe(PHPh)2          | 0.55 | 0.18 |         | 2.73            |                 |       |       |
| (MePDPBu)Fe(OH)2            | 0.40,0.21 |  | 1.34 |                 |                 |       |       |
| (MePDPBu)Fe(SPh)2           | 0.50,0.18 |  | 1.86 |                 |                 |       |       |
| (MePDPBu)Fe(SPh)3           | 0.57 |      |         |                 |                 |       |       |
Table S26. Frontier orbital energies (eV) and Becke orbital composition for 1 and 2-E and analogous (MePDPtBu)Fe(E)₂ complexes.

| E                     | α/HOMO | α/LUMO | β/HOMO | β/LUMO | Orbital Composition β LUMO |
|-----------------------|--------|--------|--------|--------|---------------------------|
| (BBNPDptBu)Fe(E)₂     |        |        |        |        |                           |
| H                     | -5.303 | -2.231 | -5.204 | -2.485 | 17.1                      |
| NH₂                   | -4.918 | -2.184 | -4.917 | -2.346 | 9.6                       |
| NHMe                  | -4.865 | -2.163 | -4.879 | -2.327 | 10.4                      |
| NHPh                  | -5.048 | -2.041 | -5.067 | -2.294 | 15.9                      |
| PHPh                  | -5.067 | -2.171 | -5.222 | -2.506 | 9.5                       |
| OH                    | -4.925 | -2.171 | -4.893 | -2.332 | 20.4                      |
| SFh                   | -4.346 | -1.766 | -4.193 | -1.976 | 15.3                      |
| SPh (2-SPh")         | -4.535 | -1.795 | -4.415 | -1.997 | 13.6                      |
| (MePDPtBu)Fe(E)₂      |        |        |        |        |                           |
| H                     | -3.930 | -1.196 | -3.320 | -1.492 | 20.5                      |
| NH₂                   | -4.437 | -0.766 | -2.736 | -0.877 | 59.7                      |
| NHMe                  | -4.264 | -0.754 | -2.784 | -0.653 | 21.5                      |
| NHPh                  | -3.630 | -1.668 | -3.589 | -1.859 | 7.9                       |
| PHPh                  | -3.831 | -0.490 | -3.812 | -1.929 | 12.0                      |
| OH                    | -5.423 | -1.018 | -3.078 | -0.890 | 14.7                      |
| SFh                   | -5.532 | -1.725 | -5.031 | -2.376 | 10.6                      |
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 functional 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 $\beta$ 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 is 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 $\beta$ LUMO (Figures S91 and S92). The experimental $E_{1/2}$ of 2-OH is quasireversible 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) | $\Delta$ (eV) | ZPE-Entropy correction (eV) | $E^0$ (calc) V (vs. Fc/Fc$^+$) | $E_{1/2}$, V (vs. Fc/Fc$^+$) |
|---------------------|--------|---------------|----------------------|---------------------------|---------------|-----------------------------|-----------------------------|-----------------------------|
| (BBNPDPtBu)Fe(H)$_2$| 0      | -86736.988    | 25.50                | -86735.892                | -2.308        | -0.088                      | -2.594                      | -2.06                       |
|                     | -1     | -86738.493    | 6.83                 | -86738.200                | -2.308        | -0.088                      | -2.594                      | -2.06                       |
| (BBNPDPtBu)Fe(NH$_2$)$_2$ | 0      | -89750.909    | 29.07                | -89749.659                | -1.913        | -0.130                      | -2.947                      | -2.12                       |
|                     | -1     | -89752.085    | 11.91                | -89751.573                | -1.913        | -0.130                      | -2.947                      | -2.12                       |
| (BBNPDPtBu)Fe(OH)$_2$ | 0      | -90833.656    | 30.76                | -90832.333                | -2.077        | -0.116                      | -2.797                      | -2.12                       |
|                     | -1     | -90834.880    | 10.91                | -90834.410                | -2.077        | -0.116                      | -2.797                      | -2.12                       |
| (BBNPDPtBu)Fe(PHPh)$_2$ | 0      | -117916.663   | 41.65                | -117915.872               | -2.351        | -0.112                      | -2.527                      | -1.96                       |
|                     | -1     | -117918.282   | 24.62                | -117917.224               | -2.351        | -0.112                      | -2.527                      | -1.96                       |

Figure S90. LUMO $\beta$ energy (eV) vs $E^0$ (calc) V (vs. Fc/Fc$^+$) for 1 and 2-E.
Figure S91. LUMO $\beta$ energy (eV) vs $E_{1/2}$ (expt.) V (vs. Fc/Fc$^+$) for 1 and 2-E.

Figure S92. $E^0$ (calc) V (vs. Fc/Fc$^+$) vs $E_{1/2}$ (expt.) V (vs. Fc/Fc$^+$) for 1 and 2-E.
| E   | \((\text{BBNPDP}^{\text{tBu}})\text{Fe}(E)_{2}\) | \((\text{MePDP}^{\text{tBu}})\text{Fe}(E)_{2}\) |
|-----|---------------------------------------------|---------------------------------------------|
| H   | ![Image](image1.png)                         | ![Image](image2.png)                         |
| NH₂ | ![Image](image3.png)                         | ![Image](image4.png)                         |
| NHMe| ![Image](image5.png)                         | ![Image](image6.png)                         |
| PHPH| ![Image](image7.png)                         | ![Image](image8.png)                         |
| OH  | ![Image](image9.png)                         | ![Image](image10.png)                        |

**Figure S93.** Figure of β LUMO at 0.03 au for 1, 2-E and analogous \((\text{MePDP}^{\text{tBu}})\text{M}(E)_{2}\) complexes.

S98
## Optimized Geometries

### 1 S=2

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Fe   | 8.59011200 | 10.67669000| -0.71950800|
| N    | 10.11120900| 12.19601200| -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    | 8.94715200 | 14.49151200| 2.82942500 |
| C    | 7.74651900 | 12.79412000| 3.06397400 |
| H    | 7.37697400 | 15.29793600| 4.16023000 |
| H    | 8.48028000 | 13.39758000| 5.20680300 |
| C    | 5.43631700 | 13.37994900| 3.86083800 |
| H    | 4.84340900 | 13.68947000| 4.72935800 |
| H    | 4.97566900 | 12.47735100| 3.44881500 |
| H    | 5.38592000 | 14.16519800| 3.10080500 |
| C    | 6.97986300 | 12.07924700| 5.39818500 |
| H    | 6.44983800 | 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 | 1.0228200 |
| 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 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 10.81931900 | 6.43323400 | 1.56107900 |
| H       | 11.75562900 | 5.93949400 | 1.25233100 |
| H       | 11.03370000 | 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  | 6.63507600 | -1.18875600 |
| 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 |
| C       | 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       | 13.21391100 | 9.46129800  | -5.59675200 |
| H       | 12.29744900 | 10.57020500 | -6.64323600 |
| C       | 11.29281500 | 7.52277100  | -5.30017600 |
| H       | 11.60232100 | 6.93011700  | -6.16883300 |
| 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  | 8.60589000  | -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

| Atoms | x    | y    | z    |
|-------|------|------|------|
| Fe    | 8.32216900 | 10.40822400 | -0.71927500 |
| N     | 9.64600400  | 11.73345200  | -0.71993100  |
| C     | 9.68449200  | 12.63497900  | 0.31491600   |
| C     | 10.65650100 | 13.63583400  | 1.27052300   |
| H     | 10.68100600 | 12.88996800  | 2.98173000   |
| C     | 11.59273200 | 13.68123700  | 4.16336700   |
| H     | 12.36023100 | 14.44914100  | 5.80689800   |
| N     | 7.91142800  | 11.26147500  | 0.97598800   |
| C     | 6.39302400  | 9.75552100   | 1.99305000   |
| H     | 6.20754500  | 9.53005400   | 0.93876600   |
| H     | 5.41609700  | 9.84774600   | 2.47126300   |
| C     | 7.25635100  | 8.86108800   | 2.65383700   |
| H     | 6.87590500  | 7.70003600   | 2.28179400   |
| H     | 11.01127600 | 5.89519500   | 1.99767400   |
| H     | 11.58201400 | 7.32807600   | 2.15315500   |
| H     | 12.68239500 | 7.26327100   | 2.15923000   |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 11.307751 | 7.710092  | 3.145432  |
| C    | 11.109127 | 8.359514  | 1.089217  |
| H    | 11.475500 | 9.343481  | 1.428737  |
| C    | 11.732370 | 8.103760  | -0.301229 |
| H    | 12.833579 | 8.096524  | -0.242808 |
| H    | 11.470907 | 8.949887  | -0.951124 |
| C    | 11.271221 | 6.800139  | -0.986963 |
| H    | 11.567460 | 6.826989  | -2.046414 |
| H    | 11.816926 | 5.951944  | -0.561616 |
| C    | 9.751394  | 6.535127  | -0.899306 |
| H    | 9.258126  | 7.168413  | -1.646932 |
| H    | 9.557484  | 5.495336  | -1.211805 |
| C    | 10.547203 | 11.772148 | -1.733820 |
| C    | 11.547547 | 12.744671 | -1.755610 |
| H    | 12.266518 | 12.769322 | -2.567251 |
| C    | 10.263165 | 10.730540 | -2.710288 |
| C    | 10.802142 | 10.294718 | -3.932766 |
| H    | 11.690138 | 10.661347 | -4.422269 |
| C    | 9.974933  | 9.268177  | -4.377940 |
| C    | 10.162359 | 8.379484  | -5.603074 |
| C    | 11.411656 | 8.860183  | -6.372810 |
| H    | 11.568912 | 8.220364  | -7.247465 |
| H    | 12.313549 | 8.805833  | -5.753878 |
| H    | 11.294796 | 9.890104  | -6.727986 |
| C    | 10.403126 | 6.915876  | -5.159654 |
| H    | 10.574289 | 6.285080  | -6.039898 |
| H    | 9.550107  | 6.500913  | -4.614068 |
| H    | 11.280909 | 6.842168  | -4.509312 |
| C    | 8.958858  | 8.441897  | -6.571995 |
| H    | 9.203131  | 7.896467  | -7.490798 |
| H    | 8.719212  | 9.475534  | -6.843375 |
| H    | 8.060859  | 7.993731  | -6.251112 |
| N    | 9.174620  | 9.997966  | -2.415182 |
| N    | 8.989586  | 9.126873  | -3.422068 |
| C    | 7.669108  | 8.478500  | -3.431442 |
| H    | 7.444278  | 8.293046  | -2.377034 |
| H    | 7.761870  | 7.501549  | -3.909501 |
| C    | 6.573604  | 9.340790  | -4.091862 |
| H    | 5.613071  | 8.960065  | -3.718770 |
| H    | 6.581678  | 9.128972  | -5.168244 |
| C    | 6.675476  | 10.864646 | -3.867443 |
| H    | 6.020767  | 11.300520 | -4.634740 |
| H    | 7.680273  | 11.199166 | -4.168040 |
| B    | 6.221798  | 11.565514 | -2.463404 |
| H    | 7.089489  | 11.244911 | -1.465907 |
| C    | 4.736408  | 11.181048 | -1.912093 |
| H    | 4.591530  | 10.094010 | -1.775873 |
| C    | 3.721825  | 11.614950 | -3.007772 |
|   |   |   |   |
|---|---|---|---|
| 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 |
| Atom | X  | Y  | Z    |
|------|----|----|------|
| 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 | 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 | -4.1422100  |
| 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 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| 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| 2.45405000|
| H       | 9.09435400 | 14.52965000| 2.83506000|
| C       | 7.71626800 | 12.80668500| 2.99955900|
| C       | 6.83988700 | 13.14114000| 4.20466200|
| C       | 7.30739000 | 14.48944100| 4.79593100|
| C       | 7.22931500 | 15.30051300| 4.06441400|
| C       | 8.34344700 | 14.43805400| 5.14841400|
| C       | 5.36840500 | 13.30494900| 3.74980500|
| H       | 6.67546000 | 14.74961000| 5.65160000|
| H       | 7.97225600 | 11.92157900| 5.63590000|
| H       | 6.50923500 | 11.11917000| 5.04063000|
| N       | 8.42591000 | 11.80047300| 1.11603900|
| N       | 7.55754600 | 11.72295600| 2.16907400|
| C       | 7.91794600 | 10.42209400| 2.39578600|
| H       | 6.62131800 | 10.04985700| 1.41280200|
| H       | 6.00099000 | 10.59581500| 2.96084000|
| C       | 7.19736400 | 8.50572200 | 3.25206000|
| H       | 8.03139000 | 9.78181600 | 4.12089100|
| C       | 9.12975800 | 9.01892000 | 2.40261800|
| H       | 9.66446200 | 8.35899900 | 3.10367700|
| H       | 9.77741200 | 9.03999400 | 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|
| Element | X    | Y    | Z    |
|---------|------|------|------|
| 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 | -0.66373000 |
| H       | 7.36157800  | 7.45499200 | -1.24661200 |
| H       | 7.06839100  | 5.79898500 | -0.75802300 |
| C       | 11.08609700 | 12.26109000 | -1.72415200 |
| C       | 12.07851800 | 13.22541200 | -2.12964700 |
| H       | 12.81177300 | 13.23655800 | -2.53061600 |
| C       | 10.84845400 | 11.24801100 | -2.71826100 |
| C       | 11.50802800 | 10.81980100 | -3.88249900 |
| H       | 12.45088800 | 11.18135000 | -4.25973600 |
| C       | 10.72904400 | 9.80799500 | -4.43288800 |
| C       | 11.06513300 | 8.93400400 | -5.63927300 |
| C       | 12.41595300 | 9.40040200 | -6.22563000 |
| H       | 12.67724400 | 8.77017100 | -7.08222500 |
| H       | 13.22487000 | 9.31870000 | -5.92121000 |
| C       | 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 |
|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| 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   | 19.44633200 | 13.57871600 | -1.85307600 |
| C   | 19.81831600 | 14.67505800 | -1.05421600 |
| C   | 19.27596800 | 14.78122400 | 0.23966600  |
| C   | 18.27941500 | 10.94460000 | -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   | 15.97630000 | 8.74609700  | -5.29055900 |
| C   | 15.46976200 | 9.07966300  | -1.95815300 |
| C   | 14.17423000 | 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   | 10.74109000 | 11.79949700 | 0.10466700  |
| C   | 11.71187200 | 12.96494100 | -0.20193200 |
| C   | 13.14352200 | 12.80375200 | 0.37119800  |
| C   | 13.19068900 | 12.92862000 | 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 | 11.7351700 | -4.07529000 |
| H | 19.84028200 | 13.46881700 | -2.86057100 |
| H | 20.50902200 | 15.42534000 | -1.42847800 |
| H | 19.54679900 | 15.61546000 | 0.88715600 |
| H | 18.35269300 | 15.54232000 | 3.24007500 |
| H | 18.55141800 | 15.74641000 | 5.69713200 |
| H | 20.54647900 | 15.61154600 | 0.88715600 |
| H | 18.35269300 | 15.54232000 | 3.24007500 |
| H | 18.55141800 | 15.74641000 | 5.69713200 |
| H | 19.54679900 | 15.61546000 | 0.88715600 |
| H | 18.35269300 | 15.54232000 | 3.24007500 |
| H | 18.55141800 | 15.74641000 | 5.69713200 |
| H | 19.39930600 | 9.30211100 | -5.32441000 |
| H | 18.35898500 | 8.53219400 | -6.53440700 |
| H | 18.13017300 | 10.24099000 | -6.13357000 |
| 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 | -5.65036000 |
| H | 15.51959400 | 11.09681600 | 3.37731700 |
| H | 15.40694000 | 11.83697400 | 4.97190000 |
| H | 17.61315800 | 10.98528700 | 5.60758900 |
| H | 16.57891800 | 9.68066800 | 5.05275300 |
| H | 18.79311600 | 10.99323000 | 3.36786900 |
| H | 18.98271600 | 9.55978800 | 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 | 17.18681100 | 6.51412800 | -0.45896000 |
| H | 15.92479600 | 6.18808800 | 1.73609700 |
| H | 15.78028200 | 7.77588100 | 0.99990200 |
| H | 16.00882000 | 8.09571300 | 3.33857600 |
| H | 17.17437000 | 6.00382400 | 4.01850200 |
| H | 17.86737100 | 7.45757200 | 4.71869600 |
| H | 19.03319800 | 5.65797500 | 2.56269100 |
| H | 19.72089900 | 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 | 13.05922000 | 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 |
1S=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   19.13364000  14.87967100  -0.21635800
C   18.30702600  13.87191500   0.68930600
C   18.01528200  11.49967400  -2.01420100
C   17.27939900   9.77411800  -3.27702500
C   17.21988000   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  -1.59656600
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   13.83482000  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   6.95090200   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       18.88128400   9.11752100 -4.03905100
H       19.77662500   9.11752100 -2.86947100
H       20.33713600   9.11752100 -1.45650500
H       19.35946900   9.11752100  0.85074500
H       18.03976400   9.11752100  3.30769600
H       18.12165400   9.11752100  5.74749000
H       16.67407100   9.11752100 -5.15904100
H       18.18545400   9.11752100 -6.27375300
H       17.93422500   9.11752100 -5.96525700
H       18.76420900   9.11752100 -3.34689800
H       17.10489200   9.11752100 -2.94758200
H       17.76217300   9.11752100 -4.53821800
H       15.86089900   9.11752100 -5.77368700
H       15.13667300   9.11752100 -4.21671200
H       15.47809900   9.11752100 -5.33653800
H       15.60956000   9.11752100 -3.15463000
H       15.36302200   9.11752100 -4.75189900
H       17.67649700   9.11752100 -5.41856600
H       16.76601700   9.11752100 -4.88224800
H       18.83774100   9.11752100 -3.18157000
H       19.13393800   9.11752100 -4.09584800
H       19.88968200   9.11752100  1.03579500
H       18.34886800   9.11752100 -0.55749100
H       19.69161700   9.11752100 -0.41909400
H       18.39061000   9.11752100 -0.70483400
H       17.37434600   9.11752100 -0.58865200
H       16.21418800   9.11752100 -1.66103000
H       15.92355300   9.11752100 -0.87720200
H       16.20572700   9.11752100  3.19347700
H       17.52728300   9.11752100  3.87619700
H       18.13872600   9.11752100  4.53165800
H       19.36597600   9.11752100  2.39077500
H       20.06724900   9.11752100  3.89647300
H       21.00864800   9.11752100  1.76168600
H       20.60267200   9.11752100  3.07044500
H       15.53625300   9.11752100 -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   | 13.02957000 | 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 |
$^{1^\text{st}} S=5/2$

| Symbol | $x$-coordinate | $y$-coordinate | $z$-coordinate |
|--------|----------------|----------------|----------------|
| 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    | 14.92793000    | 0.22170200     |
| 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      | 17.95771100    | 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      | 11.40809000    | 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 | 13.67541000 | -2.91456600 |
| H   | 20.38256500 | 15.63864400 | -1.46383000 |
| 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 | 6.60663000  |
| 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 | 15.02670000 | 6.61212200  |
| H   | 19.48074200 | 9.49185000  | -5.37854500 |
| H   | 18.46450100 | 8.68774600  | -6.58709000 |
| H   | 18.17042500 | 10.38689000 | -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   | 15.68420000 | 11.02374300 | 3.45352400  |
| H   | 15.61554500 | 11.77776700 | 5.04282500  |
| H   | 17.95683100 | 11.10798600 | 5.50744300  |
| H   | 16.91415000 | 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   | 19.43767000 | 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  |
(BBNPDpBu)ZnH₂

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  4.12119900  17.77538600
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  4.54013000  14.01105800
H  8.48237900  4.18471000  13.13138500
H  6.84023500  4.52126400  13.69898800
H  6.19209200  4.43085000  16.07279100
C  9.88302400  5.60737700  14.98604000
H  10.46772900  5.30334400  14.1100200
H  9.98576500  4.83172600  15.75221500
H  10.32962800  5.62516000  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
H  7.73925100  7.24269000  16.6245100
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  18.04661100
C  4.57541900  12.58617200  17.40046400
H  4.32984400  12.15736700  16.41886700
|    | X            | Y            | Z            |
|----|--------------|--------------|--------------|
| H  | 3.66713000  | 13.12164400  | 17.72243900  |
| C  | 4.89028700  | 11.41731000  | 18.83691100  |
| H  | 4.03842900  | 10.71859500  | 18.30347200  |
| C  | 4.97216600  | 11.87103500  | 19.85024000  |
| H  | 4.05141600  | 12.39874000  | 20.15127500  |
| H  | 4.01389000  | 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  | 23.45084000  |
| 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  |
| Atom  | X (Å) | Y (Å) | Z (Å) |
|-------|-------|-------|-------|
| 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     | 17.23287300 | 9.90458900  | 1.52349100  |
| C     | 18.51894400 | 12.71994900 | -1.38076800 |
| C     | 19.36004300 | 13.69730400 | -1.88631100 |
| C     | 19.69318600 | 14.81329100 | -1.09011200 |
| C     | 19.15856700 | 14.89261700 | 0.21213000  |
| C     | 18.33584700 | 13.88285400 | 0.68111100  |
| C     | 18.04364000 | 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 | 7.97832000  | -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     | 17.77398000 | 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     | 18.81883000 | 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   | 16.91501000 | 16.62796300 | 4.92987000  |
| H   | 17.05059900 | 16.34937000 | 6.67501400  |
| H   | 18.41840300 | 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   |
\[ (\text{MePDP}^\text{Bu})\text{FeH}_2 \text{S} = 3/2 \]

| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| 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    | 11.01422100 | 13.54446500 | 2.50210400 |
| H    | 12.78228000 | 14.86718000 | 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 | 4.33886300 |
| C    | 7.66452200  | 14.32993900 | 5.08327000 |
| H    | 7.13819000  | 14.56032100 | 6.01598500 |
| C    | 7.00431100  | 15.24743700 | 4.85983000 |
| C    | 5.49348500  | 13.69004900 | 4.02419200 |
| H    | 4.98120100  | 13.96408000 | 4.95416100 |
| C    | 4.88471400  | 12.93002600 | 3.52552400 |
| C    | 5.52076200  | 14.57274300 | 3.37633000 |
| C    | 6.87840100  | 11.96657700 | 5.27678500 |
| H    | 6.39484200  | 12.24120800 | 6.22159000 |
| C    | 7.88866900  | 11.60892100 | 5.50443900 |
| C    | 6.31412300  | 11.13296600 | 4.85027400 |
| N    | 8.24075600  | 11.82903000 | 1.14443500 |
| N    | 7.39397500  | 11.85088400 | 2.18000000 |
| 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 | -1.75265600 |
| 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  | -7.45452400 |
| 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 |
|   |          X          |          Y          |          Z          |
|---|-------------------|-------------------|-------------------|
| 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      |
|    |        X         |         Y         |        Z         |
|----|----------------|----------------|----------------|
| 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    |  9.67121000    | -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(CH₃)^−

|    |   X   |       Y       |       Z       |
|----|-------|--------------|--------------|
| 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 | 19.49998000 |
| H  | 9.94348700  | 9.44442700 | 19.06657400 |
| H  | 7.92711100  | 8.74686400 | 22.96586500 |
|  | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| 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 | 11.07686000| 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|

**BBN(CH₃)**
| Atom | X coordinate | Y coordinate | Z coordinate | Standard deviation |
|------|--------------|--------------|--------------|--------------------|
| 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   |
| H    | 3.88674000   | 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    | 4.48713000   | 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    | 5.36882000   | 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  |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| 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       | 6.99073700  | 5.74629200 | -2.87131500 |
| C       | 8.32752000  | 3.08563500 | -3.20040400 |
| H       | 7.27148300  | 2.81894700 | -3.37379000 |
| 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  |
| C       | 3.46235800  | 3.84204900 | 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 | -4.87859900 |
| 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 | -6.31301000 |
| 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 |
|   | X    | Y    | Z    |
|---|------|------|------|
| 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 | 5.63889000  | 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  5.16317000  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  3.07660000
C  2.72834700  6.28334200  3.66738800
C  1.95704300  6.00766600  1.99158600
C  3.85684500  6.84138200  3.07660000
C  2.72834700  6.28334200  3.66738800
C  0.55212900  7.30134500  4.46595500
C  1.84883000  7.15740000  5.98254000
C  3.05665000  4.16697000  3.10575500
C  0.86448300  3.59769700  1.77516300
C  1.35665400  4.16697000  3.10575500
B  0.43833900  4.21664900 -0.79770600
N  2.05496400  4.44810200 -1.15648800
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  5.11271000 -1.79224000
C -0.72337300  4.78411200 -3.28454100
C -0.41124100  3.29319000 -3.65691800
C  0.24103500  2.32610600 -2.64417200
N  4.98270400  3.30676800 -1.92272900
N  5.16168500  2.40391700 -2.93026700
C  6.11504500  5.23394800 -0.99196200
C  7.11435600  6.21409500 -1.02655100
C  5.99945300  4.17953900 -2.02000000
C  6.83178400  3.86159300 -3.08815800
C  6.27610400  2.72981900 -3.67481400
C  7.89239000  1.95712700 -4.88643200
C  7.98458400  2.72726000 -5.49067300
C  7.29961500  0.55508000 -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
|   |     X     |     Y     |     Z     |
|---|----------|----------|----------|
|  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 |
|  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 | 2.30229000 | 0.38650200 |
|  H | -0.77631300 | 4.78234200 | 1.06375800 |
|  H | 0.75361700 | 5.60370500 | 0.96143600 |
|  H | 1.69144900 | 3.01420000 | 1.32205700 |
|  H | 0.12402300 | 2.82820100 | 2.02524000 |
|  H | 1.74068500 | 3.37791000 | 3.76096400 |
|  H | 0.54040000 | 4.66807800 | 3.62405300 |
|  H | 2.84184700 | 5.35070900 | 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 | -4.77931990 |
|  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 | -3.62360000 |
| 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 | 6.81865000 |
| N       | 2.55413600 | 7.84269300 | 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       | 3.12880000 | 5.62234000 | 6.39989900 |
| C       | 2.50318000 | 5.88922000 | 5.02103100 |
| B       | 3.53830600 | 5.74572400 | 3.74895500 |
| C       | 2.77948000 | 5.72630000 | 2.28826600 |
| C       | 1.76693200 | 4.55051200 | 2.27076700 |
| C       | 2.35095700 | 3.16356000 | 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 | 10.03627000 | 3.94498400 |
| C       | 9.46841200 | 8.82970700 | 3.60003700 |
| 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  6.72181000  8.01577900
H   5.47561400  6.67882000  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  8.57680000  7.29222300
H   9.22700600  10.66994700  8.48288700
H   7.62808400  11.58827400  10.16028900
H   5.1667200  10.34211600  10.63030400
H   5.02169000  8.24388400  9.44085600
H   5.00671300  4.23378800  4.68511300
H   6.20327100  4.98966600  2.73303700
H   5.94960900  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   2.04463000  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  | 7.20668000  |
| H  | -1.64097000  | 7.84010000  | 8.06977000  |
| H  | -0.79804000  | 8.54048200  | 6.61209400  |
| H  | 0.41750900  | 10.52841800  | 9.55888600  |
| H  | -0.40753100  | 10.62073800  | 7.98637000  |
| 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  | 12.46312000  | 4.64516800  |
| H  | 9.26745500  | 11.02279200  | 3.78147700  |
| H  | 12.36266500  | 9.86379500  | 2.04046000  |
| 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  | 7.63905000  |
| 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  | 5.67969400  | 10.35100100  |
| H  | 5.55555400  | 4.64506900  | 10.93939000  |
| H  | 6.84941200  | 3.54608500  | 10.55150500  |
| H  | 4.95620600  | 4.98690000  | 8.66818300  |
| H  | 5.24224500  | 3.27357500  | 8.80368300  |
2-PHPb

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    1.84537800  0.70735400  5.15336200
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  2.81431000
C   -0.20670300  1.49600300  3.02735200
C   -3.43894600  3.11382000  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  2.78303000  2.08138500
C   -3.84912700  3.39608800  2.63384000
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  0.87083000
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   -0.55337000 10.14787500  7.81481900
C    0.49492500 11.13375900  7.23502300
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  7.85459300
C   -5.84028400  9.59364700  9.13238200
C   -5.35371100  9.87649800  7.37659000
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
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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  4.54794000  3.50658200
H   -1.64739900  6.81537000  8.73607000
H   1.06784000  4.11699700  5.82145800
H   0.76140600  4.32294700  3.46459700
H   2.39266900  3.75747400  7.34469700
H   1.12026900  2.68516900  1.78856300
H   1.95238200  1.59731500  2.86366000
H   0.14792400  0.56506400  2.43912000
H   -0.13909100  2.06514900  2.58964400
H   -1.54805400  0.69154900  4.48831600
H   -0.01646200  -0.16336500  6.10517100
H   0.49961300  -0.73584100  4.53230000
H   2.43597100  0.64309900  4.50401500
H   2.35107300  0.03772000  6.13478700
H   1.68303800  2.13781500  7.04053000
H   2.94969000  2.51038000  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  3.62700000  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
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H   -3.95865900  3.54645000  12.18928800
H   -3.93997900  1.95335800  12.72262400
H   -5.42374600  0.84724300  11.96580600
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H   -6.05989600  1.03206700  10.32649400
H   -6.42802900  3.05884500  9.14197000
|   |        |        |        |
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| 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 |
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| 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 |
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| H | -5.52983600 | 8.44081000 | 10.92927000 |
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| H | -0.96110100 | 6.85669300 | 4.96534200 |
| H | 0.31750200 | 7.69364600 | 4.14145500 |
| H | -0.37619900 | 9.84696900 | 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 | 3.00117000 | 8.72533500 | 6.65746400 |
| H | 1.82454900 | 9.13735200 | 5.42608900 |
2-OH

Fe  2.16008200  11.25459600  7.72756400
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H   3.75130300  12.13687700  9.44472100
O   3.72658200  12.19139700  8.47910300
H   0.46753800  11.86406200  6.91485100
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  11.2743600
C   0.56011400 10.21498800 11.84816100
C  -0.10604600 10.43332000 13.20365400
C   0.69752200 11.42926100 14.07447100
C  -1.56984700 10.91001800 13.0293600
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
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C   6.08137300 12.72554400 10.31765700
C   5.52669900 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
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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
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H    6.38979200  11.20038000   1.45592200
H    5.84812600  12.11169700   2.86882200
H    6.61341600  10.53590400   3.08592700
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H    3.24786700   6.52721800   5.87746000
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H    0.82453600   8.02566400  11.70363800
H    0.86379100   8.68211300  14.11368900
H   -0.60451400   9.22857000  14.93863800
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H    0.18224500  14.32083500   9.79310500
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H   -1.19340700  13.01104800   3.34240300
H   -2.50067500  13.78688000   4.19236500
H    0.44830900  13.69693600   4.94274000
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| 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|
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| H     | 6.34575800  | 14.75692900 | 11.02313500|
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| H     | 5.68338600  | 15.71325900 | 7.00180700 |
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| H     | 7.89167400  | 15.74635100 | 7.88891400 |
| H     | 7.36152800  | 15.48319500 | 9.52579700 |
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2-SPh

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C  4.30288100 10.40061100  14.38743500
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C  3.43280200 10.30934000  16.85421700
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C  3.43542800  5.30372000  14.73497200
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S  5.20635400  7.48089000  14.86356000
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C 11.74565500  6.50864100  17.61421900
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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
|   | 11.88946800 | 11.29408800 | 12.34043100 |
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| 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 |
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| 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 |
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| S | 8.52449600  | 7.47671400  | 11.82435600 |
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| H | 9.26874400  | 3.95068500  | 8.48094000  |
| H | 11.00281600 | 2.75596300  | 9.81045800  |
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| H | 10.98697300 | 11.14681600 | 9.78782300  |
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| H | 8.81169700  | 11.66362900 | 10.61352800 |
| H | 8.47764900  | 10.57013800 | 12.82842100 |
| H | 10.45896600 | 11.31675300 | 13.96700000 |
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| 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 |
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| H | 10.39878000 | 6.55504500  | 20.05147300 |
|   |   |   |   |   |
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| 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 |
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| H | 2.14487200 | 4.47942700 | 7.26450700 |
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| H | 1.31907600 | 6.58759000 | 8.22139100 |
| H | 1.44408700 | 5.93760200 | 9.86698700 |
| H | 4.88687800 | 5.88001700 | 7.20702500 |
| H | 3.33092900 | 6.18063000 | 6.64678800 |
| H | 4.30961100 | 7.45013400 | 7.78153800 |
| H | 5.82447100 | 8.12118000 | 9.87623500 |
| H | 4.05754900 | 8.17723500 | 9.73083800 |
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| 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 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| 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    | 2.43088000   | 0.53147500   | 10.34116800|
| C    | 2.03105500   | -1.57933900  | 9.70052200 |
| C    | 3.24974600   | 0.57220200   | 8.76661900 |
| C    | 0.36382100   | 2.05250400   | 5.32830500 |
| C    | 1.03963400   | -0.39241400  | 7.98333600 |
| 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   | 1.33406000 |
| 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  | -1.47057700  | 4.46616000 |
| 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    | -2.40783300  | -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  | -0.76608000|
| 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  7.57841100
C  -6.09563800  3.04077900  6.39854200
C  -5.74185200  3.30603800  6.39854200
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
H  -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  6.31263000
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  -6.39212220  -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

S151
|   |            |            |            |
|---|------------|------------|------------|
| H | -0.321968  | -3.993058  | 6.160976   |
| H | 0.952999   | -2.582324  | 7.708879   |
| H | 3.069905   | -1.451746  | 10.559774  |
| H | 1.544872   | -2.175798  | 10.028857  |
| H | 2.948433   | -2.145185  | 8.937444   |
| H | 1.910640   | 0.590234   | 11.208522  |
| H | 0.941172   | 1.551016   | 10.089910  |
| H | 0.345722   | -0.020301  | 10.642703  |
| H | 3.782698   | 0.033598   | 7.975614   |
| H | 3.051031   | 1.582642   | 8.400230   |
| H | 3.919608   | 0.658524   | 9.630017   |
| H | 1.203940   | 2.293852   | 8.144417   |
| H | -0.564987  | 2.259139   | 8.041090   |
| H | -0.497119  | 2.713233   | 5.656102   |
| H | 0.371427   | 3.934908   | 6.533595   |
| H | 2.514441   | 3.177486   | 5.785923   |
| H | 1.933554   | 1.594719   | 5.342724   |
| H | -0.101466  | 4.769936   | 4.120179   |
| H | -0.380391  | 4.274615   | 1.800161   |
| H | 0.166278   | 5.937446   | 1.934636   |
| H | 2.313352   | 5.444073   | 1.025345   |
| H | 1.192998   | 4.540681   | 0.045059   |
| H | 3.330378   | 3.309836   | 0.721833   |
| H | 1.827048   | 2.444665   | 0.972115   |
| H | 3.248527   | 2.049907   | 2.868673   |
| H | 4.698843   | 4.078797   | 2.724317   |
| H | 4.164992   | 3.689016   | 4.347768   |
| H | 3.331434   | 6.023213   | 2.588186   |
| H | 3.989013   | 6.056566   | 4.201173   |
| H | 1.509621   | 6.656250   | 3.989341   |
| H | 1.913728   | 5.476583   | 5.221876   |
| H | 1.931178   | -0.163444  | 4.085343   |
| H | 3.014227   | -2.162537  | 3.114904   |
| H | 2.417196   | -2.923619  | 0.821156   |
| H | 0.729620   | -1.648563  | -0.493300  |
| H | -0.339901  | 0.365244   | 0.478735   |
| H | -5.254215  | -0.166849  | 4.841943   |
| H | -6.334602  | -2.163146  | 5.821018   |
| H | -5.736917  | -2.913260  | 8.118202   |
| H | -4.051383  | -1.630040  | 9.427324   |
| H | -2.984520  | 0.380967   | 8.446596   |
| Z'         | 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| 14.61065500 | 1.33805700  |
|            | C             | 12.43126000| 13.98692000 | -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             | 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             | 5.77709900 | 10.99507200 | 2.65661800  |
|            | C             | 7.31950900 | 9.45978000  | 2.85820600  |
|            | H             | 6.55389000 | 8.67408900  | 2.79573000  |
|            | H             | 7.43007500 | 9.69337000  | 3.92687300  |
|            | C             | 8.65070900 | 9.83356200  | 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             | 8.89324000 | 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  |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | 10.30378600 | 6.57353900 | 2.46987600 |
| C       | 10.03770800 | 7.39123100 | 0.48604700 |
| H       | 10.94668300 | 7.99317400 | 2.46987600 |
| C       | 10.07676700 | 6.96550300 | -1.00013600 |
| H       | 10.96736700 | 6.35023800 | -1.21528000 |
| C       | 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 |
| C       | 6.68794300  | 6.03346300 | -1.22614700 |
| C       | 11.26237500 | 12.22722900 | -1.66348000 |
| H       | 11.01858700 | 11.29261400 | -2.76422400 |
| H       | 11.04564900 | 11.49668500 | -4.26364400 |
| C       | 11.73212800 | 11.04564900 | -3.94949800 |
| 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 | 9.80500000 | -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 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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  | -5.16465000|
| 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   | 7.87334000  |
| N      | 3.02722600  | 10.53669600  | 5.69896400  |
| N      | 3.49641000  | 10.14171000  | 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      | 3.77914000  | 8.82905800   | 4.43742200  |
| C      | 3.96723400  | 10.00717400  | 3.72160400  |
| C      | 4.52070700  | 10.16805800  | 2.30932500  |
| C      | 5.75704700  | 11.09764600  | 2.75643000  |
| 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      | -0.18606000 | 10.59902900  | 13.19351400 |
| C      | 0.61187700  | 11.60949500  | 14.05246700 |
| C      | -1.64011500 | 11.08931000  | 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  | 5.14466000  |
| B      | 5.60598400  | 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  | 6.93930000  |
| 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  |
| C      | -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 | 6.95069000 |
| C | -1.75516400 | 15.19366600 | 5.52382600 |
| 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  | 8.81793000  | 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 | 11.75001000 | 4.41744900 |
| H | -1.02311300 | 13.20880300 | 3.23458800 |
| H | -2.27585000 | 14.06976900 | 4.08541500 |
| H | 0.65131100  | 13.75124000 | 4.84877200 |
|   | 15.23165300 | 4.57267500    |
|---|-------------|---------------|
| H | 12.72340000 | 3.33464700    |
| H | 12.84404500 | 4.76587300    |
| H | 12.78830100 | 6.23767900    |
| H | 12.77056200 | 4.81044500    |
| H | 14.99019000 | 5.40888300    |
| H | 15.02451000 | 4.10993900    |
| H | 17.47661000 | 5.65816500    |
| H | 17.73038100 | 4.96137000    |
| H | 18.81358900 | 6.31192500    |
| H | 17.57704400 | 6.32755600    |
| H | 17.47152400 | 7.81185100    |
| H | 15.32872400 | 5.69259800    |
| H | 15.25730900 | 7.39631500    |
| H | 13.79145600 | 6.75882000    |
| H | 14.27559600 | 8.48336600    |
| H | 14.59767200 | 9.10959900    |
| H | 16.29987400 | 9.75637000    |
| H | 16.98438500 | 9.09894000    |
| H | 18.18285700 | 8.05357400    |
| H | 16.71526800 | 7.78918500    |
| Atoms | x   | y   | z   |
|-------|-----|-----|-----|
| 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 | 3.98525000 | 10.28760600 |
| C     | 4.40621800 | 5.14461000 |  9.60487500 |
| C     | 3.71894600 | 5.24643600 |  8.24574000 |
| C     | 4.70276400 | 5.79688300 |  7.18305700 |
| C     | 3.29446700 | 3.82876400 |  7.02047000 |
| C     | 2.44227400 | 6.11817500 |  8.29971200 |
| C     | 4.75190800 | 7.64798300 | 10.18664700 |
| C     | 3.62853300 | 8.30034000 | 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     | 1.37492200 | 10.08347700 | 12.52711800 |
| C     | 0.01463800 | 10.61910700 | 11.99130500 |
| C     | -0.06317300 | 12.14790900 | 11.79604500 |
| C     | 1.18229100 | 12.76009900 | 11.12078200 |
| C     | 4.11201400 | 6.20612900 | 15.14694200 |
| C     | 3.04930500 | 5.65556000 | 14.40954500 |
| C     | 2.33376400 | 4.55806200 | 14.89621200 |
| C     | 2.65938000 | 3.99026800 | 16.13009400 |
| C     | 3.70901300 | 4.53361200 | 16.87421100 |
| C     | 4.42659900 | 5.62889900 | 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 | 10.37634000 |
| 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 | 16.89723000 |
| C     | 10.22086700 | 6.10156100 | 18.10033000 |
| 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 | 11.34430200 |   |   |
| 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 | 10.97610000 | 5.40073700  | 11.85132600 |   |   |
| C | 10.71884600 | 4.25760400  | 10.08760800 |   |   |
| C | 10.36916500 | 3.75917100  | 9.33599000  |   |   |
| B | 9.97221100  | 9.02877700  | 12.40967400 |   |   |
| N | 8.03198100  | 6.07192300  | 15.08883200 |   |   |
| N | 8.77553200  | 5.56617000  | 9.83679000  |   |   |
| 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 | 9.76095000  | 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 | 9.46534600  | 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 | 10.23892000 | 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 | 12.22065000 |
| 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 | 10.05950000 |
| C       | 3.45854000 | 7.93217300 | 10.81101200 |
| C       | 3.30561500 | 9.45977800 | 10.82914000 |
| 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 | 18.63834000 |
| C       | 4.53382200 | 7.95465500 | 18.19903700 |
| C       | 4.73549000 | 8.22990600 | 16.84592300 |
| B       | 2.08408900 | 10.07552000 | 11.61138800 |
| 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 | 14.16385800 |
| 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 | 15.23882000 |
| 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 | 19.10396000 |
| 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 |
| H          | 7.96451300 | 7.70212300 | 18.80117400 |
| H          | 7.36452400 | 6.12899300 | 19.31512300 |
| H          | 8.66737200 | 3.45834200 | 17.00535900 |
| H          | 6.94833000 | 0.40346900 | 13.42343600 |
| H          | 8.66737200 | 3.45834200 | 17.00535900 |
| 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          | 2.00983000 | 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 | 7.76194000 | 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 |
(MePDP$_{18}$)Fe(NH$_2$)$_2$

| Element | X  | Y   | Z   |
|---------|----|-----|-----|
| Fe      | 4.40235100 | 4.40215800 | -0.00004300 |
| N       | 2.92701700  | 2.92703000  | 0.00001400  |
| N       | 4.80776700  | 3.10262300  | 1.75329000  |
| N       | 5.71472200  | 3.05436900  | 2.75540800  |
| N       | 6.20351000  | 4.15934400  | -0.65187100 |
| H       | 6.67458000  | 3.26632000  | -0.77450700 |
| C       | 0.93351200  | 0.93373400  | 0.00008800  |
| C       | 1.92206800  | 0.95678600  | 0.99098300  |
| C       | 2.89301400  | 1.95168100  | 1.94996800  |
| C       | 3.95421800  | 2.08723700  | 1.94996800  |
| C       | 4.32041900  | 1.37857300  | 3.11478600  |
| 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  |
| C       | 5.45731300  | -0.37020400 | 5.01673500  |
| H       | 6.36903100  | 2.88399200  | 5.81505400  |
| H       | 6.92438900  | 3.71608200  | 5.37405700  |
| C       | 6.37620300  | 3.25249200  | 6.09613900  |
| C       | 7.66410400  | 1.15855400  | 4.47267400  |
| H       | 7.59040000  | 0.28633200  | 3.81418800  |
| H       | 8.21569300  | 0.86140600  | 5.37274600  |
| C       | 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  | -3.53659900 |
| 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 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| 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 |
\[(\text{MePDP}^{\text{Su}})\text{Fe(NHMe)}_2\]

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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 | -1.01315000|
| 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 | -2.47667800|
| 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 | -3.40469900|
| C       | 6.52897000 | 1.89967000 | -4.56112000|
| 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|
|   | X-coordinates | Y-coordinates | Z-coordinates |
|---|---------------|---------------|---------------|
| 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    |
| Atom | x    | y    | z    |
|------|------|------|------|
| Fe   | 5.63977700 | 8.63906300 | 5.91898400 |
| N    | 5.50007800  | 10.83564100 | 5.84500200  |
| N    | 3.47704300  | 9.30674500  | 6.43046000  |
| N    | 2.30756200  | 8.75299100  | 7.00513000  |
| 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    | 1.73756600  | 9.70230300  | 7.34971700  |
| C    | -0.05921500 | 9.42588900  | 7.87082000  |
| 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    | 7.63504000  | 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  | 5.15356600  | 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 |  6.91872700 |
| 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 |
\((\text{MePDP}^{\text{Bu}})\text{Fe(PPH)}_2\)

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| 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    | -5.25564000 | 4.20402600 | 7.76920500 |
| C    | -5.59791200 | 3.30045700 | 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  11.98242600  
H -3.78111500  3.50032000  12.47862100  
H -3.23755700  1.88962000  11.50110100  
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 -7.87294000  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  

S172
\[(Me\text{PDP}^{\text{Bu}})\text{Fe(OH)2}\]

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| 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    | 3.56626000 | 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    | 0.99821600 | 11.28189200 | 13.96914900 |
| C    | -1.29206100 | 11.45526400 | 12.89041500 |
| 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 | 6.82526600  | 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  |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Fe   | 7.0092300 | 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 | 12.64956600 |
| 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 | 7.06829000 | 11.23996600 |
| C    | 3.80706100 | 6.60932000 | 14.78425800 |
| C    | 3.01274800 | 7.76817300 | 14.68459000 |
| C    | 1.66449500 | 7.68937600 | 14.33116500 |
| C    | 1.07101200 | 6.45169500 | 14.06684000 |
| C    | 1.84567200 | 5.29269700 | 14.16829700 |
| C    | 3.19321400 | 5.36895400 | 14.52482600 |
| C    | 8.50181300 | 1.83084400 | 14.30021000 |
| 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 | 15.12653000 |
| 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 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| 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    | 0.01974700  | 3.69085500 | 3.79712800 |
| H    | 1.07429200  | 8.60087300 | 14.2642800 |
| H    | 3.46788200  | 8.73268800 | 14.8911700 |
| H    | 8.95340000  | 7.91672000 | 15.2823260 |
| H    | 3.75911600  | 7.31486500 | 12.0006160 |

(‌BNPDPBu)Fe(NH₂)₂²⁻
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -2.835172 | 3.902001  | -1.147050 |
| C       | -3.887821 | 1.795096  | -0.180537 |
| C       | -4.025805 | 4.633624  | 1.860649  |
| C       | -4.843434 | 4.733151  | 3.152439  |
| C       | -5.254210 | 3.392510  | 3.783277  |
| B       | -5.435998 | 3.454714  | 5.421032  |
| N       | -3.927929 | 3.691671  | 5.990079  |
| H       | -3.478167 | 2.774233  | 5.909734  |
| C       | -6.466035 | 4.617666  | 5.964678  |
| C       | -7.860142 | 4.388056  | 5.331721  |
| C       | -8.471608 | 2.986820  | 5.571603  |
| C       | -7.478118 | 1.806816  | 5.436590  |
| C       | -6.068770 | 2.051429  | 6.031626  |
| C       | -6.069381 | 2.079477  | 7.579562  |
| C       | -6.793518 | 3.292740  | 8.207461  |
| C       | -6.510258 | 4.646847  | 7.513845  |
| N       | -1.429851 | 5.131412  | 7.435808  |
| N       | -1.650612 | 5.814917  | 8.592067  |
| C       | 1.511695  | 3.136904  | 6.443780  |
| C       | 0.305800  | 3.820061  | 6.428319  |
| C       | -0.216109 | 4.560291  | 7.559195  |
| C       | 0.331533  | 4.867840  | 8.825379  |
| C       | -0.599089 | 5.668323  | 9.468062  |
| C       | -0.492131 | 6.294796  | 10.854579 |
| C       | 0.805817  | 5.794833  | 11.526380 |
| C       | -1.671895 | 5.874242  | 11.764810 |
| C       | -0.399179 | 7.838210  | 10.761595 |
| C       | -2.940977 | 6.494978  | 8.762384  |
| C       | -3.440980 | 7.158744  | 7.475059  |
| C       | -2.488715 | 8.189251  | 6.846973  |
| B       | -2.635236 | 8.318087  | 5.209837  |
| N       | -2.098762 | 6.889082  | 4.637589  |
| H       | -1.078706 | 6.955594  | 4.712245  |
| H       | -2.253306 | 6.860119  | 3.629381  |
| C       | -4.154467 | 8.647315  | 4.666379  |
| C       | -4.632245 | 9.979386  | 5.296548  |
| C       | -3.708887 | 11.195892 | 5.050914  |
| C       | -2.194373 | 10.905877 | 5.187557  |
| C       | -1.721020 | 9.554761  | 4.595624  |
| C       | -1.747249 | 9.539778  | 3.047817  |
| C       | -3.160256 | 9.574933  | 2.420966  |
| C       | -4.201743 | 8.665912  | 3.117099  |
| H       | 2.897510  | 1.919251  | 5.292165  |
| H       | -1.523262 | 6.273715  | 12.776050 |
| H       | -2.636554 | 6.239200  | 11.404298 |
| H       | -1.732972 | 4.782361  | 11.836675 |
| H       | 0.464224  | 8.132206  | 10.154956 |
|   |       |       |       |
|---|-------|-------|-------|
| 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 | 3.58529000 | -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 | -5.45137000 | 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 | 6.75877990  |
| H | -4.40573600 | 7.62259700 | 7.72243300  |
| H | -1.44825600 | 7.89355800 | 7.06198500  |
| H | -2.62533400 | 9.14357700 | 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  | 2.17120000 | 11.11730000 | 7.73660000 |
| O  | 3.58620000 | 12.38650000 | 8.48700000 |
| H  | 2.94960000 | 10.52600000 | 5.68400000 |
| O  | 3.45510000 | 10.06990000 | 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  | 2.81440000 | 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  | -0.15700000 | 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 |
| Element | Carbon | Carbon life | Hydrogen |
|---------|--------|-------------|----------|
|         | 4.38310000 | 14.89830000 | 10.02040000 |
|         | 4.62060000 | 14.81360000 | 8.49190000  |
|         | 5.83620000 | 15.64770000 | 8.01620000  |
|         | 7.21940000 | 15.11800000 | 8.46500000  |
|         | 7.38700000 | 15.82100000 | 8.37580000  |
|         | 0.34800000 | 13.19880000 | 9.63320000  |
|         | -0.85960000 | 12.58340000 | 8.90160000  |
|         | -0.79440000 | 12.75630000 | 7.27310000  |
|         | -2.02950000 | 12.01920000 | 6.47530000  |
|         | -1.78970000 | 12.05100000 | 4.94450000  |
|         | -1.50950000 | 13.45000000 | 4.34650000  |
|         | -0.56650000 | 14.33750000 | 5.19300000  |
|         | -0.81540000 | 14.30570000 | 6.72110000  |
|         | -2.14990000 | 14.97240000 | 7.13880000  |
|         | -3.43030000 | 14.21490000 | 6.71210000  |
|         | -3.36810000 | 12.67870000 | 6.89000000  |
|         | 0.69250000  | 12.57380000 | 10.99150000 |
|         | 4.09870000  | 11.16700000 | 0.39490000  |
|         | 2.69510000  | 10.54250000 | 1.28400000  |
|         | 3.41220000  | 12.09440000 | 1.73340000  |
|         | 5.60320000  | 8.37320000  | 2.30020000  |
|         | 3.98150000  | 8.36210000  | 1.57820000  |
|         | 5.33900000  | 9.10110000  | 0.70770000  |
|         | 6.41360000  | 11.18210000 | 1.48620000  |
|         | 5.84030000  | 12.07650000 | 2.90100000  |
|         | 6.63320000  | 10.51680000 | 3.11930000  |
|         | 4.07850000  | 7.91520000  | 4.01720000  |
|         | 3.30510000  | 6.46750000  | 5.90400000  |
|         | 2.71250000  | 5.21190000  | 8.00280000  |
|         | 1.88320000  | 6.51980000  | 9.98640000  |
|         | 0.82160000  | 7.95900000  | 11.73170000 |
|         | 0.78300000  | 8.62280000  | 14.12690000 |
|         | -0.70680000 | 9.17570000  | 14.91550000 |
|         | -0.79540000 | 8.28000000  | 13.39030000 |
|         | 1.65360000  | 11.01320000 | 14.23810000 |
|         | 0.68340000  | 12.36830000 | 13.64830000 |
|         | 0.14050000  | 11.45000000 | 15.05670000 |
|         | -1.67590000 | 11.81440000 | 12.46300000 |
|         | -2.17650000 | 10.12550000 | 12.38830000 |
|         | -2.11080000 | 10.96550000 | 13.95310000 |
|         | 1.60520000  | 13.03040000 | 11.40340000 |
|         | -0.11520000 | 12.76170000 | 11.69890000 |
|         | 0.17840000  | 14.26770000 | 9.82560000  |
|         | 1.24560000  | 13.16970000 | 9.01000000  |
|         | -0.89770000 | 11.50430000 | 9.11400000  |
|         | -1.78230000 | 12.99960000 | 9.33310000  |
|         | -0.00800000 | 14.90520000 | 7.17560000  |
|         | -2.15130000 | 15.06150000 | 8.23500000  |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| 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 | 12.44700000 | 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 | 11.00660000|
| 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 |

$({^2\text{BBNPDPtBu}})\text{Fe(PhPh)}_2^-$

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| 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    | -4.16200000 | 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 |
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| 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 | 4.95900000 |
| 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| 6.92350000 |
| C   | 1.99520000  | 8.85380000 | 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 |
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