Vibrational Properties of Heme-Nitrosoalkane Complexes in Comparison with those of their HNO Analogs, and Reactivity Studies towards Nitric Oxide and Lewis Acids

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Supporting Information

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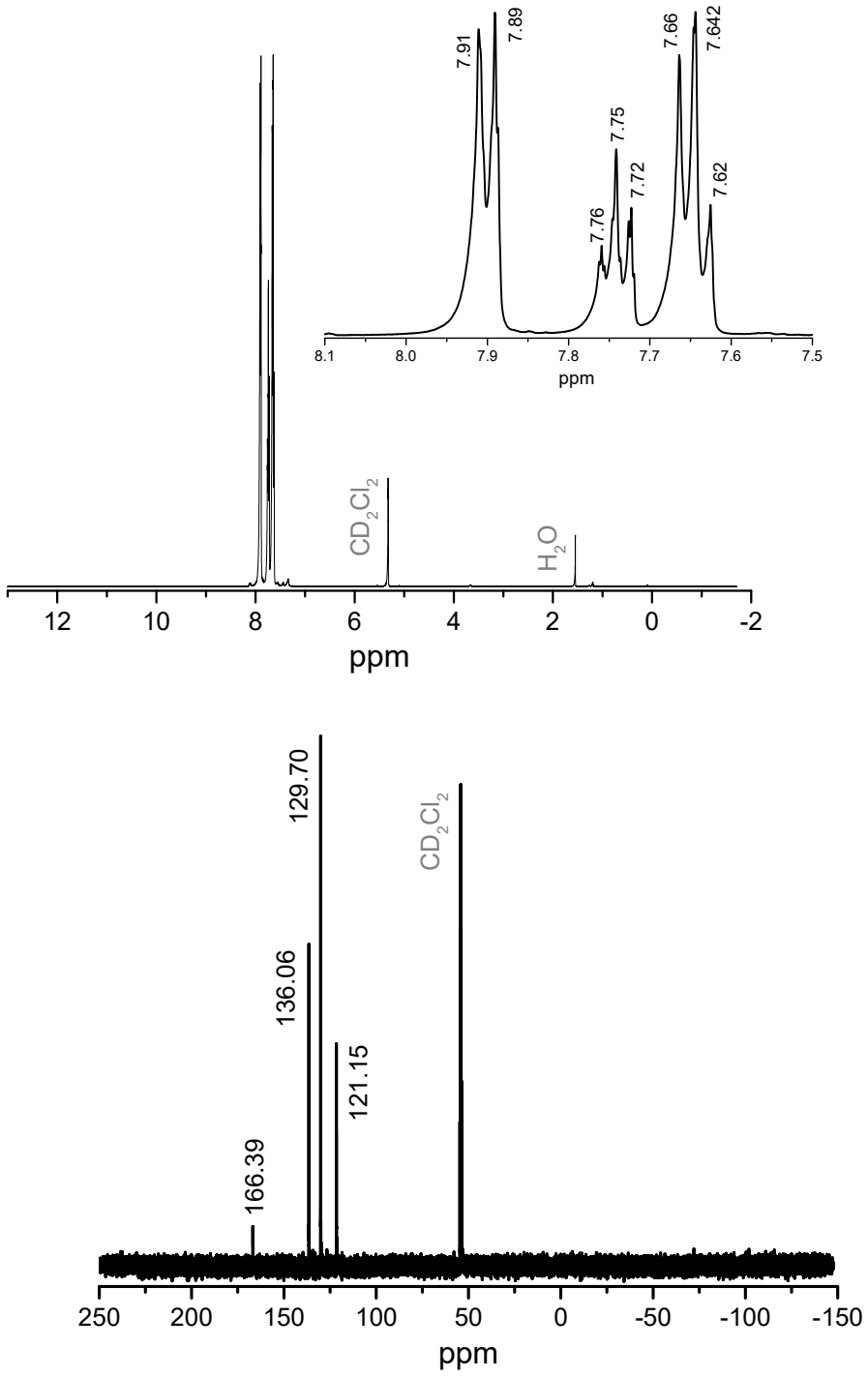

Figure S1. Top: ^{1}H-NMR spectrum of nitrosobenzene in CD_2Cl_2. Bottom: ^{13}C-NMR spectrum of nitrosobenzene recorded in CD_2Cl_2 with the line width set to 1 Hz. All spectra were recorded at room temperature.

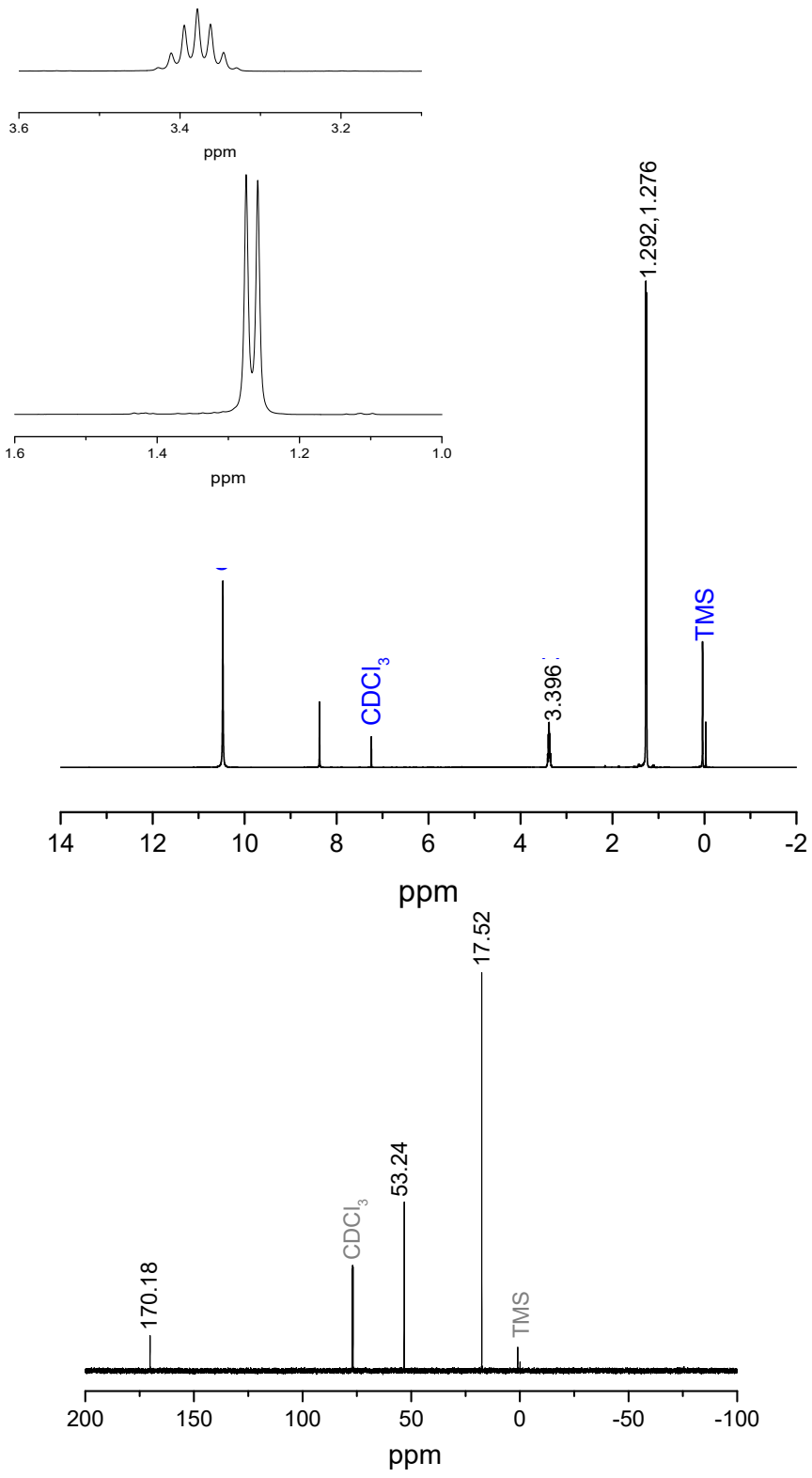

Figure S2. Top: ^{1}H-NMR spectrum of N-isopropylhydroxylamine (iPrNHOH) in $CDCl_3$. Bottom: ^{13}C-NMR spectrum of iPrNHOH in $CDCl_3$, with the line width set to 1 Hz. All spectra were recorded at room temperature.

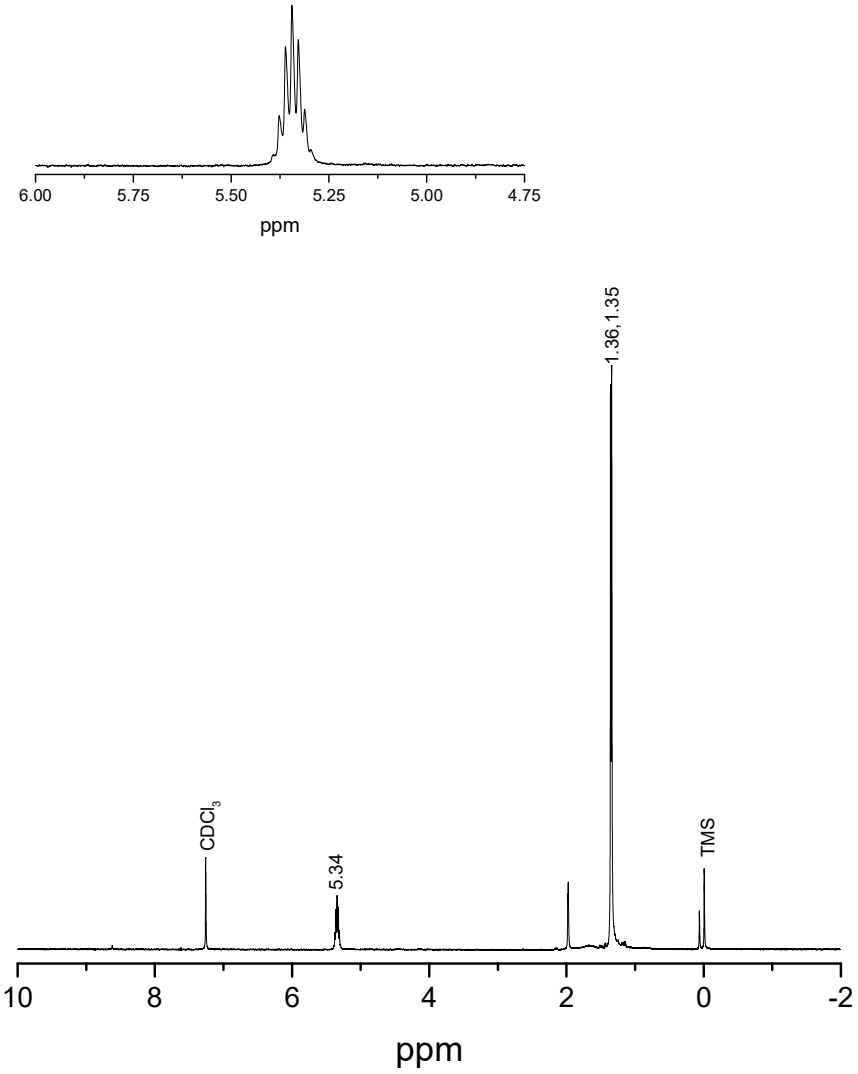

Figure S3. ^{1}H-NMR spectrum of 2-nitrosopropane (iPrNO) in $CDCl_3$ recorded at room temperature.

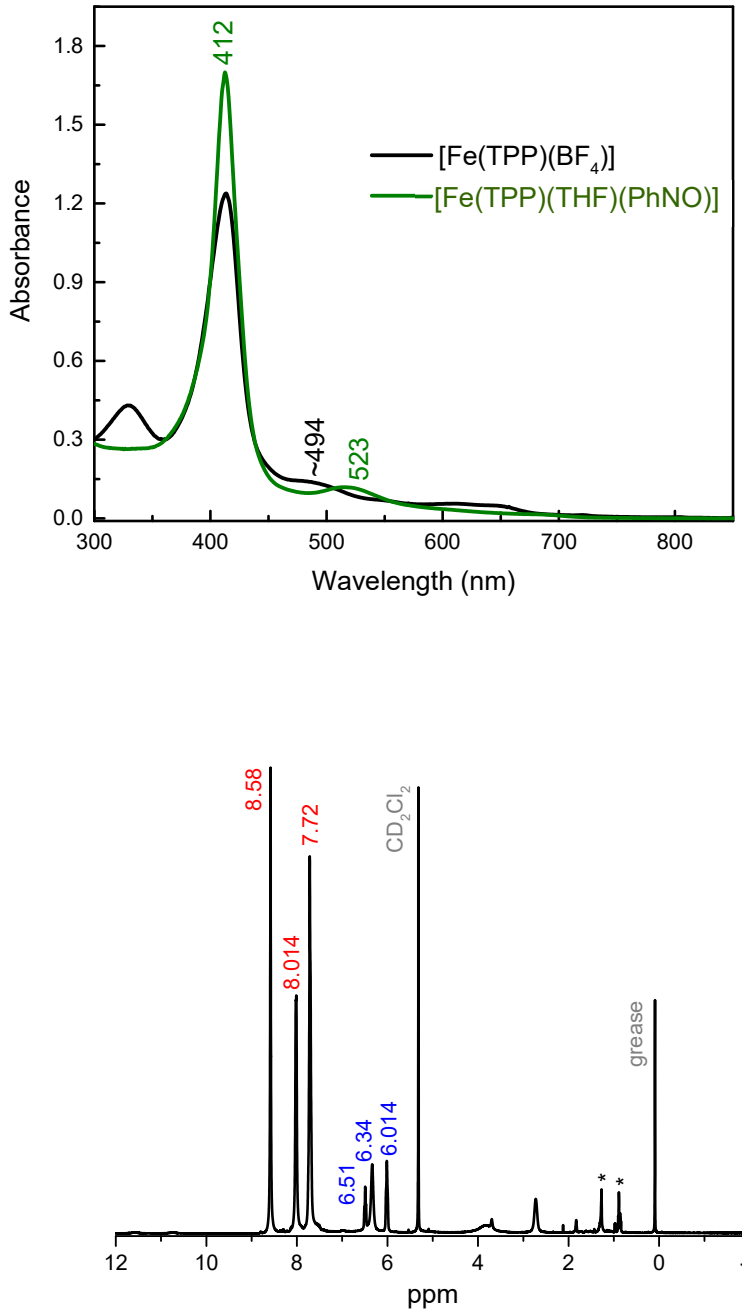

Figure S4. Top: UV-vis spectra of the precursor, [Fe(TPP)(BF_4)] (black), and of the isolated reaction product, [Fe(TPP)(THF)(PhNO)] (green), in dichloromethane at room temperature. Bottom: ^{1}H-NMR spectrum of [Fe(TPP)(THF)(PhNO)] in CD_2Cl_2 with the line width is set to 0.3 Hz. The * denotes residual hexanes from the recrystallization. All spectra were recorded at room temperature.

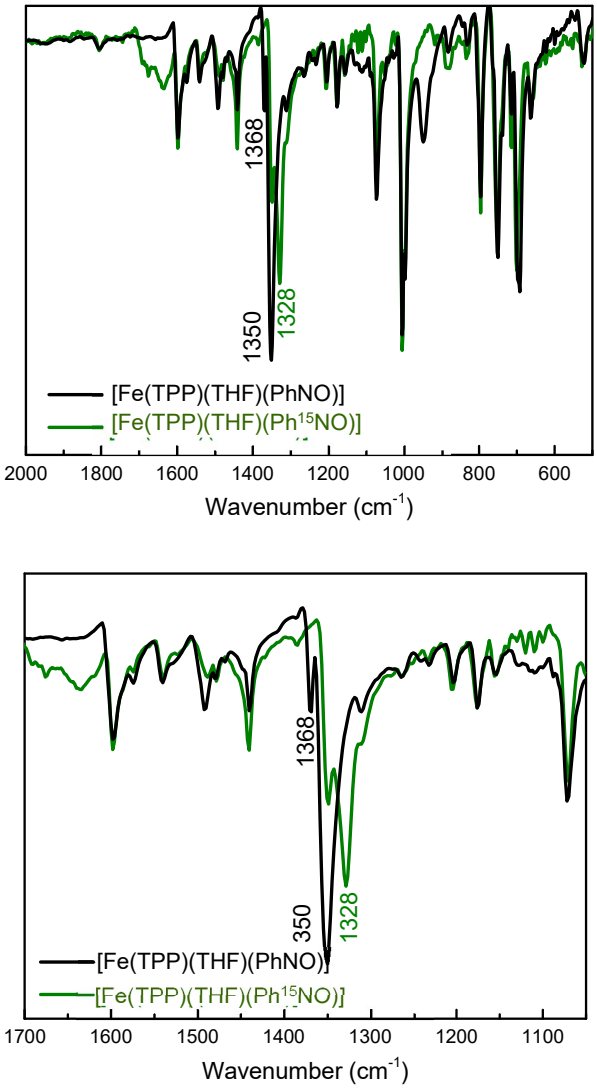

Figure S5. Top: Overlay of the IR spectra of [Fe(TPP)(THF)(PhNO)] (black), and of the ^{15}N-labeled complex, [Fe(TPP)(THF)(Ph^{15}NO)] (green), measured in KBr pellets. Bottom: Expanded view of the N-O stretching frequency region. The natural abundance isotopes complex [Fe(TPP)(THF)(PhNO)] shows two isotope sensitive features at 1368 and 1350 cm^{-1}, indicative of the presence of the bis-PhNO complex (see text). The spectra were recorded at room temperature.

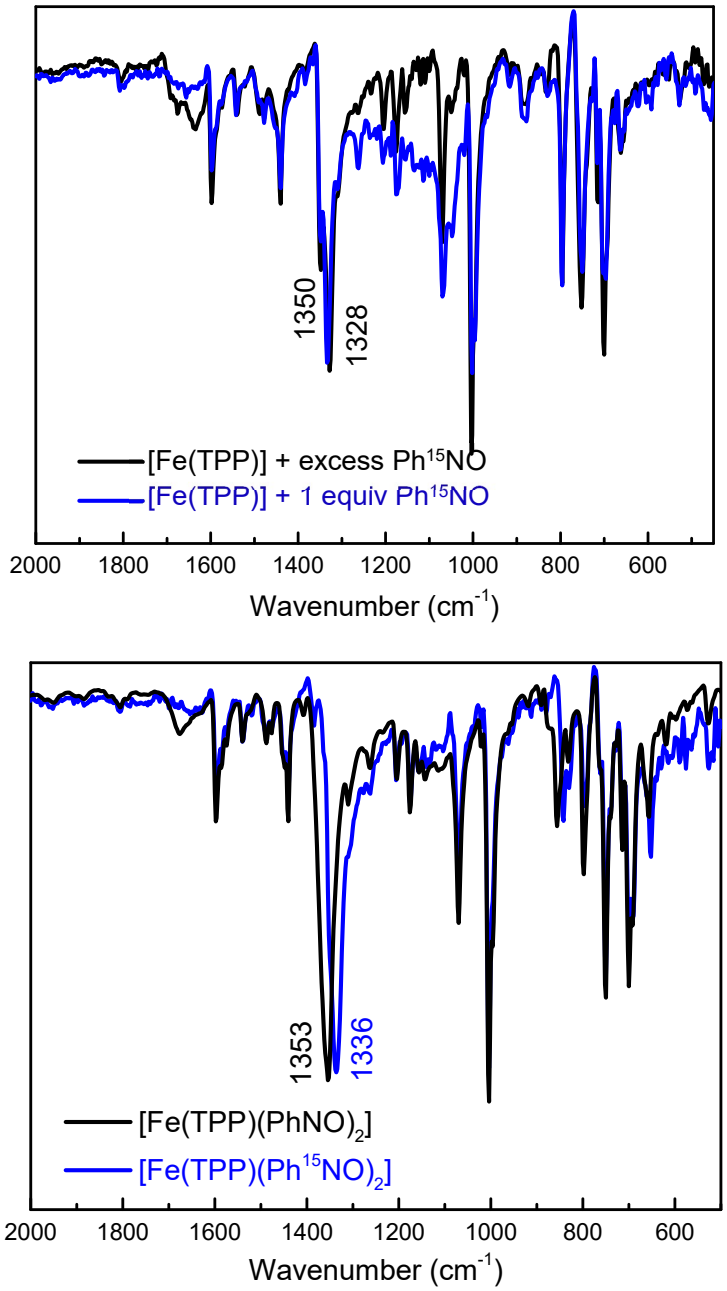

Figure S6. Top: Comparison of the IR spectra of the isolated product, [Fe(TPP)(THF)(Ph^{15}NO)], prepared by reacting [Fe(TPP)] with different equivalents of Ph^{15}NO. The N-O stretching frequency region is identical when excess Ph^{15}NO (black) versus ~1 equiv. Ph^{15}NO (blue) is used. Bottom: Overlay of the IR spectra of [Fe(TPP)(PhNO)$_2$] (black) and the ^{15}N-labeled complex, [Fe(TPP)(Ph^{15}NO)$_2$] (blue), measured in KBr pellets. The spectra were recorded at room temperature.

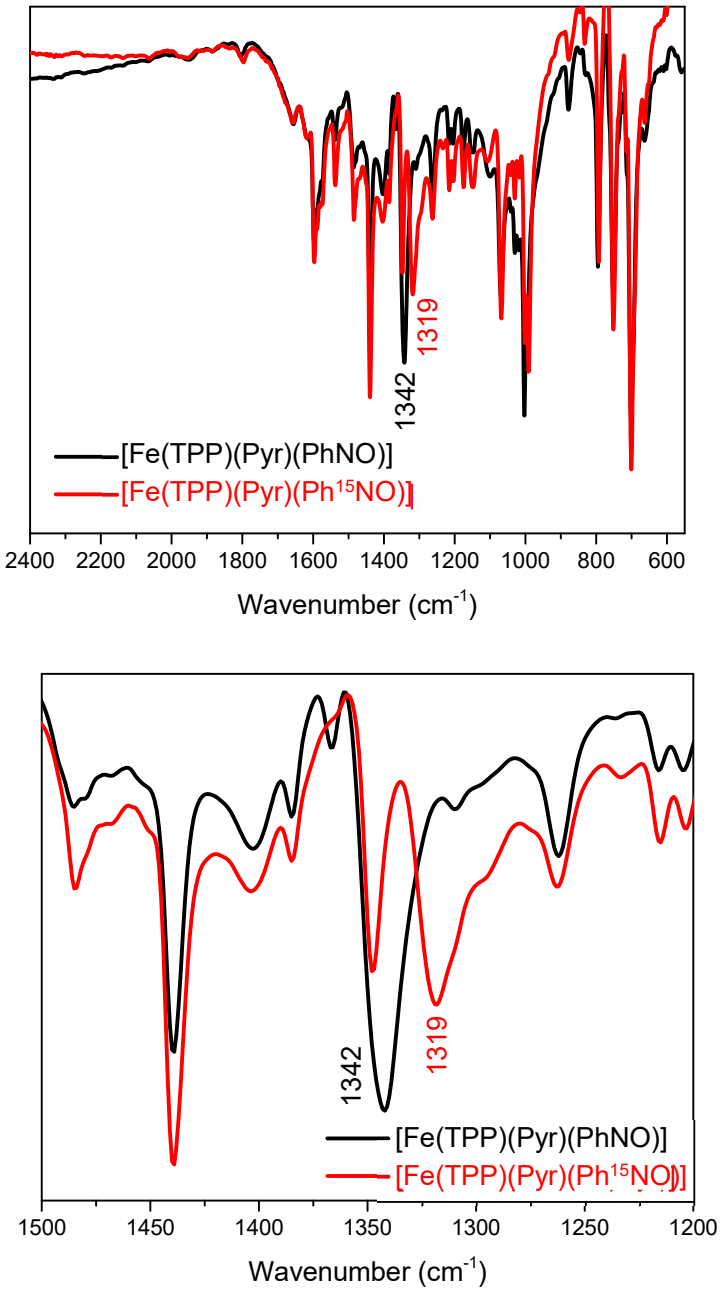

Figure S7. Top: Overlay of the IR spectra of [Fe(TPP)(Pyr)(PhNO)] (black), and of the ^{15}N-labeled complex, [Fe(TPP)(Pyr)(Ph^{15}NO)] (red, Pyr = pyridine), measured in KBr pellets. Bottom: Expanded view of the N-O stretching frequency region. The natural abundance isotopes complex [Fe(TPP)(Pyr)(PhNO)] shows an isotope sensitive feature at 1342 cm^{-1}. The spectra were recorded at room temperature.

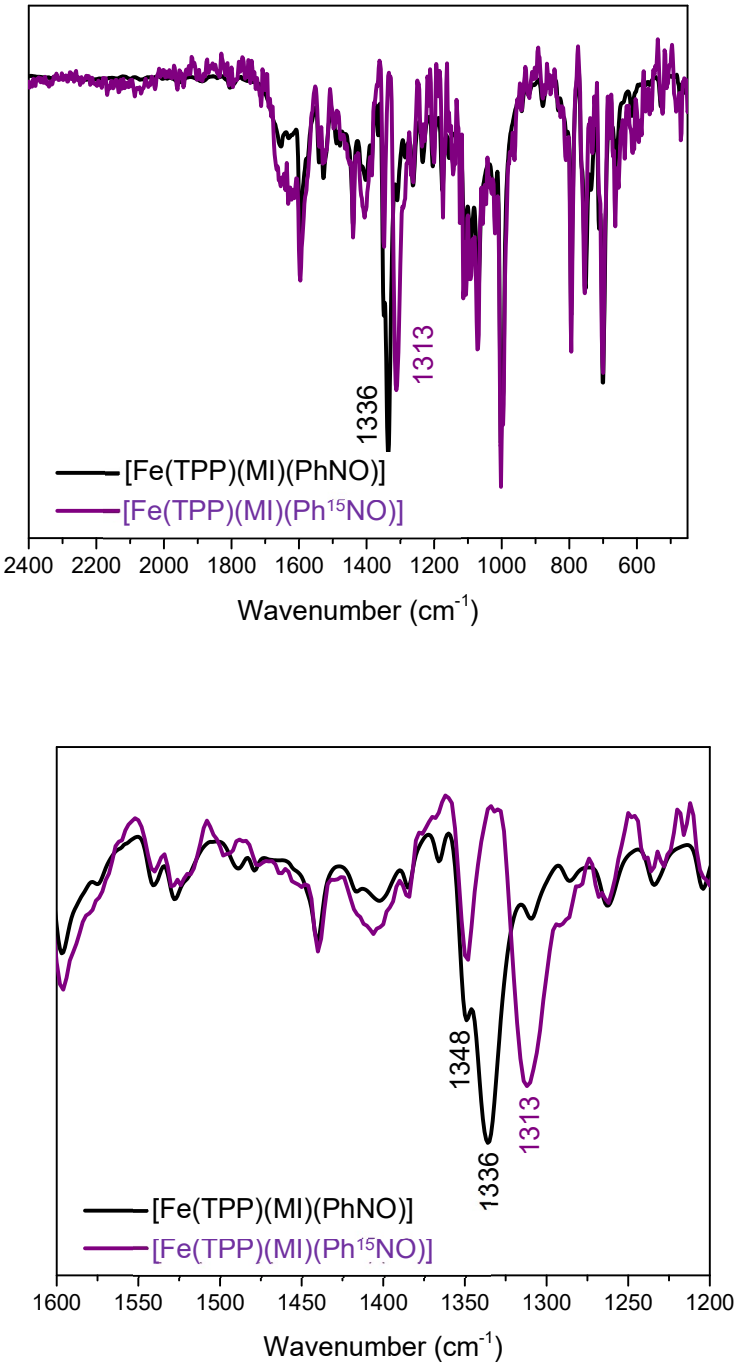

Figure S8. Top: Overlay of the IR spectra of [Fe(TPP)(MI)(PhNO)] (black), and of the ^{15}N-labeled complex, [Fe(TPP)(MI)(Ph^{15}NO)] (purple), measured in KBr pellets. Bottom: Expanded view of the N-O stretching frequency region. The natural abundance isotopes complex [Fe(TPP)(MI)(PhNO)] shows an isotope sensitive feature at 1336 cm^{-1}. MI denotes 1-methylimidazole. The spectra were recorded at room temperature.

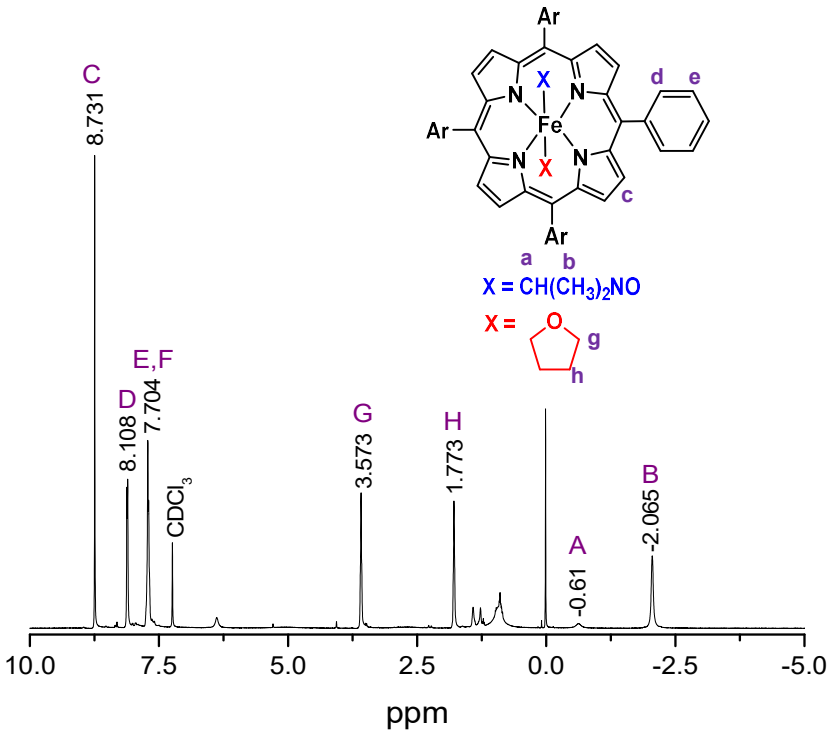

Figure S9. ^{1}H-NMR spectrum of [Fe(TPP)(THF)(iPrNO)] in $CDCl_3$, with the line width set to 0.3 Hz, measured at room temperature.

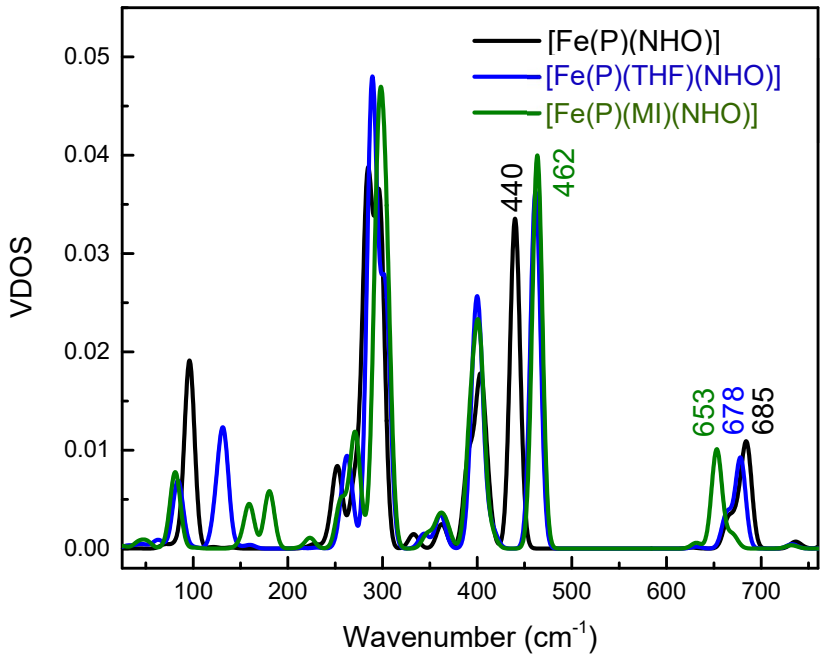

Figure S10. BP86/TZVP calculated NRVS VDOS for [Fe(P)(NHO)] (black), [Fe(P)(THF)(NHO)] (blue), and [Fe(P)(MI)(NHO)] (green).

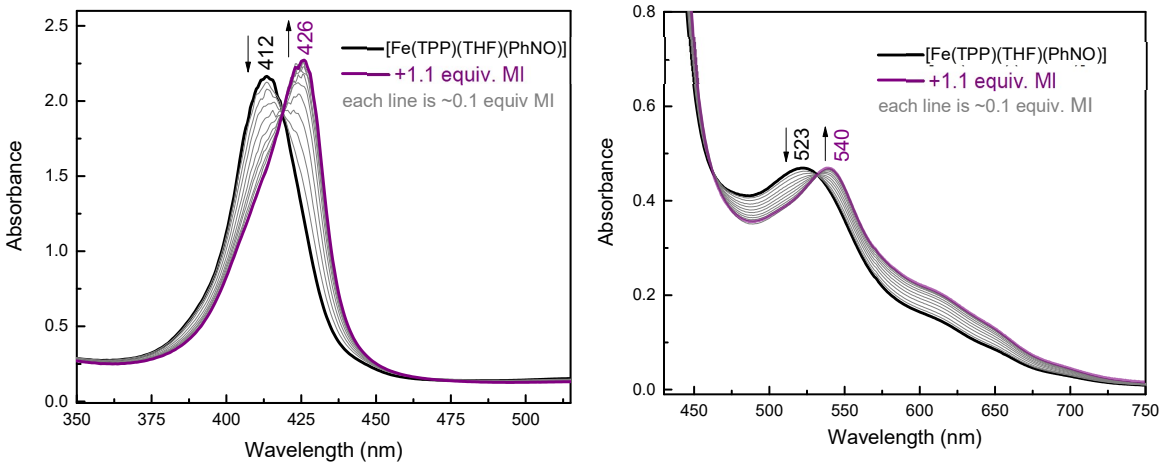

Figure S11. Left: UV-vis spectra following the titration of ~13 μM [Fe(TPP)(THF)(PhNO)] (black) with a solution of MI in dichloromethane, forming the six-coordinate complex [Fe(TPP)(MI)(PhNO)] (purple). Right: UV-vis spectra of the titration of ~51 μM [Fe(TPP)(THF)(PhNO)] (black) with a solution of MI in dichloromethane, forming the six-coordinate complex [Fe(TPP)(MI)(PhNO)] (purple). In both cases, the reaction is complete after the addition of ~1.0 equivalent MI to the solution. The spectra were recorded at room temperature.

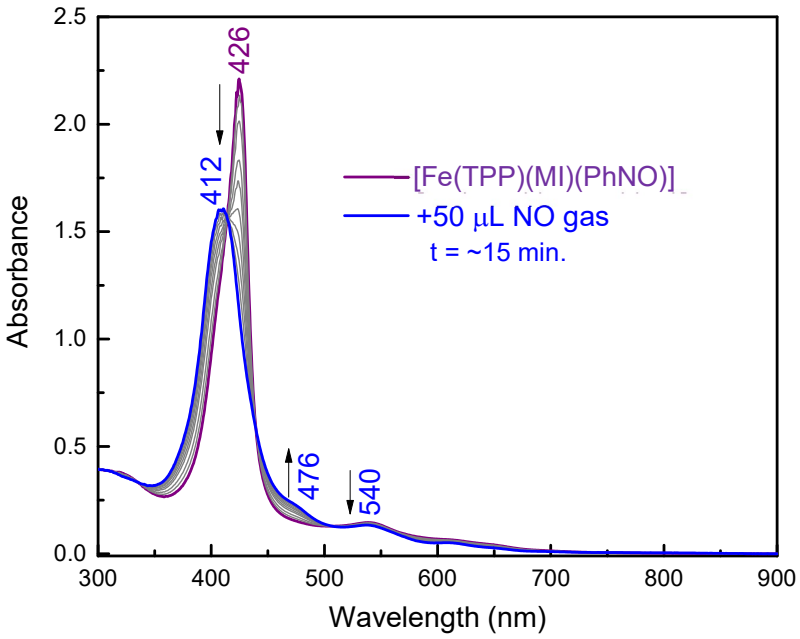

Figure S12. *In situ* UV-vis monitoring of the reaction of [Fe(TPP)(MI)(PhNO)] (purple) with 50 µL of NO gas (~6 equiv.) in dichloromethane. The product is the ferrous NO complex, [Fe(TPP)(NO)] (blue). The spectra were recorded at room temperature.

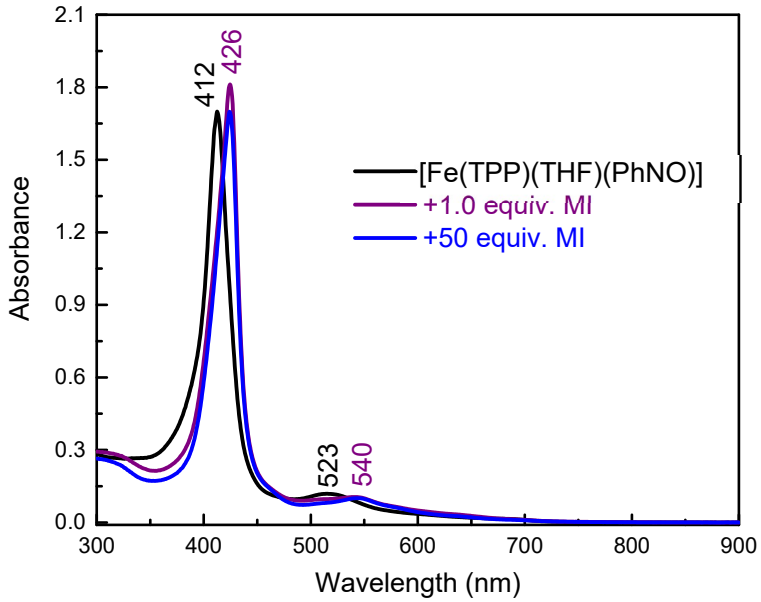

Figure S13. UV-vis spectra of a solution of [Fe(TPP)(THF)(PhNO)] (black), with ~1 equiv. MI added to the solution (purple), and 50 equiv. MI added to the same solution (blue). The spectra were recorded at room temperature.

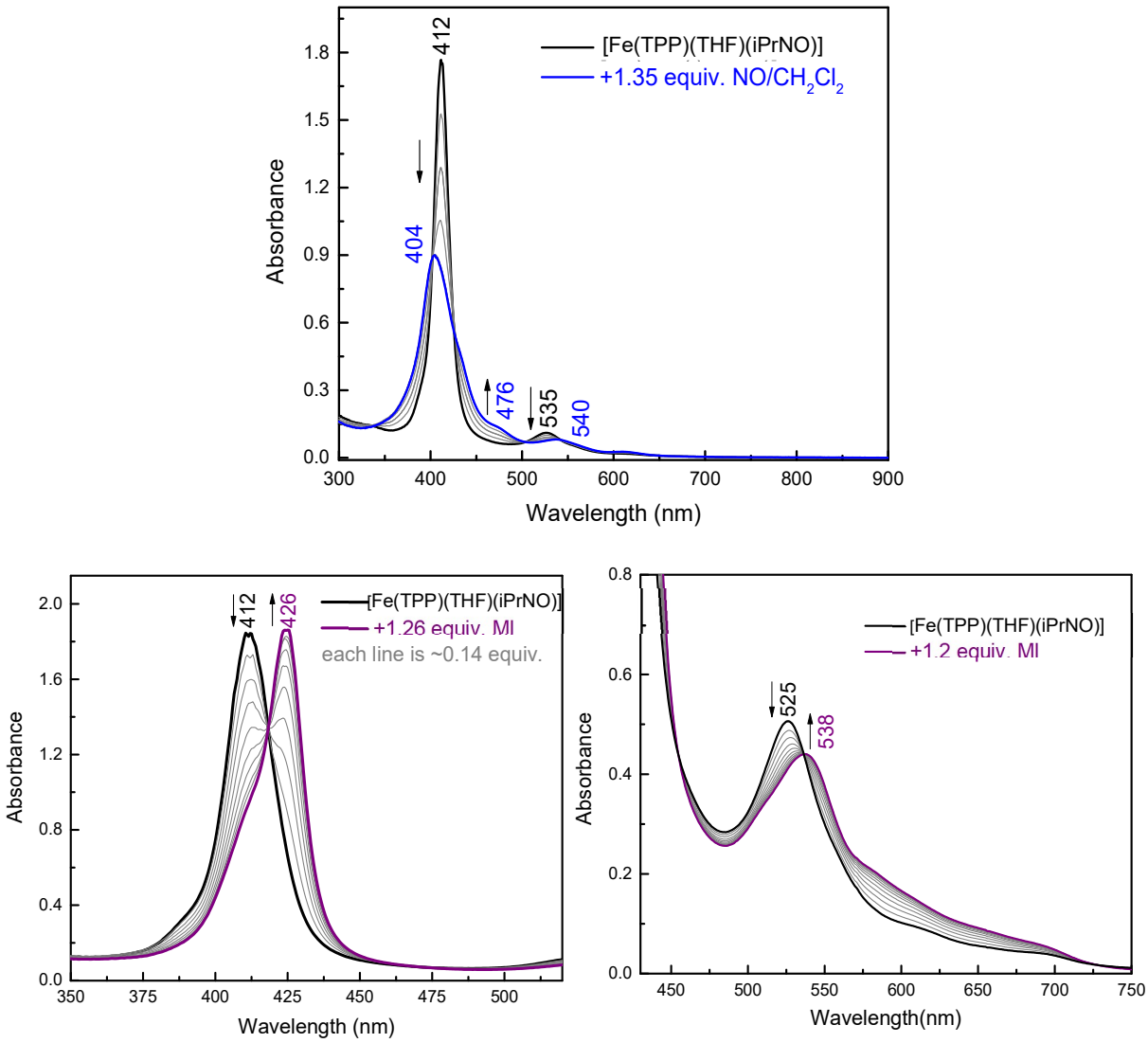

Figure S14. Top: *In situ* UV-vis monitoring of the titration of ~16 μM [Fe(TPP)(THF)(iPrNO)] (black) in CH_2Cl_2 with a NO saturated solution in dichloromethane, forming the ferrous NO complex [Fe(TPP)(NO)] (blue). Bottom left: UV-vis spectra following the titration of ~16 μM [Fe(TPP)(THF)(iPrNO)] (black) with a solution of MI in dichloromethane, forming the six-coordinate complex [Fe(TPP)(MI)(iPrNO)] (purple). Bottom right: UV-vis spectra of the titration of ~74 μM [Fe(TPP)(THF)(iPrNO)] (black) with a solution of MI in dichloromethane, forming the six-coordinate complex [Fe(TPP)(MI)(iPrNO)] (purple). The reaction is complete after the addition of ~1.0 equivalent MI to the solution.

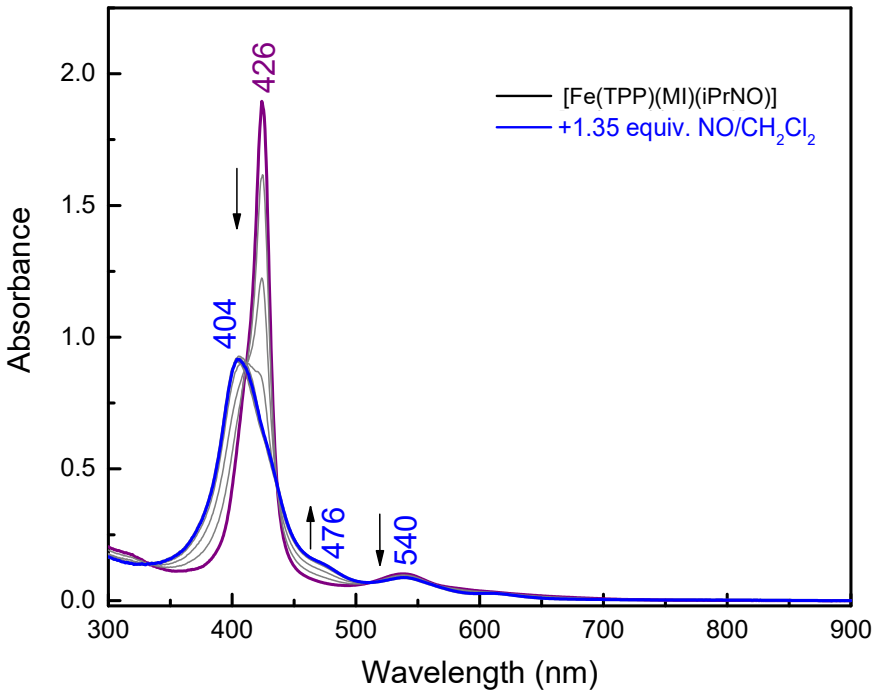

Figure S15. *In situ* UV-vis monitoring of the titration of ~16 μM [Fe(TPP)(MI)(iPrNO)] (purple) in CH_2Cl_2 with a NO saturated solution in dichloromethane, forming the ferrous NO complex [Fe(TPP)(NO)] (blue).

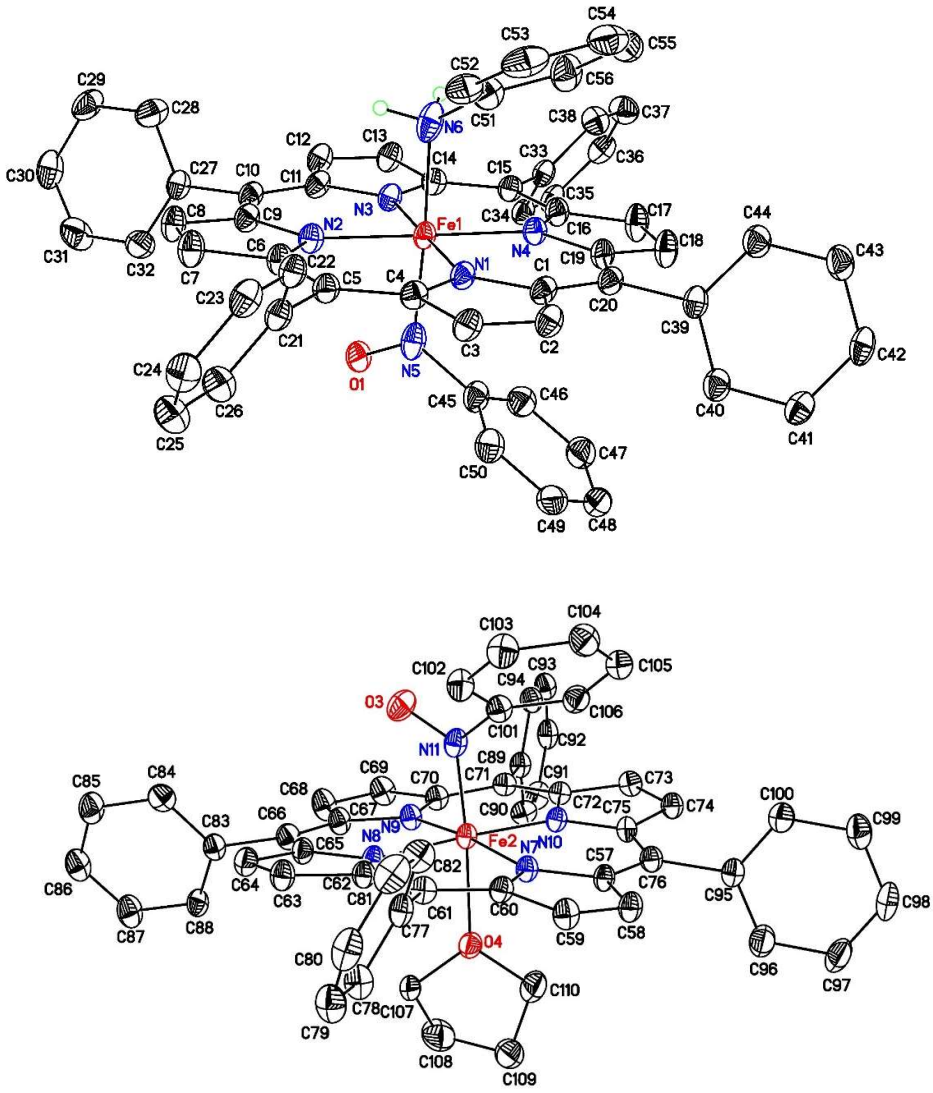

Figure S16. Structural diagrams including the atomic numbering schemes for the crystal structures of [Fe(TPP)($PhNH_2$)(PhNO)] (top) and [Fe(TPP)(THF)(PhNO)] (bottom). Hydrogen atoms (except for the amino group of $PhNH_2$) and solvent molecules are omitted for clarity.

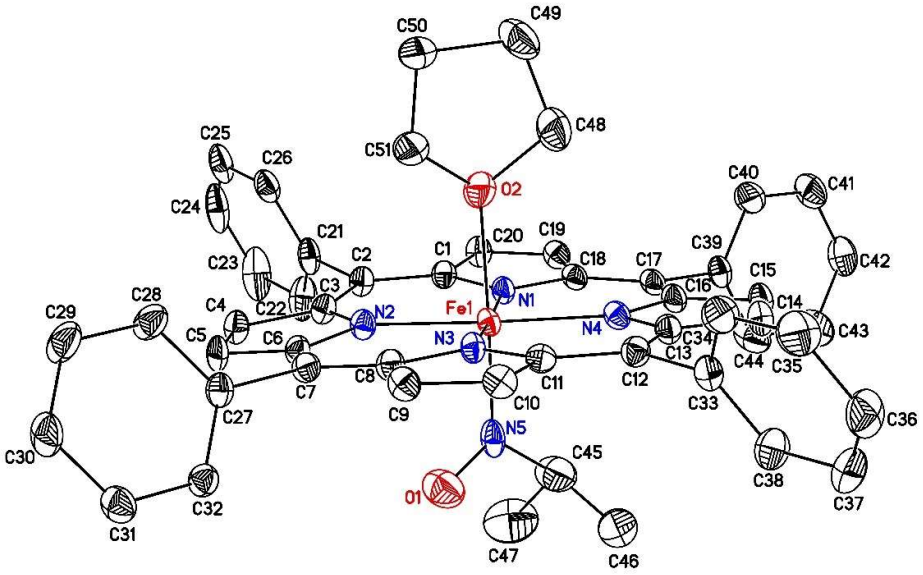

Figure S17. Structural diagram including the atomic numbering scheme for the crystal structure of [Fe(TPP)(THF)(iPrNO)]. Hydrogen atoms are omitted for clarity.

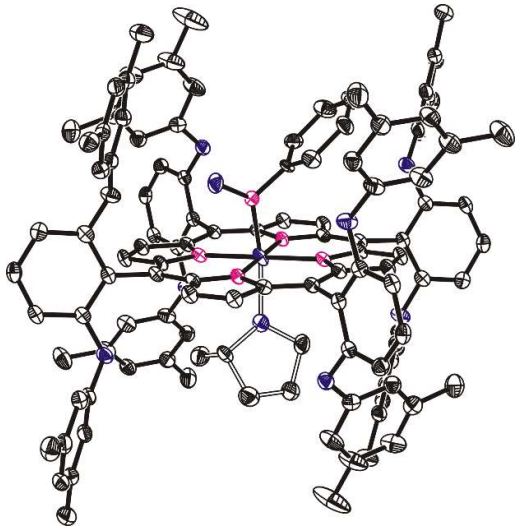

Figure S18. Structural diagram including the atomic numbering scheme for the crystal structure of [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)]. Hydrogen atoms are omitted for clarity.

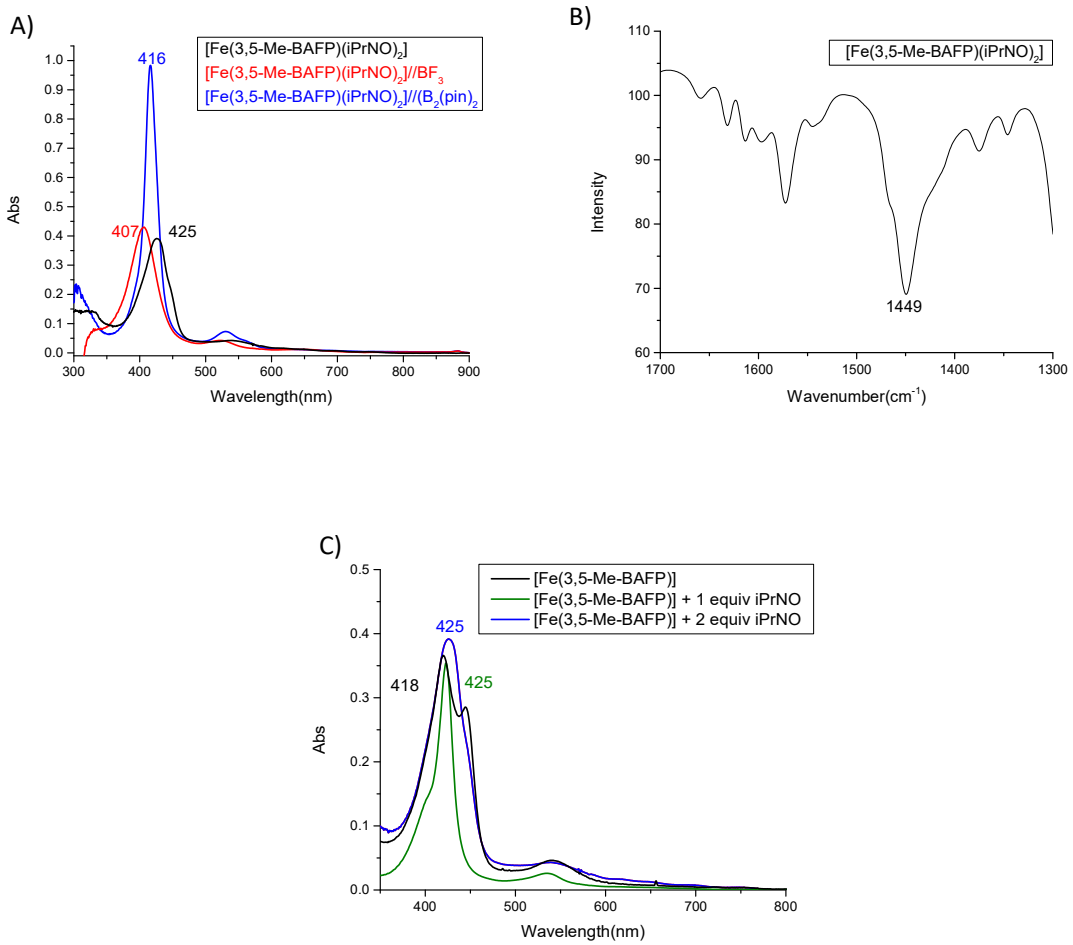

Figure S19. A) UV-Vis spectra of [Fe(3,5-Me-BAFP)(iPrNO)$_2$] (black), [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with BF_3•OEt_2 (red), and [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with $B_2(pin)_2$ (blue), all taken in THF. B) ATR IR spectrum of [Fe(3,5-Me-BAFP)(iPrNO)$_2$] with the N-O stretching frequency observed at 1449 cm^{-1}. C) UV-Vis spectra of [Fe(3,5-Me-BAFP)] (black) reacted with 1 equiv iPrNO (green) and 2 equiv iPrNO (blue) in THF.

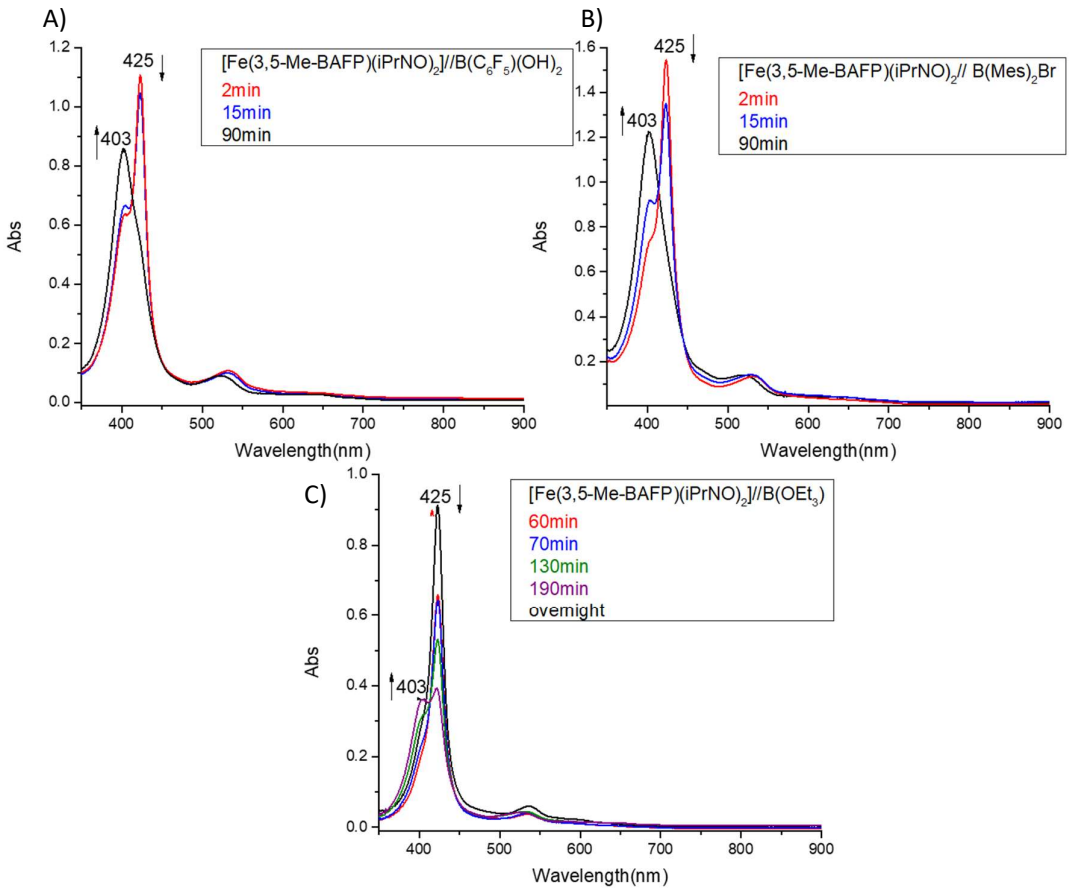

Figure S20. UV-Vis spectra of [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with different Lewis acids monitored over time. A) [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B(C$_6$F$_5$)(OH)$_2$, B) [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B(Mes)$_2$Br, and C) [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B(OEt)$_3$. All spectra were recorded in THF.

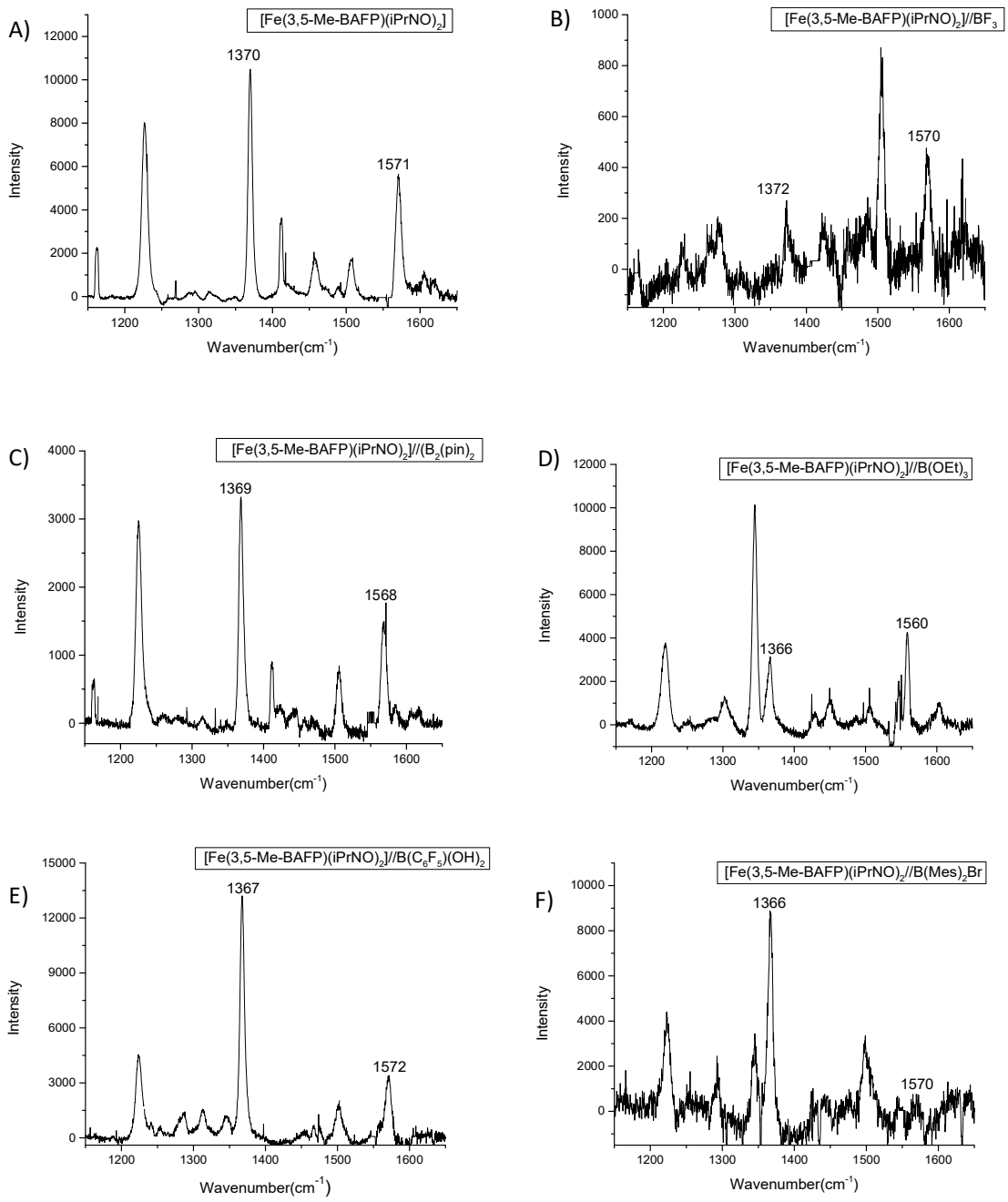

Figure S21. rRaman spectra in THF of A) 1 mM [Fe(3,5-Me-BAFP)(iPrNO)$_2$] B) 1 mM [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with BF3•OEt$_2$ C) 1 mM [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B$_2$(pin)$_2$, D) 1 mM [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B(OEt)$_3$ E) 1 mM [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B(C$_6$F$_5$)(OH)$_2$ F) 1 mM [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B(Mes)$_2$Br.

Crystal structure determination of [Fe(TPP)(THF)(iPrNO)] (University of Michigan): A brown plate of [Fe(TPP)(THF)(iPrNO)] of dimensions 0.24 x 0.14 x 0.12 mm was mounted on a Rigaku AFC10K Saturn 944+ CCD-based X-ray diffractometer equipped with a low temperature device and a Micromax-007HF Cu-target micro-focus rotating anode (λ = 1.54187 Å) operated at 1.2 kW power (40 kV, 30 mA). The X-ray intensities were measured at 85 K with the detector placed at a distance of 42.00 mm from the crystal. A total of 3857 images were collected with an oscillation width of 1.0° in ω. The exposure times were 5 s for the low angle images, 30 s for high angle. Rigaku d*trek images were exported to CrysAlisPro for processing and corrected for absorption. The integration of the data yielded a total of 103,181 reflections to a maximum 2θ value of 136.38° of which 7302 were independent and 7094 were greater than $2\sigma(I)$. The final cell constants were based on the xyz centroids of 56,915 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection; the data were processed with CrystalClear 2.0 and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 2008/4) software package,[1] using the space group P2(1)/c with Z = 4 for the formula $C_{51}H_{43}N_5O_2Fe$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized positions. Full matrix least-squares refinement based on F^2 converged at R1 = 0.0612 and wR2 = 0.1627 [based on $I > 2\sigma(I)$], R1 = 0.0621 and wR2 = 0.1635 for all data. Additional details are presented in **Tables S7-S12** and are given as Supporting Information in a CIF file, which was deposited in the CCDC (#2341278).

Crystal structure determination for [Fe(TPP)(THF)(PhNO)]/[Fe(TPP)($PhNH_2$)(PhNO)] (University of Michigan): A brown plate of [Fe(TPP)(THF)(PhNO)]/[Fe(TPP)($PhNH_2$)(PhNO)] of dimensions 0.22 x 0.14 x 0.12 mm was mounted on a Rigaku AFC10K Saturn 944+ CCD-based X-ray diffractometer equipped with a low temperature device and a Micromax-007HF Cu-target micro-focus rotating anode (λ = 1.54184 Å) operated at 1.2 kW power (40 kV, 30 mA). The X-ray intensities were measured at 85 K with the detector placed at a distance of 42.00 mm from the crystal. A total of 4223 images were collected with an oscillation width of 1.0° in ω. The exposure times were 2 s for the low angle images, 12 s for high angle. Rigaku d*trek images were exported to CrysAlisPro for processing and corrected for absorption. The integration of the data yielded a total of 137,394 reflections to a maximum 2θ value of 147.91° of which 17,016 were independent and 16,662 were greater than 2σ(I). The final cell constants were based on the xyz centroids of 67,011 reflections above 10σ(I). Analysis of the data showed negligible decay during data collection; the data were processed with CrystalClear 2.0 and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 2014/6) software package,[1] using the space group P1bar with Z = 2 for the formula $C_{114}H_{89}N_{11}O_4Fe_2$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized positions. Full matrix least-squares refinement based on F^2 converged at R1 = 0.0436 and wR2 = 0.1159 [based on I > 2σ(I)], R1 = 0.0444 and wR2 = 0.1169 for all data. Additional details are presented in **Tables S1-S6** and are given as Supporting Information in a CIF file, which was deposited in the CCDC (#2340714).

Crystal Structure Determination of [Fe(3,5-Me-BAFP)(iPrNO)$_2$] and [Fe(3,5-Me-BAFP)(iPrNH$_2$)(iPrNO)] (Purdue University): Single crystals of [Fe(3,5-Me-BAFP)(iPrNH$_2$)(iPrNO)] were coated with perfluoropolyether and quickly transferred to the goniometer head of a Bruker Quest diffractometer with kappa geometry, an I-μ-S microsource X-ray tube, laterally graded multilayer (Goebel) mirror single crystal for monochromatization, a Photon-III C14 area detector and an Oxford Cryosystems low temperature device. Examination and data collection were performed with Cu Kα radiation (λ = 1.54178 Å) at low temperatures.

Single crystals of [Fe(3,5-Me-BAFP)(iPrNO)$_2$] were coated with perfluoropolyether and quickly transferred to the goniometer head of a Bruker Quest diffractometer with a fixed chi angle, a sealed tube fine focus X-ray tube, single crystal curved graphite incident beam monochromator, a Photon II area detector and an Oxford Cryosystems low temperature device. Examination and data collection were performed with Mo Kα radiation (λ = 0.71073 Å) at low temperatures.

Data were collected, reflections were indexed and processed, and the files scaled and corrected for absorption using APEX3[2] and SADABS[3]. The space groups were assigned using XPREP within the SHELXTL suite of programs[4, 5] and solved by direct methods using ShelXS[5] or dual methods using ShelXT[6] and refined by full matrix least squares against F^2 with all reflections using Shelxl2018[7, 8] using the graphical interface Shelxle[9]. If not specified otherwise H atoms attached to carbon, boron and nitrogen atoms as well as hydroxyl hydrogens were positioned geometrically and constrained to ride on their parent atoms. C-H bond distances were constrained to 0.95 Å for aromatic and alkene C-H and CH_2 and alkyne C-H moieties, and to 1.00, 0.99 and 0.98 Å for aliphatic C-H, CH_2 and CH_3 moieties, respectively. N-H bond distances were constrained to 0.88 Å for planar (sp^2 hybridized) N-H, N-H^+ and NH_2 groups. N-H bond distances were constrained to 0.91 Å for pyramidal (sp^3 hybridized) ammonium NH_2^+ and NH_3^+ groups. O-H distances of alcohols were constrained to 0.84 Å. Methyl CH_3, ammonium NH_3^+ and hydroxyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density. H atoms of pyramidalized R_2NH and RNH_2 units were refined

and N-H distances were restrained to 0.88(2) Å. Where necessary, water H···H distances were restrained to 1.36(2) Å, and H atom positions were further restrained based on hydrogen bonding considerations. U_{iso}(H) values were set to a multiple of U_{eq}(C) with 1.5 for CH_3, NH_3^+ and OH, and 1.2 for C-H, CH_2, B-H, N-H and NH_2 units, respectively. Additional data collection and refinement details, including description of disorder (where present) can be found above. This material is based upon work supported by the National Science Foundation through the Major Research Instrumentation Program under Grant CHE-1625543 (funding for the single crystal X-ray diffractometer). Additional details are presented in **Tables S13-S21** (two crystals) and **Tables S22-S26**, respectively, and are given as Supporting Information in CIF files, which were deposited in the CCDC (#2339812 and #2339811).

Crystal structure determination for [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)] (University of Michigan): Brown block-like crystals of [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)] were grown from 2-methyl-tetrahydronfuran/hexanes solution of the compound at 22 deg. C. A crystal of dimensions 0.12 x 0.12 x 0.10 mm was mounted on a Rigaku AFC10K Saturn 944+ CCD-based X-ray diffractometer equipped with a low temperature device and Micromax-007HF Cu-target micro-focus rotating anode (λ = 1.54187 Å) operated at 1.2 kW power (40 kV, 30 mA). The X-ray intensities were measured at 85(1) K with the detector placed at a distance 42.00 mm from the crystal. A total of 4005 images were collected with an oscillation width of 1.0° in ω. The exposure time was 2 sec. for the low angle images, 10 sec. for high angle. The integration of the data yielded a total of 127,465 reflections to a maximum 2θ value of 136.46° of which 8510 were independent and 8187 were greater than 2σ (I). The final cell constants were based on the xyz centroids 78,234 reflections above 10σ (I). Analysis of the data showed negligible decay during data collection; the data were processed with CrystalClear 2.0 and corrected for absorption. The structure was solved with the Bruker SHELXT (SHELXT 2018) and refined with the Bruker SHELXL (version 2019/2) software package,[1] using the space group P2(1)/c with Z = 2 for the formula C119H107N5O10Fe. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized positions. The complex lies on an inversion center of the crystal lattice. The axial positions of the core iron atom have coordinated 2-MeTHF and nitrosobenzene molecules in a 1:1 ratio disordered over the inversion center, resulting in a fixed occupation of 0.5 for both ligands per molecule in the asymmetric unit. Full matrix least-squares refinement based on F2 converged at R1 = 0.0428 and wR2 = 0.1112 [based on I > 2σ (I)], R1 = 0.0440 and wR2 = 0.1122 for all data. Additional details are presented in **Table S27-S31** and are given as Supporting Information in a CIF file, which was deposited in the CCDC (#2357458). Acknowledgement is made for funding from NSF grant CHE-0840456 for X-ray instrumentation.

Table S1. Crystal data and structure refinement for [Fe(TPP)(THF)(PhNO)] and [Fe(TPP)($PhNH_2$)(PhNO)].

Empirical formula	$C_{114}H_{89}Fe_2N_{11}O_4$
Formula weight	1788.66
Temperature	85(2) K
Wavelength	1.54184 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.75223(16)Å alpha = 93.5688(10) deg. b = 17.0546(2) Å beta = 100.6223(10) deg. c = 23.4214(2) Å gamma = 109.2852(13) deg.
Volume	4316.45(10) $Å^3$
Z, Calculated density	2, 1.376 Mg/m^3
Absorption coefficient	3.217 mm^{-1}
F(000)	1868
Crystal size	0.220 x 0.140 x 0.120 mm
Theta range for data collection	2.769 to 73.953 deg.
Limiting indices	-14<=h<=14, -21<=k<=20, -29<=l<=29
Reflections collected / unique	137394 / 17016 [R(int) = 0.0679]
Completeness to theta =	67.684 98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.80581
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17016 / 246 / 1342
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0436, wR2 = 0.1159
R indices (all data)	R1 = 0.0444, wR2 = 0.1169
Extinction coefficient	n/a
Largest diff. peak and hole	0.895 and -0.521 $e.Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^2) for [Fe(TPP)(THF)(PhNO)] and [Fe(TPP)($PhNH_2$)(PhNO)]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	9352(1)	7387(1)	8582(1)	18(1)
Fe(2)	499(1)	2691(1)	6313(1)	17(1)
O(1)	10283(3)	8921(2)	9278(1)	27(1)
O(2)	7169(3)	6053(2)	8436(1)	31(1)
N(1)	9547(1)	7589(1)	7767(1)	19(1)
N(2)	7965(1)	7836(1)	8485(1)	20(1)
N(3)	9146(1)	7171(1)	9394(1)	20(1)
N(4)	10725(1)	6926(1)	8676(1)	20(1)
N(5)	10517(2)	8514(1)	8914(1)	28(1)
N(6)	8108(2)	6249(1)	8284(1)	31(1)
N(7)	735(1)	2252(1)	5551(1)	18(1)
N(8)	2318(1)	3311(1)	6567(1)	19(1)
N(9)	288(1)	3013(1)	7111(1)	19(1)
N(10)	-1304(1)	2020(1)	6072(1)	17(1)
N(11)	393(1)	3654(1)	6064(1)	21(1)
C(1)	10377(2)	7423(1)	7479(1)	20(1)
C(2)	10205(2)	7648(1)	6895(1)	23(1)
C(3)	9286(2)	7958(1)	6834(1)	23(1)
C(4)	8861(2)	7915(1)	7374(1)	20(1)
C(5)	7890(2)	8166(1)	7471(1)	21(1)
C(6)	7469(2)	8111(1)	7992(1)	22(1)
C(7)	6431(2)	8333(1)	8085(1)	26(1)
C(8)	6325(2)	8212(1)	8641(1)	26(1)
C(9)	7277(2)	7904(1)	8889(1)	21(1)
C(10)	7450(2)	7698(1)	9457(1)	21(1)
C(11)	8309(2)	7336(1)	9680(1)	21(1)
C(12)	8444(2)	7077(1)	10254(1)	25(1)
C(13)	9371(2)	6769(1)	10319(1)	25(1)
C(14)	9824(2)	6840(1)	9787(1)	21(1)
C(15)	10806(2)	6599(1)	9692(1)	21(1)
C(16)	11217(2)	6648(1)	9168(1)	22(1)
C(17)	12264(2)	6438(1)	9076(1)	29(1)
C(18)	12400(2)	6588(1)	8530(1)	28(1)
C(19)	11433(2)	6883(1)	8279(1)	21(1)
C(20)	11276(2)	7098(1)	7712(1)	20(1)
C(21)	7264(2)	8512(1)	6986(1)	21(1)
C(22)	6658(2)	8024(1)	6446(1)	22(1)
C(23)	6100(2)	8353(1)	5992(1)	24(1)
C(24)	6142(2)	9173(1)	6071(1)	28(1)
C(25)	6736(2)	9663(1)	6607(1)	30(1)
C(26)	7289(2)	9335(1)	7061(1)	26(1)
C(27)	6698(2)	7905(1)	9856(1)	21(1)

C(28)	5700(5)	7268(4)	9982(3)	32(1)
C(29)	5006(5)	7458(4)	10353(3)	34(1)
C(28A)	5455(5)	7495(3)	9793(2)	26(1)
C(29A)	4790(5)	7708(4)	10174(3)	30(1)
C(30)	5340(2)	8316(2)	10612(1)	34(1)
C(31)	6284(8)	8884(5)	10480(3)	35(2)
C(32)	6980(6)	8699(4)	10108(3)	30(1)
C(31A)	6616(7)	8813(6)	10682(3)	41(2)
C(32A)	7284(6)	8592(5)	10304(3)	35(2)
C(33)	11475(2)	6293(1)	10185(1)	22(1)
C(34)	12049(2)	6808(1)	10719(1)	23(1)
C(35)	12681(2)	6533(1)	11176(1)	25(1)
C(36)	12764(2)	5744(1)	11110(1)	28(1)
C(37)	12195(2)	5224(1)	10584(1)	31(1)
C(38)	11552(2)	5496(1)	10126(1)	26(1)
C(39)	12129(2)	6978(1)	7340(1)	21(1)
C(40)	12986(2)	7673(1)	7185(1)	24(1)
C(41)	13817(2)	7573(1)	6861(1)	25(1)
C(42)	13796(2)	6775(1)	6687(1)	26(1)
C(43)	12936(2)	6082(1)	6828(1)	28(1)
C(44)	12103(2)	6182(1)	7154(1)	25(1)
C(45)	11743(2)	8824(1)	8798(1)	26(1)
C(46)	12720(2)	8752(1)	9195(1)	28(1)
C(47)	13900(2)	9039(1)	9089(1)	32(1)
C(48)	14102(2)	9404(1)	8585(1)	32(1)
C(49)	13122(2)	9483(1)	8193(1)	30(1)
C(50)	11936(2)	9190(1)	8294(1)	28(1)
C(51)	8127(2)	5770(1)	7754(1)	27(1)
C(52)	7441(2)	5837(1)	7223(1)	28(1)
C(53)	7498(2)	5401(1)	6713(1)	35(1)
C(54)	8220(2)	4902(1)	6736(1)	36(1)
C(55)	8892(2)	4834(1)	7268(1)	36(1)
C(56)	8854(2)	5271(1)	7780(1)	33(1)
C(57)	-135(2)	1660(1)	5119(1)	18(1)
C(58)	416(2)	1495(1)	4646(1)	22(1)
C(59)	1612(2)	2004(1)	4785(1)	22(1)
C(60)	1806(2)	2473(1)	5348(1)	19(1)
C(61)	2942(2)	3052(1)	5645(1)	20(1)
C(62)	3158(2)	3443(1)	6214(1)	19(1)
C(63)	4330(2)	4041(1)	6525(1)	23(1)
C(64)	4207(2)	4252(1)	7067(1)	23(1)
C(65)	2942(2)	3806(1)	7092(1)	21(1)
C(66)	2445(2)	3860(1)	7582(1)	22(1)
C(67)	1196(2)	3486(1)	7583(1)	22(1)
C(68)	665(2)	3572(1)	8081(1)	29(1)
C(69)	-560(2)	3161(1)	7909(1)	26(1)
C(70)	-797(2)	2814(1)	7302(1)	20(1)
C(71)	-1972(2)	2374(1)	6962(1)	19(1)
C(72)	-2194(2)	2018(1)	6381(1)	18(1)
C(73)	-3399(2)	1517(1)	6039(1)	21(1)

C(74)	-3233(2)	1194(1)	5532(1)	21(1)
C(75)	-1927(2)	1501(1)	5554(1)	18(1)
C(76)	-1385(2)	1298(1)	5114(1)	19(1)
C(77)	4002(2)	3270(1)	5345(1)	21(1)
C(78)	5022(2)	3041(1)	5548(1)	26(1)
C(79)	6040(2)	3274(1)	5290(1)	29(1)
C(80)	6043(2)	3738(1)	4825(1)	29(1)
C(81)	5031(2)	3963(1)	4617(1)	29(1)
C(82)	4010(2)	3730(1)	4874(1)	26(1)
C(83)	3295(17)	4254(7)	8161(5)	21(2)
C(84)	3870(10)	5117(7)	8253(4)	26(2)
C(85)	4736(8)	5513(5)	8775(4)	31(2)
C(86)	4962(8)	5031(5)	9206(3)	30(2)
C(87)	4383(8)	4181(5)	9120(3)	32(2)
C(88)	3532(10)	3786(4)	8604(4)	22(2)
C(83A)	3337(17)	4417(7)	8116(5)	22(2)
C(84A)	3987(10)	5268(6)	8124(4)	25(2)
C(85A)	4834(8)	5724(5)	8625(3)	31(2)
C(86A)	5068(7)	5353(5)	9120(4)	31(2)
C(87A)	4450(9)	4505(5)	9119(3)	33(2)
C(88A)	3602(11)	4048(5)	8613(4)	27(2)
C(89)	-3057(2)	2220(1)	7245(1)	20(1)
C(90)	-3328(2)	1579(1)	7593(1)	25(1)
C(91)	-4330(2)	1423(1)	7861(1)	28(1)
C(92)	-5076(2)	1901(1)	7780(1)	26(1)
C(93)	-4825(2)	2538(1)	7431(1)	25(1)
C(94)	-3814(2)	2703(1)	7168(1)	23(1)
C(95)	-2182(2)	667(1)	4601(1)	20(1)
C(96)	-2304(2)	-171(1)	4602(1)	33(1)
C(97)	-3012(2)	-760(1)	4119(1)	37(1)
C(98)	-3610(2)	-519(1)	3638(1)	30(1)
C(99)	-3500(2)	313(1)	3633(1)	31(1)
C(100)	-2786(2)	905(1)	4112(1)	29(1)
C(101)	223(2)	3788(1)	5450(1)	22(1)
C(102)	1177(2)	4396(1)	5287(1)	27(1)
C(103)	1057(2)	4525(1)	4705(1)	30(1)
C(104)	-14(2)	4067(1)	4295(1)	29(1)
C(105)	-964(2)	3470(1)	4469(1)	27(1)
C(106)	-849(2)	3322(1)	5049(1)	24(1)
C(107)	1723(6)	1633(5)	7120(3)	26(1)
C(108)	1114(7)	802(6)	7371(4)	44(2)
C(17A)	1385(9)	1648(6)	7253(3)	44(2)
C(18A)	1569(6)	832(5)	7299(3)	34(2)
C(109)	541(2)	217(1)	6810(1)	36(1)
C(110)	120(2)	758(1)	6389(1)	43(1)
O(3)	705(1)	4315(1)	6412(1)	29(1)
O(4)	781(1)	1610(1)	6642(1)	23(1)
O(10)	-1219(6)	775(4)	9773(2)	93(2)
C(111)	-2355(9)	582(8)	9340(3)	104(3)
C(112)	-1888(8)	693(5)	8764(3)	72(2)

C(113)	-866(10)	356(8)	8793(4)	106(3)
C(114)	-343(10)	625(9)	9475(4)	114(4)
O(11)	-946(7)	212(5)	9234(4)	115(2)
C(115)	-1421(10)	869(7)	9254(4)	98(3)
C(116)	-1417(14)	1175(9)	8700(4)	127(4)
C(117)	-619(12)	998(8)	8465(5)	122(4)
C(118)	-189(7)	278(5)	8795(4)	100(3)

Table S3. Bond lengths [Å] and angles [°] for [Fe(TPP)(THF)(PhNO)] and [Fe(TPP)($PhNH_2$)(PhNO)].

Fe(1)-N(5)	1.9635(19)
Fe(1)-N(6)	1.994(2)
Fe(1)-N(4)	2.0008(16)
Fe(1)-N(2)	2.0012(16)
Fe(1)-N(1)	2.0020(15)
Fe(1)-N(3)	2.0031(15)
Fe(2)-N(11)	1.8129(17)
Fe(2)-N(7)	1.9947(15)
Fe(2)-N(9)	1.9962(15)
Fe(2)-N(10)	1.9982(15)
Fe(2)-N(8)	2.0005(15)
Fe(2)-O(4)	2.1415(14)
O(1)-N(5)	1.195(3)
O(2)-N(6)	1.171(3)
N(1)-C(1)	1.374(2)
N(1)-C(4)	1.375(2)
N(2)-C(9)	1.375(2)
N(2)-C(6)	1.376(2)
N(3)-C(14)	1.375(2)
N(3)-C(11)	1.377(2)
N(4)-C(19)	1.371(2)
N(4)-C(16)	1.373(2)
N(5)-C(45)	1.444(3)
N(5)-H(5NA)	0.9100
N(5)-H(5NB)	0.9100
N(6)-C(51)	1.449(3)
N(6)-H(6NA)	0.9100
N(6)-H(6NB)	0.9100
N(7)-C(60)	1.371(2)
N(7)-C(57)	1.378(2)
N(8)-C(62)	1.375(2)
N(8)-C(65)	1.376(2)
N(9)-C(70)	1.374(2)
N(9)-C(67)	1.378(2)
N(10)-C(72)	1.378(2)
N(10)-C(75)	1.379(2)
N(11)-O(3)	1.253(2)
N(11)-C(101)	1.457(2)
C(1)-C(20)	1.391(3)
C(1)-C(2)	1.441(2)
C(2)-C(3)	1.340(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.442(2)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.393(3)
C(5)-C(6)	1.395(2)

C(5)-C(21)	1.497(3)
C(6)-C(7)	1.439(3)
C(7)-C(8)	1.354(3)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.432(3)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.393(3)
C(10)-C(11)	1.389(3)
C(10)-C(27)	1.499(2)
C(11)-C(12)	1.438(3)
C(12)-C(13)	1.347(3)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.438(2)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.396(3)
C(15)-C(16)	1.398(2)
C(15)-C(33)	1.493(3)
C(16)-C(17)	1.437(3)
C(17)-C(18)	1.349(3)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.435(3)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.394(3)
C(20)-C(39)	1.497(2)
C(21)-C(26)	1.393(3)
C(21)-C(22)	1.395(3)
C(22)-C(23)	1.393(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.382(3)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.387(3)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.388(3)
C(25)-H(25A)	0.9500
C(26)-H(26A)	0.9500
C(27)-C(32)	1.352(7)
C(27)-C(28A)	1.371(6)
C(27)-C(28)	1.403(6)
C(27)-C(32A)	1.413(7)
C(28)-C(29)	1.387(8)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.444(7)
C(29)-H(29A)	0.9500
C(28A)-C(29A)	1.393(8)
C(28A)-H(28B)	0.9500
C(29A)-C(30)	1.314(6)
C(29A)-H(29B)	0.9500
C(30)-C(31)	1.312(9)
C(30)-C(31A)	1.430(9)
C(30)-H(30)	0.9500

C(31)-C(32)	1.387(11)
C(31)-H(31A)	0.9500
C(32)-H(32A)	0.9500
C(31A)-C(32A)	1.397(11)
C(31A)-H(31B)	0.9500
C(32A)-H(32B)	0.9500
C(33)-C(38)	1.392(3)
C(33)-C(34)	1.397(3)
C(34)-C(35)	1.384(3)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.383(3)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.387(3)
C(36)-H(36A)	0.9500
C(37)-C(38)	1.389(3)
C(37)-H(37A)	0.9500
C(38)-H(38A)	0.9500
C(39)-C(44)	1.388(3)
C(39)-C(40)	1.397(3)
C(40)-C(41)	1.388(3)
C(40)-H(40A)	0.9500
C(41)-C(42)	1.387(3)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.381(3)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.393(3)
C(43)-H(43A)	0.9500
C(44)-H(44A)	0.9500
C(45)-C(46)	1.383(3)
C(45)-C(50)	1.391(3)
C(46)-C(47)	1.385(3)
C(46)-H(46A)	0.9500
C(47)-C(48)	1.391(3)
C(47)-H(47A)	0.9500
C(48)-C(49)	1.384(3)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.387(3)
C(49)-H(49A)	0.9500
C(50)-H(50A)	0.9500
C(51)-C(52)	1.386(3)
C(51)-C(56)	1.387(3)
C(52)-C(53)	1.391(3)
C(52)-H(52A)	0.9500
C(53)-C(54)	1.383(4)
C(53)-H(53A)	0.9500
C(54)-C(55)	1.380(4)
C(54)-H(54A)	0.9500
C(55)-C(56)	1.388(3)
C(55)-H(55A)	0.9500
C(56)-H(56A)	0.9500

C(57)-C(76)	1.390(2)
C(57)-C(58)	1.440(2)
C(58)-C(59)	1.351(3)
C(58)-H(58A)	0.9500
C(59)-C(60)	1.439(2)
C(59)-H(59A)	0.9500
C(60)-C(61)	1.394(2)
C(61)-C(62)	1.391(2)
C(61)-C(77)	1.496(2)
C(62)-C(63)	1.442(2)
C(63)-C(64)	1.345(3)
C(63)-H(63A)	0.9500
C(64)-C(65)	1.443(3)
C(64)-H(64A)	0.9500
C(65)-C(66)	1.391(3)
C(66)-C(67)	1.393(3)
C(66)-C(83)	1.495(8)
C(66)-C(83A)	1.509(9)
C(67)-C(68)	1.443(3)
C(68)-C(69)	1.345(3)
C(68)-H(68A)	0.9500
C(69)-C(70)	1.445(2)
C(69)-H(69A)	0.9500
C(70)-C(71)	1.393(3)
C(71)-C(72)	1.395(2)
C(71)-C(89)	1.499(2)
C(72)-C(73)	1.440(2)
C(73)-C(74)	1.352(3)
C(73)-H(73A)	0.9500
C(74)-C(75)	1.438(2)
C(74)-H(74A)	0.9500
C(75)-C(76)	1.390(3)
C(76)-C(95)	1.496(2)
C(77)-C(78)	1.390(3)
C(77)-C(82)	1.393(3)
C(78)-C(79)	1.392(3)
C(78)-H(78A)	0.9500
C(79)-C(80)	1.385(3)
C(79)-H(79A)	0.9500
C(80)-C(81)	1.382(3)
C(80)-H(80A)	0.9500
C(81)-C(82)	1.392(3)
C(81)-H(81A)	0.9500
C(82)-H(82A)	0.9500
C(83)-C(84)	1.385(9)
C(83)-C(88)	1.389(9)
C(84)-C(85)	1.404(9)
C(84)-H(84A)	0.9500
C(85)-C(86)	1.382(8)
C(85)-H(85A)	0.9500

C(86)-C(87)	1.367(8)
C(86)-H(86A)	0.9500
C(87)-C(88)	1.387(8)
C(87)-H(87A)	0.9500
C(88)-H(88A)	0.9500
C(83A)-C(88A)	1.390(9)
C(83A)-C(84A)	1.397(9)
C(84A)-C(85A)	1.385(8)
C(84A)-H(84B)	0.9500
C(85A)-C(86A)	1.382(8)
C(85A)-H(85B)	0.9500
C(86A)-C(87A)	1.387(8)
C(86A)-H(86B)	0.9500
C(87A)-C(88A)	1.394(9)
C(87A)-H(87B)	0.9500
C(88A)-H(88B)	0.9500
C(89)-C(90)	1.392(3)
C(89)-C(94)	1.394(3)
C(90)-C(91)	1.392(3)
C(90)-H(90A)	0.9500
C(91)-C(92)	1.378(3)
C(91)-H(91A)	0.9500
C(92)-C(93)	1.387(3)
C(92)-H(92A)	0.9500
C(93)-C(94)	1.394(3)
C(93)-H(93A)	0.9500
C(94)-H(94A)	0.9500
C(95)-C(100)	1.389(3)
C(95)-C(96)	1.389(3)
C(96)-C(97)	1.393(3)
C(96)-H(96A)	0.9500
C(97)-C(98)	1.376(3)
C(97)-H(97A)	0.9500
C(98)-C(99)	1.382(3)
C(98)-H(98A)	0.9500
C(99)-C(100)	1.390(3)
C(99)-H(99A)	0.9500
C(100)-H(10D)	0.9500
C(101)-C(106)	1.383(3)
C(101)-C(102)	1.386(3)
C(102)-C(103)	1.383(3)
C(102)-H(10E)	0.9500
C(103)-C(104)	1.389(3)
C(103)-H(10H)	0.9500
C(104)-C(105)	1.385(3)
C(104)-H(10C)	0.9500
C(105)-C(106)	1.387(3)
C(105)-H(10A)	0.9500
C(106)-H(10B)	0.9500
C(107)-O(4)	1.410(7)

C(107)-C(108)	1.568(12)
C(107)-H(10I)	0.9900
C(107)-H(10L)	0.9900
C(108)-C(109)	1.497(10)
C(108)-H(10J)	0.9900
C(108)-H(10K)	0.9900
C(17A)-O(4)	1.463(8)
C(17A)-C(18A)	1.484(14)
C(17A)-H(10M)	0.9900
C(17A)-H(10N)	0.9900
C(18A)-C(109)	1.542(8)
C(18A)-H(10P)	0.9900
C(18A)-H(10Q)	0.9900
C(109)-C(110)	1.517(3)
C(109)-H(10F)	0.9900
C(109)-H(10G)	0.9900
C(109)-H(10R)	0.9900
C(109)-H(10S)	0.9900
C(110)-O(4)	1.430(2)
C(110)-H(11A)	0.9900
C(110)-H(11B)	0.9900
O(10)-C(114)	1.425(10)
O(10)-C(111)	1.445(9)
C(111)-C(112)	1.547(11)
C(111)-H(11C)	0.9900
C(111)-H(11D)	0.9900
C(112)-C(113)	1.486(11)
C(112)-H(11E)	0.9900
C(112)-H(11F)	0.9900
C(113)-C(114)	1.580(11)
C(113)-H(11G)	0.9900
C(113)-H(11H)	0.9900
C(114)-H(11I)	0.9900
C(114)-H(11J)	0.9900
O(11)-C(115)	1.410(10)
O(11)-C(118)	1.466(10)
C(115)-C(116)	1.428(10)
C(115)-H(11K)	0.9900
C(115)-H(11L)	0.9900
C(116)-C(117)	1.278(12)
C(116)-H(11M)	0.9900
C(116)-H(11N)	0.9900
C(117)-C(118)	1.655(12)
C(117)-H(11O)	0.9900
C(117)-H(11P)	0.9900
C(118)-H(11Q)	0.9900
C(118)-H(11R)	0.9900

N(5)-Fe(1)-N(6)	176.37(7)
N(5)-Fe(1)-N(4)	91.11(7)

N(6)-Fe(1)-N(4)	91.02(7)
N(5)-Fe(1)-N(2)	89.52(7)
N(6)-Fe(1)-N(2)	88.34(7)
N(4)-Fe(1)-N(2)	179.36(7)
N(5)-Fe(1)-N(1)	92.14(6)
N(6)-Fe(1)-N(1)	90.80(7)
N(4)-Fe(1)-N(1)	89.83(6)
N(2)-Fe(1)-N(1)	90.24(6)
N(5)-Fe(1)-N(3)	88.52(7)
N(6)-Fe(1)-N(3)	88.54(7)
N(4)-Fe(1)-N(3)	90.08(6)
N(2)-Fe(1)-N(3)	89.84(6)
N(1)-Fe(1)-N(3)	179.33(6)
N(11)-Fe(2)-N(7)	94.09(7)
N(11)-Fe(2)-N(9)	92.45(7)
N(7)-Fe(2)-N(9)	173.45(6)
N(11)-Fe(2)-N(10)	96.47(7)
N(7)-Fe(2)-N(10)	89.45(6)
N(9)-Fe(2)-N(10)	90.21(6)
N(11)-Fe(2)-N(8)	86.39(7)
N(7)-Fe(2)-N(8)	90.14(6)
N(9)-Fe(2)-N(8)	89.87(6)
N(10)-Fe(2)-N(8)	177.13(6)
N(11)-Fe(2)-O(4)	175.25(6)
N(7)-Fe(2)-O(4)	86.67(6)
N(9)-Fe(2)-O(4)	86.78(6)
N(10)-Fe(2)-O(4)	88.22(6)
N(8)-Fe(2)-O(4)	88.92(6)
C(1)-N(1)-C(4)	105.60(14)
C(1)-N(1)-Fe(1)	127.49(13)
C(4)-N(1)-Fe(1)	126.91(12)
C(9)-N(2)-C(6)	105.63(15)
C(9)-N(2)-Fe(1)	127.26(12)
C(6)-N(2)-Fe(1)	127.06(12)
C(14)-N(3)-C(11)	105.57(15)
C(14)-N(3)-Fe(1)	127.21(12)
C(11)-N(3)-Fe(1)	127.21(13)
C(19)-N(4)-C(16)	105.83(15)
C(19)-N(4)-Fe(1)	126.87(12)
C(16)-N(4)-Fe(1)	127.12(12)
O(1)-N(5)-C(45)	117.7(2)
O(1)-N(5)-Fe(1)	119.88(18)
C(45)-N(5)-Fe(1)	121.75(13)
C(45)-N(5)-H(5NA)	106.9
Fe(1)-N(5)-H(5NA)	106.9
C(45)-N(5)-H(5NB)	106.9
Fe(1)-N(5)-H(5NB)	106.9
H(5NA)-N(5)-H(5NB)	106.7
O(2)-N(6)-C(51)	116.3(2)
O(2)-N(6)-Fe(1)	118.8(2)

C(51)-N(6)-Fe(1)	121.79(13)
C(51)-N(6)-H(6NA)	106.9
Fe(1)-N(6)-H(6NA)	106.9
C(51)-N(6)-H(6NB)	106.9
Fe(1)-N(6)-H(6NB)	106.9
H(6NA)-N(6)-H(6NB)	106.7
C(60)-N(7)-C(57)	105.39(14)
C(60)-N(7)-Fe(2)	127.09(12)
C(57)-N(7)-Fe(2)	127.53(12)
C(62)-N(8)-C(65)	105.93(14)
C(62)-N(8)-Fe(2)	126.01(12)
C(65)-N(8)-Fe(2)	127.20(12)
C(70)-N(9)-C(67)	105.56(14)
C(70)-N(9)-Fe(2)	127.13(12)
C(67)-N(9)-Fe(2)	127.32(12)
C(72)-N(10)-C(75)	105.64(14)
C(72)-N(10)-Fe(2)	126.51(12)
C(75)-N(10)-Fe(2)	127.77(12)
O(3)-N(11)-C(101)	113.46(15)
O(3)-N(11)-Fe(2)	121.62(13)
C(101)-N(11)-Fe(2)	123.47(12)
N(1)-C(1)-C(20)	125.83(16)
N(1)-C(1)-C(2)	110.25(16)
C(20)-C(1)-C(2)	123.91(16)
C(3)-C(2)-C(1)	106.89(16)
C(3)-C(2)-H(2A)	126.6
C(1)-C(2)-H(2A)	126.6
C(2)-C(3)-C(4)	107.37(17)
C(2)-C(3)-H(3A)	126.3
C(4)-C(3)-H(3A)	126.3
N(1)-C(4)-C(5)	126.12(16)
N(1)-C(4)-C(3)	109.88(16)
C(5)-C(4)-C(3)	124.00(17)
C(4)-C(5)-C(6)	123.77(17)
C(4)-C(5)-C(21)	117.85(16)
C(6)-C(5)-C(21)	118.38(17)
N(2)-C(6)-C(5)	125.82(18)
N(2)-C(6)-C(7)	110.19(16)
C(5)-C(6)-C(7)	123.99(17)
C(8)-C(7)-C(6)	106.69(17)
C(8)-C(7)-H(7A)	126.7
C(6)-C(7)-H(7A)	126.7
C(7)-C(8)-C(9)	107.23(17)
C(7)-C(8)-H(8A)	126.4
C(9)-C(8)-H(8A)	126.4
N(2)-C(9)-C(10)	125.95(17)
N(2)-C(9)-C(8)	110.24(16)
C(10)-C(9)-C(8)	123.81(17)
C(11)-C(10)-C(9)	123.64(17)
C(11)-C(10)-C(27)	118.21(16)

C(9)-C(10)-C(27)	118.11(17)
N(3)-C(11)-C(10)	125.98(16)
N(3)-C(11)-C(12)	110.11(17)
C(10)-C(11)-C(12)	123.92(17)
C(13)-C(12)-C(11)	107.06(16)
C(13)-C(12)-H(12A)	126.5
C(11)-C(12)-H(12A)	126.5
C(12)-C(13)-C(14)	107.12(17)
C(12)-C(13)-H(13A)	126.4
C(14)-C(13)-H(13A)	126.4
N(3)-C(14)-C(15)	125.87(16)
N(3)-C(14)-C(13)	110.10(17)
C(15)-C(14)-C(13)	124.03(17)
C(14)-C(15)-C(16)	123.58(18)
C(14)-C(15)-C(33)	118.07(16)
C(16)-C(15)-C(33)	118.33(17)
N(4)-C(16)-C(15)	126.06(18)
N(4)-C(16)-C(17)	110.00(16)
C(15)-C(16)-C(17)	123.90(18)
C(18)-C(17)-C(16)	107.00(18)
C(18)-C(17)-H(17A)	126.5
C(16)-C(17)-H(17A)	126.5
C(17)-C(18)-C(19)	107.03(17)
C(17)-C(18)-H(18A)	126.5
C(19)-C(18)-H(18A)	126.5
N(4)-C(19)-C(20)	126.55(17)
N(4)-C(19)-C(18)	110.13(16)
C(20)-C(19)-C(18)	123.31(17)
C(1)-C(20)-C(19)	123.28(17)
C(1)-C(20)-C(39)	118.66(16)
C(19)-C(20)-C(39)	118.06(17)
C(26)-C(21)-C(22)	118.41(17)
C(26)-C(21)-C(5)	120.75(17)
C(22)-C(21)-C(5)	120.83(17)
C(23)-C(22)-C(21)	120.78(18)
C(23)-C(22)-H(22A)	119.6
C(21)-C(22)-H(22A)	119.6
C(24)-C(23)-C(22)	120.12(18)
C(24)-C(23)-H(23A)	119.9
C(22)-C(23)-H(23A)	119.9
C(23)-C(24)-C(25)	119.62(18)
C(23)-C(24)-H(24A)	120.2
C(25)-C(24)-H(24A)	120.2
C(24)-C(25)-C(26)	120.3(2)
C(24)-C(25)-H(25A)	119.8
C(26)-C(25)-H(25A)	119.8
C(25)-C(26)-C(21)	120.75(18)
C(25)-C(26)-H(26A)	119.6
C(21)-C(26)-H(26A)	119.6
C(32)-C(27)-C(28)	118.9(4)

C(28A)-C(27)-C(32A)	117.5(4)
C(32)-C(27)-C(10)	121.0(3)
C(28A)-C(27)-C(10)	123.9(3)
C(28)-C(27)-C(10)	120.2(3)
C(32A)-C(27)-C(10)	118.4(3)
C(29)-C(28)-C(27)	120.3(5)
C(29)-C(28)-H(28A)	119.9
C(27)-C(28)-H(28A)	119.9
C(28)-C(29)-C(30)	118.9(5)
C(28)-C(29)-H(29A)	120.5
C(30)-C(29)-H(29A)	120.5
C(27)-C(28A)-C(29A)	122.1(5)
C(27)-C(28A)-H(28B)	119.0
C(29A)-C(28A)-H(28B)	119.0
C(30)-C(29A)-C(28A)	120.8(5)
C(30)-C(29A)-H(29B)	119.6
C(28A)-C(29A)-H(29B)	119.6
C(29A)-C(30)-C(31A)	120.5(4)
C(31)-C(30)-C(29)	118.2(4)
C(31)-C(30)-H(30)	120.9
C(29)-C(30)-H(30)	120.9
C(30)-C(31)-C(32)	123.2(7)
C(30)-C(31)-H(31A)	118.4
C(32)-C(31)-H(31A)	118.4
C(27)-C(32)-C(31)	120.6(6)
C(27)-C(32)-H(32A)	119.7
C(31)-C(32)-H(32A)	119.7
C(32A)-C(31A)-C(30)	118.4(6)
C(32A)-C(31A)-H(31B)	120.8
C(30)-C(31A)-H(31B)	120.8
C(31A)-C(32A)-C(27)	120.4(6)
C(31A)-C(32A)-H(32B)	119.8
C(27)-C(32A)-H(32B)	119.8
C(38)-C(33)-C(34)	118.15(18)
C(38)-C(33)-C(15)	121.40(17)
C(34)-C(33)-C(15)	120.45(18)
C(35)-C(34)-C(33)	120.90(19)
C(35)-C(34)-H(34A)	119.5
C(33)-C(34)-H(34A)	119.5
C(36)-C(35)-C(34)	120.46(18)
C(36)-C(35)-H(35A)	119.8
C(34)-C(35)-H(35A)	119.8
C(35)-C(36)-C(37)	119.37(18)
C(35)-C(36)-H(36A)	120.3
C(37)-C(36)-H(36A)	120.3
C(36)-C(37)-C(38)	120.2(2)
C(36)-C(37)-H(37A)	119.9
C(38)-C(37)-H(37A)	119.9
C(37)-C(38)-C(33)	120.89(19)
C(37)-C(38)-H(38A)	119.6

C(33)-C(38)-H(38A)	119.6
C(44)-C(39)-C(40)	118.92(17)
C(44)-C(39)-C(20)	120.99(17)
C(40)-C(39)-C(20)	120.08(17)
C(41)-C(40)-C(39)	120.67(18)
C(41)-C(40)-H(40A)	119.7
C(39)-C(40)-H(40A)	119.7
C(42)-C(41)-C(40)	119.76(18)
C(42)-C(41)-H(41A)	120.1
C(40)-C(41)-H(41A)	120.1
C(43)-C(42)-C(41)	120.04(18)
C(43)-C(42)-H(42A)	120.0
C(41)-C(42)-H(42A)	120.0
C(42)-C(43)-C(44)	120.24(19)
C(42)-C(43)-H(43A)	119.9
C(44)-C(43)-H(43A)	119.9
C(39)-C(44)-C(43)	120.34(18)
C(39)-C(44)-H(44A)	119.8
C(43)-C(44)-H(44A)	119.8
C(46)-C(45)-C(50)	120.50(19)
C(46)-C(45)-N(5)	119.20(18)
C(50)-C(45)-N(5)	120.30(18)
C(45)-C(46)-C(47)	120.0(2)
C(45)-C(46)-H(46A)	120.0
C(47)-C(46)-H(46A)	120.0
C(46)-C(47)-C(48)	120.0(2)
C(46)-C(47)-H(47A)	120.0
C(48)-C(47)-H(47A)	120.0
C(49)-C(48)-C(47)	119.8(2)
C(49)-C(48)-H(48A)	120.1
C(47)-C(48)-H(48A)	120.1
C(48)-C(49)-C(50)	120.6(2)
C(48)-C(49)-H(49A)	119.7
C(50)-C(49)-H(49A)	119.7
C(49)-C(50)-C(45)	119.2(2)
C(49)-C(50)-H(50A)	120.4
C(45)-C(50)-H(50A)	120.4
C(52)-C(51)-C(56)	120.65(19)
C(52)-C(51)-N(6)	119.19(19)
C(56)-C(51)-N(6)	120.13(18)
C(51)-C(52)-C(53)	119.0(2)
C(51)-C(52)-H(52A)	120.5
C(53)-C(52)-H(52A)	120.5
C(54)-C(53)-C(52)	120.7(2)
C(54)-C(53)-H(53A)	119.7
C(52)-C(53)-H(53A)	119.7
C(55)-C(54)-C(53)	119.9(2)
C(55)-C(54)-H(54A)	120.0
C(53)-C(54)-H(54A)	120.0
C(54)-C(55)-C(56)	120.1(2)

C(54)-C(55)-H(55A)	119.9
C(56)-C(55)-H(55A)	119.9
C(51)-C(56)-C(55)	119.7(2)
C(51)-C(56)-H(56A)	120.2
C(55)-C(56)-H(56A)	120.2
N(7)-C(57)-C(76)	125.89(16)
N(7)-C(57)-C(58)	110.31(15)
C(76)-C(57)-C(58)	123.71(16)
C(59)-C(58)-C(57)	106.79(16)
C(59)-C(58)-H(58A)	126.6
C(57)-C(58)-H(58A)	126.6
C(58)-C(59)-C(60)	106.97(16)
C(58)-C(59)-H(59A)	126.5
C(60)-C(59)-H(59A)	126.5
N(7)-C(60)-C(61)	125.69(16)
N(7)-C(60)-C(59)	110.53(15)
C(61)-C(60)-C(59)	123.76(16)
C(62)-C(61)-C(60)	123.67(16)
C(62)-C(61)-C(77)	117.27(16)
C(60)-C(61)-C(77)	119.06(16)
N(8)-C(62)-C(61)	126.08(16)
N(8)-C(62)-C(63)	109.77(15)
C(61)-C(62)-C(63)	124.13(16)
C(64)-C(63)-C(62)	107.38(16)
C(64)-C(63)-H(63A)	126.3
C(62)-C(63)-H(63A)	126.3
C(63)-C(64)-C(65)	106.91(16)
C(63)-C(64)-H(64A)	126.5
C(65)-C(64)-H(64A)	126.5
N(8)-C(65)-C(66)	125.41(16)
N(8)-C(65)-C(64)	109.98(16)
C(66)-C(65)-C(64)	124.60(16)
C(65)-C(66)-C(67)	123.81(17)
C(65)-C(66)-C(83)	119.1(9)
C(67)-C(66)-C(83)	116.7(8)
C(65)-C(66)-C(83A)	115.3(8)
C(67)-C(66)-C(83A)	120.7(8)
N(9)-C(67)-C(66)	125.72(16)
N(9)-C(67)-C(68)	110.16(16)
C(66)-C(67)-C(68)	124.08(17)
C(69)-C(68)-C(67)	107.06(17)
C(69)-C(68)-H(68A)	126.5
C(67)-C(68)-H(68A)	126.5
C(68)-C(69)-C(70)	107.00(17)
C(68)-C(69)-H(69A)	126.5
C(70)-C(69)-H(69A)	126.5
N(9)-C(70)-C(71)	125.71(16)
N(9)-C(70)-C(69)	110.22(16)
C(71)-C(70)-C(69)	124.02(17)
C(70)-C(71)-C(72)	123.81(16)

C(70)-C(71)-C(89)	118.35(15)
C(72)-C(71)-C(89)	117.69(16)
N(10)-C(72)-C(71)	125.65(16)
N(10)-C(72)-C(73)	110.00(15)
C(71)-C(72)-C(73)	124.07(16)
C(74)-C(73)-C(72)	107.14(16)
C(74)-C(73)-H(73A)	126.4
C(72)-C(73)-H(73A)	126.4
C(73)-C(74)-C(75)	107.00(16)
C(73)-C(74)-H(74A)	126.5
C(75)-C(74)-H(74A)	126.5
N(10)-C(75)-C(76)	125.48(16)
N(10)-C(75)-C(74)	110.16(15)
C(76)-C(75)-C(74)	124.36(16)
C(75)-C(76)-C(57)	123.48(16)
C(75)-C(76)-C(95)	118.80(16)
C(57)-C(76)-C(95)	117.72(16)
C(78)-C(77)-C(82)	118.89(17)
C(78)-C(77)-C(61)	120.21(17)
C(82)-C(77)-C(61)	120.85(18)
C(77)-C(78)-C(79)	120.83(19)
C(77)-C(78)-H(78A)	119.6
C(79)-C(78)-H(78A)	119.6
C(80)-C(79)-C(78)	119.8(2)
C(80)-C(79)-H(79A)	120.1
C(78)-C(79)-H(79A)	120.1
C(81)-C(80)-C(79)	119.85(18)
C(81)-C(80)-H(80A)	120.1
C(79)-C(80)-H(80A)	120.1
C(80)-C(81)-C(82)	120.44(19)
C(80)-C(81)-H(81A)	119.8
C(82)-C(81)-H(81A)	119.8
C(81)-C(82)-C(77)	120.2(2)
C(81)-C(82)-H(82A)	119.9
C(77)-C(82)-H(82A)	119.9
C(84)-C(83)-C(88)	119.4(7)
C(84)-C(83)-C(66)	118.2(8)
C(88)-C(83)-C(66)	122.4(8)
C(83)-C(84)-C(85)	120.4(7)
C(83)-C(84)-H(84A)	119.8
C(85)-C(84)-H(84A)	119.8
C(86)-C(85)-C(84)	118.9(7)
C(86)-C(85)-H(85A)	120.6
C(84)-C(85)-H(85A)	120.6
C(87)-C(86)-C(85)	120.8(6)
C(87)-C(86)-H(86A)	119.6
C(85)-C(86)-H(86A)	119.6
C(86)-C(87)-C(88)	120.6(7)
C(86)-C(87)-H(87A)	119.7
C(88)-C(87)-H(87A)	119.7

C(87)-C(88)-C(83)	119.8(7)
C(87)-C(88)-H(88A)	120.1
C(83)-C(88)-H(88A)	120.1
C(88A)-C(83A)-C(84A)	118.1(7)
C(88A)-C(83A)-C(66)	118.1(8)
C(84A)-C(83A)-C(66)	123.6(8)
C(85A)-C(84A)-C(83A)	119.8(7)
C(85A)-C(84A)-H(84B)	120.1
C(83A)-C(84A)-H(84B)	120.1
C(86A)-C(85A)-C(84A)	121.5(7)
C(86A)-C(85A)-H(85B)	119.3
C(84A)-C(85A)-H(85B)	119.3
C(85A)-C(86A)-C(87A)	119.8(6)
C(85A)-C(86A)-H(86B)	120.1
C(87A)-C(86A)-H(86B)	120.1
C(86A)-C(87A)-C(88A)	118.6(7)
C(86A)-C(87A)-H(87B)	120.7
C(88A)-C(87A)-H(87B)	120.7
C(83A)-C(88A)-C(87A)	122.3(7)
C(83A)-C(88A)-H(88B)	118.9
C(87A)-C(88A)-H(88B)	118.9
C(90)-C(89)-C(94)	118.61(17)
C(90)-C(89)-C(71)	119.70(17)
C(94)-C(89)-C(71)	121.70(16)
C(89)-C(90)-C(91)	120.89(19)
C(89)-C(90)-H(90A)	119.6
C(91)-C(90)-H(90A)	119.6
C(92)-C(91)-C(90)	120.08(18)
C(92)-C(91)-H(91A)	120.0
C(90)-C(91)-H(91A)	120.0
C(91)-C(92)-C(93)	119.79(18)
C(91)-C(92)-H(92A)	120.1
C(93)-C(92)-H(92A)	120.1
C(92)-C(93)-C(94)	120.26(19)
C(92)-C(93)-H(93A)	119.9
C(94)-C(93)-H(93A)	119.9
C(93)-C(94)-C(89)	120.37(18)
C(93)-C(94)-H(94A)	119.8
C(89)-C(94)-H(94A)	119.8
C(100)-C(95)-C(96)	118.80(17)
C(100)-C(95)-C(76)	121.15(17)
C(96)-C(95)-C(76)	120.03(17)
C(95)-C(96)-C(97)	120.5(2)
C(95)-C(96)-H(96A)	119.8
C(97)-C(96)-H(96A)	119.8
C(98)-C(97)-C(96)	120.3(2)
C(98)-C(97)-H(97A)	119.9
C(96)-C(97)-H(97A)	119.9
C(97)-C(98)-C(99)	119.68(18)
C(97)-C(98)-H(98A)	120.2

C(99)-C(98)-H(98A)	120.2
C(98)-C(99)-C(100)	120.3(2)
C(98)-C(99)-H(99A)	119.9
C(100)-C(99)-H(99A)	119.9
C(95)-C(100)-C(99)	120.4(2)
C(95)-C(100)-H(10D)	119.8
C(99)-C(100)-H(10D)	119.8
C(106)-C(101)-C(102)	121.59(18)
C(106)-C(101)-N(11)	121.03(16)
C(102)-C(101)-N(11)	117.38(16)
C(103)-C(102)-C(101)	118.81(18)
C(103)-C(102)-H(10E)	120.6
C(101)-C(102)-H(10E)	120.6
C(102)-C(103)-C(104)	120.53(18)
C(102)-C(103)-H(10H)	119.7
C(104)-C(103)-H(10H)	119.7
C(105)-C(104)-C(103)	119.71(18)
C(105)-C(104)-H(10C)	120.1
C(103)-C(104)-H(10C)	120.1
C(104)-C(105)-C(106)	120.50(18)
C(104)-C(105)-H(10A)	119.7
C(106)-C(105)-H(10A)	119.7
C(101)-C(106)-C(105)	118.83(18)
C(101)-C(106)-H(10B)	120.6
C(105)-C(106)-H(10B)	120.6
O(4)-C(107)-C(108)	102.1(5)
O(4)-C(107)-H(10I)	111.4
C(108)-C(107)-H(10I)	111.4
O(4)-C(107)-H(10L)	111.4
C(108)-C(107)-H(10L)	111.4
H(10I)-C(107)-H(10L)	109.2
C(109)-C(108)-C(107)	99.6(5)
C(109)-C(108)-H(10J)	111.9
C(107)-C(108)-H(10J)	111.9
C(109)-C(108)-H(10K)	111.9
C(107)-C(108)-H(10K)	111.9
H(10J)-C(108)-H(10K)	109.6
O(4)-C(17A)-C(18A)	105.8(6)
O(4)-C(17A)-H(10M)	110.6
C(18A)-C(17A)-H(10M)	110.6
O(4)-C(17A)-H(10N)	110.6
C(18A)-C(17A)-H(10N)	110.6
H(10M)-C(17A)-H(10N)	108.7
C(17A)-C(18A)-C(109)	104.5(6)
C(17A)-C(18A)-H(10P)	110.9
C(109)-C(18A)-H(10P)	110.9
C(17A)-C(18A)-H(10Q)	110.9
C(109)-C(18A)-H(10Q)	110.9
H(10P)-C(18A)-H(10Q)	108.9
C(108)-C(109)-C(110)	103.3(4)

C(110)-C(109)-C(18A)	105.8(3)
C(108)-C(109)-H(10F)	111.1
C(110)-C(109)-H(10F)	111.1
C(108)-C(109)-H(10G)	111.1
C(110)-C(109)-H(10G)	111.1
H(10F)-C(109)-H(10G)	109.1
C(110)-C(109)-H(10R)	110.6
C(18A)-C(109)-H(10R)	110.6
C(110)-C(109)-H(10S)	110.6
C(18A)-C(109)-H(10S)	110.6
H(10R)-C(109)-H(10S)	108.7
O(4)-C(110)-C(109)	106.67(18)
O(4)-C(110)-H(11A)	110.4
C(109)-C(110)-H(11A)	110.4
O(4)-C(110)-H(11B)	110.4
C(109)-C(110)-H(11B)	110.4
H(11A)-C(110)-H(11B)	108.6
C(107)-O(4)-C(110)	109.0(3)
C(110)-O(4)-C(17A)	110.2(4)
C(107)-O(4)-Fe(2)	124.9(3)
C(110)-O(4)-Fe(2)	126.00(12)
C(17A)-O(4)-Fe(2)	121.1(4)
C(114)-O(10)-C(111)	106.8(6)
O(10)-C(111)-C(112)	102.1(7)
O(10)-C(111)-H(11C)	111.3
C(112)-C(111)-H(11C)	111.3
O(10)-C(111)-H(11D)	111.3
C(112)-C(111)-H(11D)	111.3
H(11C)-C(111)-H(11D)	109.2
C(113)-C(112)-C(111)	108.6(7)
C(113)-C(112)-H(11E)	110.0
C(111)-C(112)-H(11E)	110.0
C(113)-C(112)-H(11F)	110.0
C(111)-C(112)-H(11F)	110.0
H(11E)-C(112)-H(11F)	108.4
C(112)-C(113)-C(114)	95.2(7)
C(112)-C(113)-H(11G)	112.7
C(114)-C(113)-H(11G)	112.7
C(112)-C(113)-H(11H)	112.7
C(114)-C(113)-H(11H)	112.7
H(11G)-C(113)-H(11H)	110.2
O(10)-C(114)-C(113)	113.1(8)
O(10)-C(114)-H(11I)	109.0
C(113)-C(114)-H(11I)	109.0
O(10)-C(114)-H(11J)	109.0
C(113)-C(114)-H(11J)	109.0
H(11I)-C(114)-H(11J)	107.8
C(115)-O(11)-C(118)	111.8(8)
O(11)-C(115)-C(116)	106.5(8)
O(11)-C(115)-H(11K)	110.4

C(116)-C(115)-H(11K)	110.4
O(11)-C(115)-H(11L)	110.4
C(116)-C(115)-H(11L)	110.4
H(11K)-C(115)-H(11L)	108.6
C(117)-C(116)-C(115)	109.8(9)
C(117)-C(116)-H(11M)	109.7
C(115)-C(116)-H(11M)	109.7
C(117)-C(116)-H(11N)	109.7
C(115)-C(116)-H(11N)	109.7
H(11M)-C(116)-H(11N)	108.2
C(116)-C(117)-C(118)	110.5(7)
C(116)-C(117)-H(11O)	109.6
C(118)-C(117)-H(11O)	109.6
C(116)-C(117)-H(11P)	109.6
C(118)-C(117)-H(11P)	109.6
H(11O)-C(117)-H(11P)	108.1
O(11)-C(118)-C(117)	96.1(6)
O(11)-C(118)-H(11Q)	112.5
C(117)-C(118)-H(11Q)	112.5
O(11)-C(118)-H(11R)	112.5
C(117)-C(118)-H(11R)	112.5
H(11Q)-C(118)-H(11R)	110.0

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for [Fe(TPP)(THF)(PhNO)] and [Fe(TPP)($PhNH_2$)(PhNO)]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U11 + ... + 2hka^*b^*U12]$.

	U11	U22	U33	U23	U13	U12
Fe(1)	19(1)	23(1)	15(1)	3(1)	8(1)	9(1)
Fe(2)	16(1)	19(1)	13(1)	0(1)	5(1)	4(1)
O(1)	30(1)	27(1)	25(1)	-5(1)	13(1)	11(1)
O(2)	26(1)	33(2)	36(2)	6(1)	14(1)	7(1)
N(1)	19(1)	22(1)	17(1)	1(1)	7(1)	7(1)
N(2)	22(1)	26(1)	16(1)	2(1)	8(1)	10(1)
N(3)	21(1)	26(1)	17(1)	3(1)	7(1)	9(1)
N(4)	22(1)	23(1)	15(1)	1(1)	7(1)	9(1)
N(5)	28(1)	43(1)	19(1)	4(1)	10(1)	19(1)
N(6)	25(1)	51(1)	21(1)	0(1)	9(1)	17(1)
N(7)	17(1)	20(1)	15(1)	0(1)	4(1)	5(1)
N(8)	19(1)	20(1)	15(1)	-2(1)	4(1)	4(1)
N(9)	18(1)	24(1)	15(1)	0(1)	5(1)	6(1)

N(10)	18(1)	19(1)	13(1)	0(1)	5(1)	4(1)
N(11)	19(1)	24(1)	19(1)	-2(1)	6(1)	5(1)
C(1)	20(1)	23(1)	16(1)	1(1)	8(1)	6(1)
C(2)	23(1)	29(1)	18(1)	2(1)	9(1)	10(1)
C(3)	23(1)	29(1)	18(1)	5(1)	9(1)	9(1)
C(4)	22(1)	22(1)	16(1)	2(1)	6(1)	7(1)
C(5)	22(1)	23(1)	19(1)	2(1)	8(1)	8(1)
C(6)	23(1)	27(1)	18(1)	3(1)	8(1)	11(1)
C(7)	27(1)	37(1)	21(1)	5(1)	8(1)	18(1)
C(8)	26(1)	37(1)	21(1)	4(1)	10(1)	17(1)
C(9)	21(1)	25(1)	18(1)	1(1)	8(1)	8(1)
C(10)	20(1)	24(1)	18(1)	1(1)	8(1)	6(1)
C(11)	20(1)	28(1)	16(1)	1(1)	8(1)	6(1)
C(12)	25(1)	35(1)	17(1)	3(1)	9(1)	11(1)
C(13)	24(1)	34(1)	18(1)	7(1)	9(1)	11(1)
C(14)	24(1)	25(1)	16(1)	3(1)	7(1)	9(1)
C(15)	23(1)	23(1)	19(1)	3(1)	8(1)	8(1)
C(16)	25(1)	26(1)	19(1)	3(1)	9(1)	12(1)
C(17)	34(1)	44(1)	20(1)	7(1)	10(1)	25(1)
C(18)	32(1)	42(1)	21(1)	6(1)	12(1)	23(1)
C(19)	24(1)	26(1)	18(1)	2(1)	8(1)	11(1)
C(20)	21(1)	23(1)	17(1)	0(1)	7(1)	7(1)
C(21)	20(1)	27(1)	18(1)	4(1)	9(1)	9(1)
C(22)	21(1)	26(1)	20(1)	3(1)	9(1)	10(1)
C(23)	22(1)	34(1)	17(1)	2(1)	6(1)	9(1)
C(24)	28(1)	34(1)	24(1)	9(1)	7(1)	14(1)
C(25)	37(1)	28(1)	28(1)	6(1)	7(1)	16(1)
C(26)	31(1)	28(1)	22(1)	1(1)	6(1)	12(1)
C(27)	21(1)	28(1)	15(1)	2(1)	6(1)	11(1)
C(28)	31(3)	31(3)	29(3)	-8(2)	16(2)	1(2)
C(29)	26(3)	39(3)	32(3)	-5(2)	15(2)	3(2)
C(28A)	23(2)	30(3)	21(3)	-5(2)	5(2)	6(2)
C(29A)	26(2)	35(3)	31(3)	3(2)	15(2)	11(2)
C(30)	36(1)	51(1)	23(1)	-1(1)	14(1)	23(1)
C(31)	53(5)	30(3)	30(4)	0(3)	21(3)	18(3)
C(32)	35(4)	26(2)	35(4)	7(3)	19(3)	11(2)
C(31A)	41(4)	46(4)	28(4)	-22(3)	9(3)	9(3)
C(32A)	26(3)	40(4)	33(4)	-14(3)	6(3)	6(2)
C(33)	21(1)	28(1)	19(1)	4(1)	9(1)	9(1)
C(34)	21(1)	26(1)	22(1)	2(1)	9(1)	7(1)
C(35)	18(1)	36(1)	18(1)	0(1)	6(1)	7(1)
C(36)	22(1)	38(1)	23(1)	10(1)	5(1)	9(1)
C(37)	32(1)	28(1)	31(1)	7(1)	3(1)	12(1)
C(38)	29(1)	28(1)	22(1)	1(1)	3(1)	10(1)
C(39)	21(1)	29(1)	16(1)	2(1)	6(1)	12(1)
C(40)	24(1)	28(1)	21(1)	-1(1)	7(1)	10(1)
C(41)	22(1)	32(1)	21(1)	2(1)	7(1)	8(1)
C(42)	25(1)	39(1)	18(1)	0(1)	10(1)	14(1)
C(43)	33(1)	30(1)	24(1)	0(1)	11(1)	14(1)
C(44)	28(1)	28(1)	23(1)	3(1)	10(1)	11(1)

C(45)	26(1)	30(1)	23(1)	-1(1)	9(1)	11(1)
C(46)	29(1)	29(1)	26(1)	1(1)	6(1)	10(1)
C(47)	26(1)	31(1)	38(1)	0(1)	4(1)	10(1)
C(48)	27(1)	25(1)	43(1)	-2(1)	13(1)	6(1)
C(49)	37(1)	24(1)	31(1)	1(1)	15(1)	8(1)
C(50)	31(1)	33(1)	23(1)	1(1)	9(1)	13(1)
C(51)	29(1)	30(1)	20(1)	-1(1)	7(1)	8(1)
C(52)	26(1)	28(1)	25(1)	2(1)	3(1)	2(1)
C(53)	33(1)	36(1)	22(1)	3(1)	4(1)	-5(1)
C(54)	42(1)	28(1)	32(1)	-5(1)	19(1)	-2(1)
C(55)	43(1)	26(1)	42(1)	5(1)	23(1)	9(1)
C(56)	38(1)	40(1)	28(1)	7(1)	16(1)	17(1)
C(57)	19(1)	20(1)	13(1)	-1(1)	4(1)	5(1)
C(58)	24(1)	25(1)	15(1)	-2(1)	5(1)	7(1)
C(59)	21(1)	28(1)	17(1)	0(1)	7(1)	7(1)
C(60)	20(1)	20(1)	16(1)	0(1)	6(1)	6(1)
C(61)	21(1)	22(1)	18(1)	4(1)	7(1)	7(1)
C(62)	17(1)	21(1)	18(1)	1(1)	4(1)	4(1)
C(63)	18(1)	24(1)	23(1)	0(1)	6(1)	3(1)
C(64)	21(1)	23(1)	22(1)	-2(1)	3(1)	5(1)
C(65)	20(1)	21(1)	17(1)	-2(1)	1(1)	5(1)
C(66)	22(1)	27(1)	18(1)	-3(1)	4(1)	10(1)
C(67)	23(1)	28(1)	14(1)	-3(1)	3(1)	9(1)
C(68)	25(1)	44(1)	16(1)	-5(1)	5(1)	12(1)
C(69)	26(1)	38(1)	17(1)	0(1)	9(1)	12(1)
C(70)	22(1)	24(1)	16(1)	1(1)	7(1)	8(1)
C(71)	21(1)	22(1)	17(1)	3(1)	8(1)	8(1)
C(72)	18(1)	20(1)	17(1)	2(1)	6(1)	6(1)
C(73)	18(1)	24(1)	20(1)	3(1)	7(1)	6(1)
C(74)	18(1)	22(1)	19(1)	1(1)	4(1)	4(1)
C(75)	16(1)	20(1)	15(1)	1(1)	3(1)	3(1)
C(76)	20(1)	22(1)	16(1)	2(1)	4(1)	6(1)
C(77)	20(1)	23(1)	17(1)	-2(1)	6(1)	2(1)
C(78)	23(1)	31(1)	21(1)	2(1)	7(1)	6(1)
C(79)	21(1)	37(1)	27(1)	-2(1)	8(1)	7(1)
C(80)	25(1)	30(1)	27(1)	-4(1)	13(1)	-1(1)
C(81)	35(1)	27(1)	25(1)	4(1)	17(1)	5(1)
C(82)	28(1)	28(1)	24(1)	3(1)	11(1)	9(1)
C(83)	19(3)	27(4)	17(3)	-4(2)	4(2)	9(3)
C(84)	26(3)	31(4)	23(3)	2(2)	6(3)	13(3)
C(85)	30(3)	35(4)	24(4)	-10(3)	2(3)	11(3)
C(86)	27(3)	43(5)	19(2)	-8(3)	3(2)	14(3)
C(87)	30(3)	42(4)	20(2)	-4(3)	3(2)	11(3)
C(88)	25(3)	24(4)	13(2)	-1(3)	1(2)	5(3)
C(83A)	21(3)	28(4)	19(3)	-5(3)	4(2)	12(3)
C(84A)	23(3)	25(4)	22(3)	-8(2)	4(3)	7(2)
C(85A)	26(3)	34(4)	30(4)	-15(2)	0(3)	12(3)
C(86A)	25(3)	40(4)	24(3)	-15(3)	0(2)	12(3)
C(87A)	37(3)	40(5)	16(2)	-12(3)	-1(2)	16(4)
C(88A)	28(3)	26(4)	25(3)	-5(3)	7(2)	8(3)

C(89)	20(1)	24(1)	15(1)	-1(1)	6(1)	6(1)
C(90)	28(1)	26(1)	24(1)	4(1)	11(1)	11(1)
C(91)	30(1)	29(1)	23(1)	4(1)	12(1)	5(1)
C(92)	21(1)	35(1)	19(1)	-4(1)	7(1)	4(1)
C(93)	21(1)	33(1)	21(1)	-3(1)	4(1)	10(1)
C(94)	23(1)	27(1)	18(1)	2(1)	4(1)	8(1)
C(95)	18(1)	23(1)	18(1)	-1(1)	6(1)	4(1)
C(96)	39(1)	25(1)	27(1)	1(1)	-2(1)	5(1)
C(97)	42(1)	22(1)	36(1)	-7(1)	1(1)	4(1)
C(98)	23(1)	34(1)	24(1)	-10(1)	5(1)	-1(1)
C(99)	29(1)	39(1)	20(1)	-3(1)	2(1)	10(1)
C(100)	33(1)	28(1)	23(1)	-2(1)	2(1)	11(1)
C(101)	22(1)	24(1)	19(1)	2(1)	6(1)	9(1)
C(102)	25(1)	27(1)	24(1)	2(1)	4(1)	5(1)
C(103)	30(1)	30(1)	27(1)	6(1)	10(1)	5(1)
C(104)	35(1)	31(1)	20(1)	5(1)	5(1)	10(1)
C(105)	28(1)	25(1)	25(1)	1(1)	1(1)	9(1)
C(106)	23(1)	22(1)	27(1)	2(1)	5(1)	6(1)
C(107)	28(3)	22(2)	22(3)	-3(2)	-6(2)	8(2)
C(108)	49(5)	39(3)	42(3)	17(2)	0(3)	14(4)
C(17A)	62(6)	40(3)	25(3)	4(2)	-5(3)	22(3)
C(18A)	38(4)	30(3)	29(3)	3(2)	-2(3)	12(3)
C(109)	31(1)	28(1)	44(1)	7(1)	1(1)	6(1)
C(110)	48(1)	22(1)	44(1)	-1(1)	-10(1)	6(1)
O(3)	38(1)	24(1)	24(1)	-2(1)	9(1)	9(1)
O(4)	26(1)	21(1)	20(1)	1(1)	2(1)	6(1)
O(10)	108(4)	97(4)	60(3)	0(3)	4(3)	25(3)
C(111)	89(5)	146(9)	66(4)	-21(5)	-3(4)	44(5)
C(112)	109(5)	59(4)	49(4)	-11(3)	-7(3)	45(4)
C(113)	99(6)	141(9)	72(5)	8(5)	-31(4)	62(6)
C(114)	92(6)	159(11)	82(5)	-18(6)	-9(4)	53(6)
O(11)	90(5)	106(5)	113(5)	-12(4)	-13(4)	14(4)
C(115)	107(7)	139(8)	66(5)	33(5)	28(5)	59(6)
C(116)	216(12)	149(10)	48(4)	26(6)	22(6)	106(10)
C(117)	151(9)	161(9)	82(6)	47(6)	55(6)	72(8)
C(118)	47(4)	93(5)	139(7)	-66(4)	5(4)	19(4)

Table S5. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for [Fe(TPP)(THF)(PhNO)] and [Fe(TPP)($PhNH_2$)(PhNO)].

	x	y	z	U(eq)
H(5NA)	10140	8883	8795	33
H(5NB)	10609	8547	9310	33
H(6NA)	8153	5927	8577	37
H(6NB)	7351	6301	8231	37
H(2A)	10657	7589	6608	27
H(3A)	8972	8168	6496	27
H(7A)	5920	8527	7809	31
H(8A)	5729	8312	8832	31
H(12A)	7968	7116	10534	30
H(13A)	9671	6548	10653	29
H(17A)	12764	6233	9349	35
H(18A)	13019	6512	8346	34
H(22A)	6627	7460	6388	26
H(23A)	5690	8013	5626	29
H(24A)	5767	9399	5760	33
H(25A)	6765	10226	6664	36
H(26A)	7689	9675	7428	32
H(28A)	5497	6706	9812	39
H(29A)	4322	7030	10435	40
H(28B)	5033	7052	9481	31
H(29B)	3929	7410	10116	36
H(30)	4889	8464	10872	41
H(31A)	6502	9450	10647	43
H(32A)	7660	9135	10030	36
H(31B)	7000	9282	10979	49
H(32B)	8137	8905	10349	42
H(34A)	12005	7353	10769	27
H(35A)	13060	6890	11537	30
H(36A)	13207	5560	11423	33
H(37A)	12246	4680	10535	37
H(38A)	11159	5133	9768	32
H(40A)	13000	8220	7302	29
H(41A)	14398	8049	6758	30
H(42A)	14374	6704	6472	31
H(43A)	12912	5536	6701	33
H(44A)	11515	5703	7250	30
H(46A)	12583	8505	9540	34
H(47A)	14571	8988	9361	38
H(48A)	14909	9598	8510	38
H(49A)	13263	9740	7852	36
H(50A)	11264	9240	8022	34
H(52A)	6939	6175	7207	34

H(53A)	7037	5446	6346	42
H(54A)	8253	4606	6385	44
H(55A)	9381	4487	7284	43
H(56A)	9323	5229	8145	40
H(58A)	16	1104	4301	26
H(59A)	2211	2045	4555	27
H(63A)	5056	4248	6375	28
H(64A)	4833	4623	7375	28
H(68A)	1098	3864	8459	35
H(69A)	-1155	3108	8143	32
H(73A)	-4165	1430	6149	25
H(74A)	-3860	833	5220	25
H(78A)	5023	2723	5866	31
H(79A)	6732	3115	5433	35
H(80A)	6738	3900	4649	35
H(81A)	5033	4280	4297	35
H(82A)	3318	3886	4727	31
H(84A)	3678	5443	7961	31
H(85A)	5159	6102	8832	37
H(86A)	5527	5295	9566	36
H(87A)	4565	3858	9416	38
H(88A)	3112	3197	8553	27
H(84B)	3849	5534	7786	30
H(85B)	5263	6304	8629	37
H(86B)	5651	5677	9460	37
H(87B)	4601	4242	9456	39
H(88B)	3190	3465	8607	32
H(90A)	-2823	1244	7648	30
H(91A)	-4498	987	8101	33
H(92A)	-5761	1793	7962	31
H(93A)	-5344	2864	7372	30
H(94A)	-3639	3147	6935	28
H(96A)	-1903	-344	4935	40
H(97A)	-3081	-1331	4122	44
H(98A)	-4097	-922	3310	37
H(99A)	-3914	481	3301	37
H(10D)	-2709	1476	4104	34
H(10E)	1901	4719	5569	32
H(10H)	1713	4929	4585	35
H(10C)	-96	4163	3897	35
H(10A)	-1699	3160	4189	32
H(10B)	-1495	2907	5168	29
H(10I)	1931	2131	7413	31
H(10L)	2478	1634	6989	31
H(10J)	1737	632	7627	53
H(10K)	486	847	7588	53
H(10M)	859	1730	7520	52
H(10N)	2188	2116	7357	52
H(10P)	1486	654	7689	40
H(10Q)	2395	869	7238	40

H(10F)	-167	-268	6857	43
H(10G)	1152	11	6673	43
H(10R)	863	-164	6608	43
H(10S)	-153	-123	6974	43
H(11A)	306	653	6002	51
H(11B)	-781	631	6336	51
H(11C)	-2788	976	9412	124
H(11D)	-2916	1	9335	124
H(11E)	-2569	388	8426	87
H(11F)	-1589	1294	8714	87
H(11G)	-266	638	8559	127
H(11H)	-1165	-259	8681	127
H(11I)	-82	177	9644	136
H(11J)	396	1140	9541	136
H(11K)	-899	1320	9575	117
H(11L)	-2272	661	9321	117
H(11M)	-2246	918	8440	153
H(11N)	-1214	1790	8755	153
H(11O)	112	1510	8495	146
H(11P)	-977	787	8044	146
H(11Q)	-426	-253	8531	120
H(11R)	706	479	8972	120

Table S6. Torsion angles [°] for [Fe(TPP)(THF)(PhNO)] and [Fe(TPP)($PhNH_2$)(PhNO)].

N(7)-Fe(2)-N(11)-O(3)	-151.96(14)
N(9)-Fe(2)-N(11)-O(3)	27.64(15)
N(10)-Fe(2)-N(11)-O(3)	118.12(14)
N(8)-Fe(2)-N(11)-O(3)	-62.08(14)
N(7)-Fe(2)-N(11)-C(101)	13.42(15)
N(9)-Fe(2)-N(11)-C(101)	-166.98(14)
N(10)-Fe(2)-N(11)-C(101)	-76.49(14)
N(8)-Fe(2)-N(11)-C(101)	103.30(14)
C(4)-N(1)-C(1)-C(20)	178.85(17)
Fe(1)-N(1)-C(1)-C(20)	-1.9(3)
C(4)-N(1)-C(1)-C(2)	-0.1(2)
Fe(1)-N(1)-C(1)-C(2)	179.15(12)
N(1)-C(1)-C(2)-C(3)	0.7(2)
C(20)-C(1)-C(2)-C(3)	-178.23(18)
C(1)-C(2)-C(3)-C(4)	-1.0(2)
C(1)-N(1)-C(4)-C(5)	178.98(18)
Fe(1)-N(1)-C(4)-C(5)	-0.3(3)
C(1)-N(1)-C(4)-C(3)	-0.6(2)
Fe(1)-N(1)-C(4)-C(3)	-179.79(12)
C(2)-C(3)-C(4)-N(1)	1.0(2)
C(2)-C(3)-C(4)-C(5)	-178.53(18)
N(1)-C(4)-C(5)-C(6)	-0.5(3)
C(3)-C(4)-C(5)-C(6)	178.96(18)
N(1)-C(4)-C(5)-C(21)	179.54(17)
C(3)-C(4)-C(5)-C(21)	-1.0(3)
C(9)-N(2)-C(6)-C(5)	178.86(18)
Fe(1)-N(2)-C(6)-C(5)	-3.4(3)
C(9)-N(2)-C(6)-C(7)	-1.6(2)
Fe(1)-N(2)-C(6)-C(7)	176.17(13)
C(4)-C(5)-C(6)-N(2)	2.4(3)
C(21)-C(5)-C(6)-N(2)	-177.61(17)
C(4)-C(5)-C(6)-C(7)	-177.08(19)
C(21)-C(5)-C(6)-C(7)	2.9(3)
N(2)-C(6)-C(7)-C(8)	1.6(2)
C(5)-C(6)-C(7)-C(8)	-178.84(19)
C(6)-C(7)-C(8)-C(9)	-0.9(2)
C(6)-N(2)-C(9)-C(10)	-179.75(18)
Fe(1)-N(2)-C(9)-C(10)	2.5(3)
C(6)-N(2)-C(9)-C(8)	1.0(2)
Fe(1)-N(2)-C(9)-C(8)	-176.72(13)
C(7)-C(8)-C(9)-N(2)	0.0(2)
C(7)-C(8)-C(9)-C(10)	-179.31(19)
N(2)-C(9)-C(10)-C(11)	-4.6(3)
C(8)-C(9)-C(10)-C(11)	174.55(19)
N(2)-C(9)-C(10)-C(27)	173.28(17)
C(8)-C(9)-C(10)-C(27)	-7.6(3)
C(14)-N(3)-C(11)-C(10)	178.12(18)

Fe(1)-N(3)-C(11)-C(10)	-0.9(3)
C(14)-N(3)-C(11)-C(12)	-1.9(2)
Fe(1)-N(3)-C(11)-C(12)	179.09(13)
C(9)-C(10)-C(11)-N(3)	3.7(3)
C(27)-C(10)-C(11)-N(3)	-174.13(17)
C(9)-C(10)-C(11)-C(12)	-176.25(18)
C(27)-C(10)-C(11)-C(12)	5.9(3)
N(3)-C(11)-C(12)-C(13)	1.0(2)
C(10)-C(11)-C(12)-C(13)	-179.05(18)
C(11)-C(12)-C(13)-C(14)	0.4(2)
C(11)-N(3)-C(14)-C(15)	-178.24(18)
Fe(1)-N(3)-C(14)-C(15)	0.8(3)
C(11)-N(3)-C(14)-C(13)	2.1(2)
Fe(1)-N(3)-C(14)-C(13)	-178.87(13)
C(12)-C(13)-C(14)-N(3)	-1.6(2)
C(12)-C(13)-C(14)-C(15)	178.77(18)
N(3)-C(14)-C(15)-C(16)	-1.5(3)
C(13)-C(14)-C(15)-C(16)	178.14(19)
N(3)-C(14)-C(15)-C(33)	176.82(17)
C(13)-C(14)-C(15)-C(33)	-3.6(3)
C(19)-N(4)-C(16)-C(15)	178.65(18)
Fe(1)-N(4)-C(16)-C(15)	3.3(3)
C(19)-N(4)-C(16)-C(17)	0.7(2)
Fe(1)-N(4)-C(16)-C(17)	-174.64(14)
C(14)-C(15)-C(16)-N(4)	-0.7(3)
C(33)-C(15)-C(16)-N(4)	-178.95(17)
C(14)-C(15)-C(16)-C(17)	176.96(19)
C(33)-C(15)-C(16)-C(17)	-1.3(3)
N(4)-C(16)-C(17)-C(18)	-0.1(2)
C(15)-C(16)-C(17)-C(18)	-178.06(19)
C(16)-C(17)-C(18)-C(19)	-0.6(2)
C(16)-N(4)-C(19)-C(20)	179.60(18)
Fe(1)-N(4)-C(19)-C(20)	-5.0(3)
C(16)-N(4)-C(19)-C(18)	-1.1(2)
Fe(1)-N(4)-C(19)-C(18)	174.30(13)
C(17)-C(18)-C(19)-N(4)	1.1(2)
C(17)-C(18)-C(19)-C(20)	-179.61(19)
N(1)-C(1)-C(20)-C(19)	1.1(3)
C(2)-C(1)-C(20)-C(19)	179.92(18)
N(1)-C(1)-C(20)-C(39)	-178.29(17)
C(2)-C(1)-C(20)-C(39)	0.5(3)
N(4)-C(19)-C(20)-C(1)	2.5(3)
C(18)-C(19)-C(20)-C(1)	-176.70(19)
N(4)-C(19)-C(20)-C(39)	-178.05(17)
C(18)-C(19)-C(20)-C(39)	2.7(3)
C(4)-C(5)-C(21)-C(26)	-117.4(2)
C(6)-C(5)-C(21)-C(26)	62.7(2)
C(4)-C(5)-C(21)-C(22)	61.7(2)
C(6)-C(5)-C(21)-C(22)	-118.3(2)
C(26)-C(21)-C(22)-C(23)	0.5(3)

C(5)-C(21)-C(22)-C(23)	-178.59(17)
C(21)-C(22)-C(23)-C(24)	0.1(3)
C(22)-C(23)-C(24)-C(25)	-0.4(3)
C(23)-C(24)-C(25)-C(26)	0.2(3)
C(24)-C(25)-C(26)-C(21)	0.4(3)
C(22)-C(21)-C(26)-C(25)	-0.7(3)
C(5)-C(21)-C(26)-C(25)	178.35(18)
C(11)-C(10)-C(27)-C(32)	101.6(4)
C(9)-C(10)-C(27)-C(32)	-76.4(4)
C(11)-C(10)-C(27)-C(28A)	-110.9(4)
C(9)-C(10)-C(27)-C(28A)	71.1(4)
C(11)-C(10)-C(27)-C(28)	-77.1(4)
C(9)-C(10)-C(27)-C(28)	104.9(4)
C(11)-C(10)-C(27)-C(32A)	72.7(4)
C(9)-C(10)-C(27)-C(32A)	-105.3(4)
C(32)-C(27)-C(28)-C(29)	0.9(8)
C(10)-C(27)-C(28)-C(29)	179.7(5)
C(27)-C(28)-C(29)-C(30)	-0.9(9)
C(32A)-C(27)-C(28A)-C(29A)	-3.6(7)
C(10)-C(27)-C(28A)-C(29A)	180.0(4)
C(27)-C(28A)-C(29A)-C(30)	-0.1(9)
C(28A)-C(29A)-C(30)-C(31A)	4.6(8)
C(28)-C(29)-C(30)-C(31)	0.7(8)
C(29)-C(30)-C(31)-C(32)	-0.6(9)
C(28)-C(27)-C(32)-C(31)	-0.8(8)
C(10)-C(27)-C(32)-C(31)	-179.5(5)
C(30)-C(31)-C(32)-C(27)	0.7(10)
C(29A)-C(30)-C(31A)-C(32A)	-5.3(9)
C(30)-C(31A)-C(32A)-C(27)	1.5(11)
C(28A)-C(27)-C(32A)-C(31A)	2.8(9)
C(10)-C(27)-C(32A)-C(31A)	179.4(6)
C(14)-C(15)-C(33)-C(38)	121.2(2)
C(16)-C(15)-C(33)-C(38)	-60.4(3)
C(14)-C(15)-C(33)-C(34)	-59.1(2)
C(16)-C(15)-C(33)-C(34)	119.3(2)
C(38)-C(33)-C(34)-C(35)	0.3(3)
C(15)-C(33)-C(34)-C(35)	-179.40(17)
C(33)-C(34)-C(35)-C(36)	0.5(3)
C(34)-C(35)-C(36)-C(37)	-0.8(3)
C(35)-C(36)-C(37)-C(38)	0.2(3)
C(36)-C(37)-C(38)-C(33)	0.6(3)
C(34)-C(33)-C(38)-C(37)	-0.8(3)
C(15)-C(33)-C(38)-C(37)	178.83(18)
C(1)-C(20)-C(39)-C(44)	-114.1(2)
C(19)-C(20)-C(39)-C(44)	66.4(2)
C(1)-C(20)-C(39)-C(40)	67.2(2)
C(19)-C(20)-C(39)-C(40)	-112.3(2)
C(44)-C(39)-C(40)-C(41)	-1.4(3)
C(20)-C(39)-C(40)-C(41)	177.30(17)
C(39)-C(40)-C(41)-C(42)	0.2(3)

C(40)-C(41)-C(42)-C(43)	1.2(3)
C(41)-C(42)-C(43)-C(44)	-1.4(3)
C(40)-C(39)-C(44)-C(43)	1.2(3)
C(20)-C(39)-C(44)-C(43)	-177.45(18)
C(42)-C(43)-C(44)-C(39)	0.1(3)
O(1)-N(5)-C(45)-C(46)	75.2(3)
Fe(1)-N(5)-C(45)-C(46)	-95.2(2)
O(1)-N(5)-C(45)-C(50)	-104.7(3)
Fe(1)-N(5)-C(45)-C(50)	84.9(2)
C(50)-C(45)-C(46)-C(47)	-0.6(3)
N(5)-C(45)-C(46)-C(47)	179.53(19)
C(45)-C(46)-C(47)-C(48)	0.3(3)
C(46)-C(47)-C(48)-C(49)	0.5(3)
C(47)-C(48)-C(49)-C(50)	-1.0(3)
C(48)-C(49)-C(50)-C(45)	0.7(3)
C(46)-C(45)-C(50)-C(49)	0.1(3)
N(5)-C(45)-C(50)-C(49)	179.97(19)
O(2)-N(6)-C(51)-C(52)	67.7(3)
Fe(1)-N(6)-C(51)-C(52)	-92.0(2)
O(2)-N(6)-C(51)-C(56)	-114.2(3)
Fe(1)-N(6)-C(51)-C(56)	86.1(2)
C(56)-C(51)-C(52)-C(53)	-0.5(3)
N(6)-C(51)-C(52)-C(53)	177.62(18)
C(51)-C(52)-C(53)-C(54)	0.6(3)
C(52)-C(53)-C(54)-C(55)	0.0(3)
C(53)-C(54)-C(55)-C(56)	-0.6(3)
C(52)-C(51)-C(56)-C(55)	-0.1(3)
N(6)-C(51)-C(56)-C(55)	-178.22(19)
C(54)-C(55)-C(56)-C(51)	0.7(3)
C(60)-N(7)-C(57)-C(76)	-175.06(18)
Fe(2)-N(7)-C(57)-C(76)	5.4(3)
C(60)-N(7)-C(57)-C(58)	1.5(2)
Fe(2)-N(7)-C(57)-C(58)	-178.03(12)
N(7)-C(57)-C(58)-C(59)	-1.6(2)
C(76)-C(57)-C(58)-C(59)	175.09(18)
C(57)-C(58)-C(59)-C(60)	0.9(2)
C(57)-N(7)-C(60)-C(61)	-179.32(18)
Fe(2)-N(7)-C(60)-C(61)	0.2(3)
C(57)-N(7)-C(60)-C(59)	-0.9(2)
Fe(2)-N(7)-C(60)-C(59)	178.62(13)
C(58)-C(59)-C(60)-N(7)	0.0(2)
C(58)-C(59)-C(60)-C(61)	178.42(18)
N(7)-C(60)-C(61)-C(62)	4.9(3)
C(59)-C(60)-C(61)-C(62)	-173.30(18)
N(7)-C(60)-C(61)-C(77)	-175.62(17)
C(59)-C(60)-C(61)-C(77)	6.2(3)
C(65)-N(8)-C(62)-C(61)	178.07(18)
Fe(2)-N(8)-C(62)-C(61)	-12.0(3)
C(65)-N(8)-C(62)-C(63)	-0.5(2)
Fe(2)-N(8)-C(62)-C(63)	169.40(13)

C(60)-C(61)-C(62)-N(8)	1.4(3)
C(77)-C(61)-C(62)-N(8)	-178.09(17)
C(60)-C(61)-C(62)-C(63)	179.79(18)
C(77)-C(61)-C(62)-C(63)	0.3(3)
N(8)-C(62)-C(63)-C(64)	1.5(2)
C(61)-C(62)-C(63)-C(64)	-177.11(18)
C(62)-C(63)-C(64)-C(65)	-1.8(2)
C(62)-N(8)-C(65)-C(66)	-179.22(19)
Fe(2)-N(8)-C(65)-C(66)	11.0(3)
C(62)-N(8)-C(65)-C(64)	-0.6(2)
Fe(2)-N(8)-C(65)-C(64)	-170.37(13)
C(63)-C(64)-C(65)-N(8)	1.6(2)
C(63)-C(64)-C(65)-C(66)	-179.79(19)
N(8)-C(65)-C(66)-C(67)	-7.7(3)
C(64)-C(65)-C(66)-C(67)	173.86(19)
N(8)-C(65)-C(66)-C(83)	165.1(6)
C(64)-C(65)-C(66)-C(83)	-13.3(6)
N(8)-C(65)-C(66)-C(83A)	177.1(6)
C(64)-C(65)-C(66)-C(83A)	-1.3(6)
C(70)-N(9)-C(67)-C(66)	-176.87(19)
Fe(2)-N(9)-C(67)-C(66)	2.7(3)
C(70)-N(9)-C(67)-C(68)	0.8(2)
Fe(2)-N(9)-C(67)-C(68)	-179.56(14)
C(65)-C(66)-C(67)-N(9)	0.5(3)
C(83)-C(66)-C(67)-N(9)	-172.5(6)
C(83A)-C(66)-C(67)-N(9)	175.4(6)
C(65)-C(66)-C(67)-C(68)	-176.9(2)
C(83)-C(66)-C(67)-C(68)	10.1(7)
C(83A)-C(66)-C(67)-C(68)	-2.0(6)
N(9)-C(67)-C(68)-C(69)	-0.6(2)
C(66)-C(67)-C(68)-C(69)	177.2(2)
C(67)-C(68)-C(69)-C(70)	0.1(2)
C(67)-N(9)-C(70)-C(71)	176.65(19)
Fe(2)-N(9)-C(70)-C(71)	-3.0(3)
C(67)-N(9)-C(70)-C(69)	-0.8(2)
Fe(2)-N(9)-C(70)-C(69)	179.61(13)
C(68)-C(69)-C(70)-N(9)	0.4(2)
C(68)-C(69)-C(70)-C(71)	-177.04(19)
N(9)-C(70)-C(71)-C(72)	5.1(3)
C(69)-C(70)-C(71)-C(72)	-177.84(19)
N(9)-C(70)-C(71)-C(89)	-179.46(17)
C(69)-C(70)-C(71)-C(89)	-2.4(3)
C(75)-N(10)-C(72)-C(71)	171.62(18)
Fe(2)-N(10)-C(72)-C(71)	-11.5(3)
C(75)-N(10)-C(72)-C(73)	-2.48(19)
Fe(2)-N(10)-C(72)-C(73)	174.44(12)
C(70)-C(71)-C(72)-N(10)	2.6(3)
C(89)-C(71)-C(72)-N(10)	-172.95(17)
C(70)-C(71)-C(72)-C(73)	175.87(18)
C(89)-C(71)-C(72)-C(73)	0.4(3)

N(10)-C(72)-C(73)-C(74)	2.0(2)
C(71)-C(72)-C(73)-C(74)	-172.19(18)
C(72)-C(73)-C(74)-C(75)	-0.7(2)
C(72)-N(10)-C(75)-C(76)	-177.93(17)
Fe(2)-N(10)-C(75)-C(76)	5.2(3)
C(72)-N(10)-C(75)-C(74)	2.0(2)
Fe(2)-N(10)-C(75)-C(74)	-174.82(12)
C(73)-C(74)-C(75)-N(10)	-0.8(2)
C(73)-C(74)-C(75)-C(76)	179.14(18)
N(10)-C(75)-C(76)-C(57)	-6.1(3)
C(74)-C(75)-C(76)-C(57)	173.97(18)
N(10)-C(75)-C(76)-C(95)	174.74(17)
C(74)-C(75)-C(76)-C(95)	-5.2(3)
N(7)-C(57)-C(76)-C(75)	0.5(3)
C(58)-C(57)-C(76)-C(75)	-175.58(18)
N(7)-C(57)-C(76)-C(95)	179.75(17)
C(58)-C(57)-C(76)-C(95)	3.6(3)
C(62)-C(61)-C(77)-C(78)	66.6(2)
C(60)-C(61)-C(77)-C(78)	-112.9(2)
C(62)-C(61)-C(77)-C(82)	-110.8(2)
C(60)-C(61)-C(77)-C(82)	69.7(2)
C(82)-C(77)-C(78)-C(79)	0.6(3)
C(61)-C(77)-C(78)-C(79)	-176.91(18)
C(77)-C(78)-C(79)-C(80)	-0.1(3)
C(78)-C(79)-C(80)-C(81)	-0.3(3)
C(79)-C(80)-C(81)-C(82)	0.2(3)
C(80)-C(81)-C(82)-C(77)	0.3(3)
C(78)-C(77)-C(82)-C(81)	-0.7(3)
C(61)-C(77)-C(82)-C(81)	176.81(18)
C(65)-C(66)-C(83)-C(84)	73.6(17)
C(67)-C(66)-C(83)-C(84)	-113.1(14)
C(65)-C(66)-C(83)-C(88)	-105.9(15)
C(67)-C(66)-C(83)-C(88)	67.4(18)
C(88)-C(83)-C(84)-C(85)	3(2)
C(66)-C(83)-C(84)-C(85)	-176.1(13)
C(83)-C(84)-C(85)-C(86)	-2.9(17)
C(84)-C(85)-C(86)-C(87)	1.9(13)
C(85)-C(86)-C(87)-C(88)	-1.6(13)
C(86)-C(87)-C(88)-C(83)	2.2(17)
C(84)-C(83)-C(88)-C(87)	-3(2)
C(66)-C(83)-C(88)-C(87)	176.4(14)
C(65)-C(66)-C(83A)-C(88A)	-115.9(14)
C(67)-C(66)-C(83A)-C(88A)	68.7(17)
C(65)-C(66)-C(83A)-C(84A)	58.7(18)
C(67)-C(66)-C(83A)-C(84A)	-116.6(15)
C(88A)-C(83A)-C(84A)-C(85A)	-2(2)
C(66)-C(83A)-C(84A)-C(85A)	-176.9(14)
C(83A)-C(84A)-C(85A)-C(86A)	0.9(17)
C(84A)-C(85A)-C(86A)-C(87A)	0.2(13)
C(85A)-C(86A)-C(87A)-C(88A)	0.0(13)

C(84A)-C(83A)-C(88A)-C(87A)	3(2)
C(66)-C(83A)-C(88A)-C(87A)	177.5(13)
C(86A)-C(87A)-C(88A)-C(83A)	-1.4(18)
C(70)-C(71)-C(89)-C(90)	-79.1(2)
C(72)-C(71)-C(89)-C(90)	96.6(2)
C(70)-C(71)-C(89)-C(94)	101.1(2)
C(72)-C(71)-C(89)-C(94)	-83.2(2)
C(94)-C(89)-C(90)-C(91)	-0.2(3)
C(71)-C(89)-C(90)-C(91)	179.94(17)
C(89)-C(90)-C(91)-C(92)	0.6(3)
C(90)-C(91)-C(92)-C(93)	-0.2(3)
C(91)-C(92)-C(93)-C(94)	-0.6(3)
C(92)-C(93)-C(94)-C(89)	1.0(3)
C(90)-C(89)-C(94)-C(93)	-0.6(3)
C(71)-C(89)-C(94)-C(93)	179.23(17)
C(75)-C(76)-C(95)-C(100)	87.8(2)
C(57)-C(76)-C(95)-C(100)	-91.5(2)
C(75)-C(76)-C(95)-C(96)	-93.9(2)
C(57)-C(76)-C(95)-C(96)	86.8(2)
C(100)-C(95)-C(96)-C(97)	0.5(3)
C(76)-C(95)-C(96)-C(97)	-177.9(2)
C(95)-C(96)-C(97)-C(98)	-0.8(4)
C(96)-C(97)-C(98)-C(99)	0.5(3)
C(97)-C(98)-C(99)-C(100)	0.2(3)
C(96)-C(95)-C(100)-C(99)	0.1(3)
C(76)-C(95)-C(100)-C(99)	178.49(18)
C(98)-C(99)-C(100)-C(95)	-0.4(3)
O(3)-N(11)-C(101)-C(106)	-128.32(19)
Fe(2)-N(11)-C(101)-C(106)	65.2(2)
O(3)-N(11)-C(101)-C(102)	51.8(2)
Fe(2)-N(11)-C(101)-C(102)	-114.64(18)
C(106)-C(101)-C(102)-C(103)	-1.4(3)
N(11)-C(101)-C(102)-C(103)	178.52(18)
C(101)-C(102)-C(103)-C(104)	1.7(3)
C(102)-C(103)-C(104)-C(105)	-0.8(3)
C(103)-C(104)-C(105)-C(106)	-0.5(3)
C(102)-C(101)-C(106)-C(105)	0.1(3)
N(11)-C(101)-C(106)-C(105)	-179.78(18)
C(104)-C(105)-C(106)-C(101)	0.8(3)
O(4)-C(107)-C(108)-C(109)	43.5(6)
O(4)-C(17A)-C(18A)-C(109)	-26.4(7)
C(107)-C(108)-C(109)-C(110)	-36.4(5)
C(17A)-C(18A)-C(109)-C(110)	19.0(6)
C(108)-C(109)-C(110)-O(4)	18.1(4)
C(18A)-C(109)-C(110)-O(4)	-4.3(4)
C(108)-C(107)-O(4)-C(110)	-34.0(5)
C(108)-C(107)-O(4)-Fe(2)	150.7(4)
C(109)-C(110)-O(4)-C(107)	10.9(4)
C(109)-C(110)-O(4)-C(17A)	-12.6(4)
C(109)-C(110)-O(4)-Fe(2)	-173.82(14)

C(18A)-C(17A)-O(4)-C(110)	25.1(7)
C(18A)-C(17A)-O(4)-Fe(2)	-172.6(4)
C(114)-O(10)-C(111)-C(112)	-23.8(11)
O(10)-C(111)-C(112)-C(113)	39.1(10)
C(111)-C(112)-C(113)-C(114)	-34.1(11)
C(111)-O(10)-C(114)-C(113)	3.0(14)
C(112)-C(113)-C(114)-O(10)	19.7(13)
C(118)-O(11)-C(115)-C(116)	22.4(13)
O(11)-C(115)-C(116)-C(117)	-23.4(17)
C(115)-C(116)-C(117)-C(118)	15.3(17)
C(115)-O(11)-C(118)-C(117)	-12.6(10)
C(116)-C(117)-C(118)-O(11)	-1.9(13)

Table S7. Crystal data and structure refinement for [Fe(TPP)(THF)(iPrNO)].

Empirical formula	$C_{51}H_{43}FeN_5O_2$
Formula weight	813.75
Temperature	85(2) K
Wavelength	1.54178 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 13.4128(9) Å alpha = 90 deg. b = 15.7751(10) Å beta = 94.719(7) deg. c = 18.9793(13) Å gamma = 90 deg.
Volume	4002.2(5) $Å^3$
Z, Calculated density	4, 1.351 Mg/m^3
Absorption coefficient	3.407 mm^{-1}
F(000)	1704
Crystal size	0.24 x 0.14 x 0.12 mm
Theta range for data collection	4.34 to 68.19 deg.
Limiting indices	-16<=h<=16, -18<=k<=18, -22<=l<=22
Reflections collected / unique	103181 / 7302 [R(int) = 0.0540]
Completeness to theta =	68.19 99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6853 and 0.4952
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7302 / 124 / 571
Goodness-of-fit on F^2	1.053
Final R indices [I>2sigma(I)]	R1 = 0.0612, wR2 = 0.1627
R indices (all data)	R1 = 0.0621, wR2 = 0.1635
Largest diff. peak and hole	1.775 and -0.556 e.$Å^{-3}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Fe(TPP)(THF)(iPrNO)]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	2599(1)	5421(1)	2384(1)	17(1)
O(1)	2460(2)	4626(1)	1129(1)	41(1)
N(1)	1679(1)	4907(1)	3053(1)	18(1)
N(2)	3494(1)	4416(1)	2512(1)	19(1)
N(3)	3557(1)	5970(1)	1782(1)	18(1)
N(4)	1717(1)	6445(1)	2287(1)	18(1)
N(5)	1974(2)	4926(1)	1580(1)	24(1)
C(1)	1821(2)	4169(2)	3434(1)	20(1)
C(2)	2616(2)	3609(2)	3389(1)	21(1)
C(3)	3360(2)	3712(2)	2923(1)	20(1)
C(4)	4098(2)	3082(2)	2807(1)	24(1)
C(5)	4693(2)	3405(2)	2334(1)	23(1)
C(6)	4333(2)	4247(2)	2164(1)	19(1)
C(7)	4800(2)	4816(2)	1739(1)	19(1)
C(8)	4434(2)	5624(2)	1574(1)	19(1)
C(9)	4913(2)	6218(2)	1136(1)	21(1)
C(10)	4314(2)	6900(2)	1054(1)	21(1)
C(11)	3470(2)	6752(2)	1454(1)	18(1)
C(12)	2666(2)	7310(2)	1490(1)	20(1)
C(13)	1860(2)	7165(2)	1893(1)	19(1)
C(14)	1051(2)	7753(2)	1960(1)	23(1)
C(15)	417(2)	7389(2)	2383(1)	24(1)
C(16)	825(2)	6573(2)	2588(1)	20(1)
C(17)	378(2)	6010(2)	3033(1)	19(1)
C(18)	795(2)	5245(2)	3258(1)	19(1)
C(19)	380(2)	4700(2)	3767(1)	22(1)
C(20)	1023(2)	4048(2)	3888(1)	22(1)
C(21)	2708(2)	2867(2)	3883(1)	25(1)
C(22)	2075(2)	2173(2)	3814(2)	38(1)
C(23)	2198(2)	1493(2)	4286(2)	48(1)
C(24)	2931(2)	1513(2)	4835(2)	43(1)
C(25)	3554(2)	2200(2)	4917(2)	36(1)
C(26)	3447(2)	2876(2)	4445(1)	28(1)
C(27)	5760(2)	4551(1)	1448(1)	20(1)
C(28)	6630(2)	4440(2)	1895(1)	28(1)
C(29)	7516(2)	4191(2)	1629(2)	34(1)
C(30)	7554(2)	4070(2)	908(2)	30(1)
C(31)	6702(2)	4184(2)	456(1)	26(1)
C(32)	5810(2)	4411(2)	727(1)	21(1)
C(33)	2640(2)	8111(2)	1058(1)	21(1)
C(34)	3353(2)	8750(2)	1190(1)	28(1)
C(35)	3289(2)	9500(2)	806(2)	35(1)

C(36)	2517(2)	9627(2)	286(2)	35(1)
C(37)	1807(2)	9000(2)	147(2)	34(1)
C(38)	1872(2)	8248(2)	526(1)	29(1)
C(39)	-622(2)	6252(2)	3268(1)	21(1)
C(40)	-711(2)	6679(2)	3898(2)	34(1)
C(41)	-1636(2)	6930(2)	4095(2)	36(1)
C(42)	-2487(2)	6763(2)	3657(2)	35(1)
C(43)	-2414(2)	6324(2)	3035(2)	45(1)
C(44)	-1482(2)	6061(2)	2847(2)	37(1)
C(45)	880(2)	4917(2)	1435(2)	43(1)
C(46)	590(3)	5488(3)	827(2)	70(1)
C(47)	557(3)	4016(3)	1296(2)	58(1)
O(2)	3371(1)	5973(1)	3270(1)	32(1)
C(48)	3048(3)	6732(3)	3638(2)	44(1)
C(49)	3838(3)	6932(3)	4219(2)	42(1)
C(50)	4641(3)	6224(3)	4157(2)	40(1)
C(51)	4458(3)	5957(3)	3399(2)	34(1)
O(2A)	3371(1)	5973(1)	3270(1)	32(1)
C(48A)	3191(10)	6826(8)	3510(9)	41(1)
C(49A)	3993(11)	6937(11)	4127(9)	51(1)
C(50A)	4842(8)	6510(8)	3682(10)	58(2)
C(51A)	4295(9)	5657(8)	3633(10)	45(2)

Table S9. Bond lengths [Å] and angles [°] for [Fe(TPP)(THF)(iPrNO)].

Fe(1)-N(5)	1.853(2)
Fe(1)-N(3)	1.988(2)
Fe(1)-N(2)	1.991(2)
Fe(1)-N(4)	2.002(2)
Fe(1)-N(1)	2.012(2)
Fe(1)-O(2)	2.0899(19)
O(1)-N(5)	1.212(3)
N(1)-C(1)	1.375(3)
N(1)-C(18)	1.385(3)
N(2)-C(3)	1.377(3)
N(2)-C(6)	1.379(3)
N(3)-C(11)	1.381(3)
N(3)-C(8)	1.384(3)
N(4)-C(13)	1.381(3)
N(4)-C(16)	1.382(3)
N(5)-C(45)	1.470(4)
C(1)-C(2)	1.392(3)
C(1)-C(20)	1.442(3)
C(2)-C(3)	1.397(3)
C(2)-C(21)	1.499(3)
C(3)-C(4)	1.432(3)
C(4)-C(5)	1.348(4)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.441(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.389(3)
C(7)-C(8)	1.393(3)
C(7)-C(27)	1.501(3)
C(8)-C(9)	1.437(3)
C(9)-C(10)	1.345(3)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.434(3)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.399(3)
C(12)-C(13)	1.394(3)
C(12)-C(33)	1.504(3)
C(13)-C(14)	1.441(3)
C(14)-C(15)	1.345(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.440(3)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.394(3)
C(17)-C(18)	1.384(3)
C(17)-C(39)	1.497(3)
C(18)-C(19)	1.439(3)
C(19)-C(20)	1.349(3)
C(19)-H(19A)	0.9500
C(20)-H(20A)	0.9500

C(21)-C(22)	1.385(4)
C(21)-C(26)	1.395(4)
C(22)-C(23)	1.399(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.373(5)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.369(5)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.392(4)
C(25)-H(25A)	0.9500
C(26)-H(26A)	0.9500
C(27)-C(32)	1.392(3)
C(27)-C(28)	1.398(3)
C(28)-C(29)	1.386(4)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.386(4)
C(29)-H(29A)	0.9500
C(30)-C(31)	1.383(4)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.388(4)
C(31)-H(31A)	0.9500
C(32)-H(32A)	0.9500
C(33)-C(34)	1.397(4)
C(33)-C(38)	1.399(4)
C(34)-C(35)	1.388(4)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.386(4)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.383(4)
C(36)-H(36A)	0.9500
C(37)-C(38)	1.387(4)
C(37)-H(37A)	0.9500
C(38)-H(38A)	0.9500
C(39)-C(44)	1.382(4)
C(39)-C(40)	1.386(4)
C(40)-C(41)	1.383(4)
C(40)-H(40A)	0.9500
C(41)-C(42)	1.382(4)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.378(4)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.391(4)
C(43)-H(43A)	0.9500
C(44)-H(44A)	0.9500
C(45)-C(46)	1.489(6)
C(45)-C(47)	1.504(5)
C(45)-H(45A)	1.0000
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800

C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
O(2)-C(51)	1.458(4)
O(2)-C(48)	1.470(4)
C(48)-C(49)	1.497(6)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(50)	1.564(5)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-C(51)	1.499(5)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(48A)-C(49A)	1.533(14)
C(48A)-H(48C)	0.9900
C(48A)-H(48D)	0.9900
C(49A)-C(50A)	1.619(16)
C(49A)-H(49C)	0.9900
C(49A)-H(49D)	0.9900
C(50A)-C(51A)	1.532(13)
C(50A)-H(50C)	0.9900
C(50A)-H(50D)	0.9900
C(51A)-H(51C)	0.9900
C(51A)-H(51D)	0.9900

N(5)-Fe(1)-N(3)	88.81(8)
N(5)-Fe(1)-N(2)	89.59(9)
N(3)-Fe(1)-N(2)	90.32(8)
N(5)-Fe(1)-N(4)	92.28(8)
N(3)-Fe(1)-N(4)	89.99(8)
N(2)-Fe(1)-N(4)	178.11(8)
N(5)-Fe(1)-N(1)	95.23(8)
N(3)-Fe(1)-N(1)	175.96(8)
N(2)-Fe(1)-N(1)	89.83(8)
N(4)-Fe(1)-N(1)	89.74(8)
N(5)-Fe(1)-O(2)	177.16(8)
N(3)-Fe(1)-O(2)	88.84(8)
N(2)-Fe(1)-O(2)	88.83(8)
N(4)-Fe(1)-O(2)	89.31(8)
N(1)-Fe(1)-O(2)	87.13(8)
C(1)-N(1)-C(18)	105.27(19)
C(1)-N(1)-Fe(1)	127.35(15)
C(18)-N(1)-Fe(1)	127.29(16)
C(3)-N(2)-C(6)	105.35(19)
C(3)-N(2)-Fe(1)	127.33(16)
C(6)-N(2)-Fe(1)	127.12(16)
C(11)-N(3)-C(8)	105.44(19)

C(11)-N(3)-Fe(1)	127.80(15)
C(8)-N(3)-Fe(1)	126.70(16)
C(13)-N(4)-C(16)	105.47(19)
C(13)-N(4)-Fe(1)	127.34(16)
C(16)-N(4)-Fe(1)	127.18(16)
O(1)-N(5)-C(45)	116.8(2)
O(1)-N(5)-Fe(1)	120.79(18)
C(45)-N(5)-Fe(1)	122.33(18)
N(1)-C(1)-C(2)	125.4(2)
N(1)-C(1)-C(20)	110.4(2)
C(2)-C(1)-C(20)	124.2(2)
C(1)-C(2)-C(3)	123.7(2)
C(1)-C(2)-C(21)	118.8(2)
C(3)-C(2)-C(21)	117.4(2)
N(2)-C(3)-C(2)	125.8(2)
N(2)-C(3)-C(4)	110.4(2)
C(2)-C(3)-C(4)	123.8(2)
C(5)-C(4)-C(3)	107.2(2)
C(5)-C(4)-H(4A)	126.4
C(3)-C(4)-H(4A)	126.4
C(4)-C(5)-C(6)	107.0(2)
C(4)-C(5)-H(5A)	126.5
C(6)-C(5)-H(5A)	126.5
N(2)-C(6)-C(7)	125.3(2)
N(2)-C(6)-C(5)	110.0(2)
C(7)-C(6)-C(5)	124.6(2)
C(6)-C(7)-C(8)	123.7(2)
C(6)-C(7)-C(27)	118.4(2)
C(8)-C(7)-C(27)	117.9(2)
N(3)-C(8)-C(7)	126.0(2)
N(3)-C(8)-C(9)	109.8(2)
C(7)-C(8)-C(9)	124.1(2)
C(10)-C(9)-C(8)	107.3(2)
C(10)-C(9)-H(9A)	126.4
C(8)-C(9)-H(9A)	126.4
C(9)-C(10)-C(11)	107.4(2)
C(9)-C(10)-H(10A)	126.3
C(11)-C(10)-H(10A)	126.3
N(3)-C(11)-C(12)	125.3(2)
N(3)-C(11)-C(10)	110.0(2)
C(12)-C(11)-C(10)	124.6(2)
C(13)-C(12)-C(11)	124.0(2)
C(13)-C(12)-C(33)	117.0(2)
C(11)-C(12)-C(33)	119.1(2)
N(4)-C(13)-C(12)	125.5(2)
N(4)-C(13)-C(14)	110.1(2)
C(12)-C(13)-C(14)	124.4(2)
C(15)-C(14)-C(13)	107.2(2)
C(15)-C(14)-H(14A)	126.4
C(13)-C(14)-H(14A)	126.4

C(14)-C(15)-C(16)	107.3(2)
C(14)-C(15)-H(15A)	126.3
C(16)-C(15)-H(15A)	126.3
N(4)-C(16)-C(17)	126.0(2)
N(4)-C(16)-C(15)	110.0(2)
C(17)-C(16)-C(15)	124.1(2)
C(18)-C(17)-C(16)	124.1(2)
C(18)-C(17)-C(39)	118.6(2)
C(16)-C(17)-C(39)	117.3(2)
C(17)-C(18)-N(1)	125.6(2)
C(17)-C(18)-C(19)	124.1(2)
N(1)-C(18)-C(19)	110.3(2)
C(20)-C(19)-C(18)	107.0(2)
C(20)-C(19)-H(19A)	126.5
C(18)-C(19)-H(19A)	126.5
C(19)-C(20)-C(1)	107.1(2)
C(19)-C(20)-H(20A)	126.5
C(1)-C(20)-H(20A)	126.5
C(22)-C(21)-C(26)	118.2(2)
C(22)-C(21)-C(2)	122.6(2)
C(26)-C(21)-C(2)	119.2(2)
C(21)-C(22)-C(23)	120.4(3)
C(21)-C(22)-H(22A)	119.8
C(23)-C(22)-H(22A)	119.8
C(24)-C(23)-C(22)	120.5(3)
C(24)-C(23)-H(23A)	119.8
C(22)-C(23)-H(23A)	119.8
C(25)-C(24)-C(23)	119.8(3)
C(25)-C(24)-H(24A)	120.1
C(23)-C(24)-H(24A)	120.1
C(24)-C(25)-C(26)	120.3(3)
C(24)-C(25)-H(25A)	119.9
C(26)-C(25)-H(25A)	119.9
C(25)-C(26)-C(21)	120.8(3)
C(25)-C(26)-H(26A)	119.6
C(21)-C(26)-H(26A)	119.6
C(32)-C(27)-C(28)	118.1(2)
C(32)-C(27)-C(7)	121.2(2)
C(28)-C(27)-C(7)	120.7(2)
C(29)-C(28)-C(27)	120.8(2)
C(29)-C(28)-H(28A)	119.6
C(27)-C(28)-H(28A)	119.6
C(30)-C(29)-C(28)	120.1(2)
C(30)-C(29)-H(29A)	120.0
C(28)-C(29)-H(29A)	120.0
C(31)-C(30)-C(29)	119.9(2)
C(31)-C(30)-H(30A)	120.1
C(29)-C(30)-H(30A)	120.1
C(30)-C(31)-C(32)	119.8(2)
C(30)-C(31)-H(31A)	120.1

C(32)-C(31)-H(31A)	120.1
C(31)-C(32)-C(27)	121.2(2)
C(31)-C(32)-H(32A)	119.4
C(27)-C(32)-H(32A)	119.4
C(34)-C(33)-C(38)	118.0(2)
C(34)-C(33)-C(12)	121.6(2)
C(38)-C(33)-C(12)	120.3(2)
C(35)-C(34)-C(33)	120.6(3)
C(35)-C(34)-H(34A)	119.7
C(33)-C(34)-H(34A)	119.7
C(36)-C(35)-C(34)	120.5(3)
C(36)-C(35)-H(35A)	119.8
C(34)-C(35)-H(35A)	119.8
C(37)-C(36)-C(35)	119.6(3)
C(37)-C(36)-H(36A)	120.2
C(35)-C(36)-H(36A)	120.2
C(36)-C(37)-C(38)	120.0(3)
C(36)-C(37)-H(37A)	120.0
C(38)-C(37)-H(37A)	120.0
C(37)-C(38)-C(33)	121.2(3)
C(37)-C(38)-H(38A)	119.4
C(33)-C(38)-H(38A)	119.4
C(44)-C(39)-C(40)	118.5(2)
C(44)-C(39)-C(17)	119.9(2)
C(40)-C(39)-C(17)	121.6(2)
C(41)-C(40)-C(39)	121.1(3)
C(41)-C(40)-H(40A)	119.5
C(39)-C(40)-H(40A)	119.5
C(42)-C(41)-C(40)	119.8(3)
C(42)-C(41)-H(41A)	120.1
C(40)-C(41)-H(41A)	120.1
C(43)-C(42)-C(41)	119.8(3)
C(43)-C(42)-H(42A)	120.1
C(41)-C(42)-H(42A)	120.1
C(42)-C(43)-C(44)	119.9(3)
C(42)-C(43)-H(43A)	120.0
C(44)-C(43)-H(43A)	120.0
C(39)-C(44)-C(43)	120.8(3)
C(39)-C(44)-H(44A)	119.6
C(43)-C(44)-H(44A)	119.6
N(5)-C(45)-C(46)	109.4(3)
N(5)-C(45)-C(47)	108.1(3)
C(46)-C(45)-C(47)	112.5(3)
N(5)-C(45)-H(45A)	108.9
C(46)-C(45)-H(45A)	108.9
C(47)-C(45)-H(45A)	108.9
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5

H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(45)-C(47)-H(47A)	109.5
C(45)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(45)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(51)-O(2)-C(48)	105.2(3)
C(51)-O(2)-Fe(1)	123.47(18)
C(48)-O(2)-Fe(1)	125.2(2)
O(2)-C(48)-C(49)	107.7(3)
O(2)-C(48)-H(48A)	110.2
C(49)-C(48)-H(48A)	110.2
O(2)-C(48)-H(48B)	110.2
C(49)-C(48)-H(48B)	110.2
H(48A)-C(48)-H(48B)	108.5
C(48)-C(49)-C(50)	104.1(3)
C(48)-C(49)-H(49A)	110.9
C(50)-C(49)-H(49A)	110.9
C(48)-C(49)-H(49B)	110.9
C(50)-C(49)-H(49B)	110.9
H(49A)-C(49)-H(49B)	109.0
C(51)-C(50)-C(49)	102.3(3)
C(51)-C(50)-H(50A)	111.3
C(49)-C(50)-H(50A)	111.3
C(51)-C(50)-H(50B)	111.3
C(49)-C(50)-H(50B)	111.3
H(50A)-C(50)-H(50B)	109.2
O(2)-C(51)-C(50)	103.9(3)
O(2)-C(51)-H(51A)	111.0
C(50)-C(51)-H(51A)	111.0
O(2)-C(51)-H(51B)	111.0
C(50)-C(51)-H(51B)	111.0
H(51A)-C(51)-H(51B)	109.0
C(49A)-C(48A)-H(48C)	111.2
C(49A)-C(48A)-H(48D)	111.2
H(48C)-C(48A)-H(48D)	109.1
C(48A)-C(49A)-C(50A)	91.9(10)
C(48A)-C(49A)-H(49C)	113.3
C(50A)-C(49A)-H(49C)	113.3
C(48A)-C(49A)-H(49D)	113.3
C(50A)-C(49A)-H(49D)	113.3
H(49C)-C(49A)-H(49D)	110.6
C(51A)-C(50A)-C(49A)	92.5(10)
C(51A)-C(50A)-H(50C)	113.2
C(49A)-C(50A)-H(50C)	113.2
C(51A)-C(50A)-H(50D)	113.2
C(49A)-C(50A)-H(50D)	113.2
H(50C)-C(50A)-H(50D)	110.6

C(50A)-C(51A)-H(51C)	112.5
C(50A)-C(51A)-H(51D)	112.5
H(51C)-C(51A)-H(51D)	110.0

Table S10. Anisotropic displacement parameters ($Å^2$ x 10^3) for [Fe(TPP)(THF)(iPrNO)]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U11 + ... + 2hkabU12]$.

	U11	U22	U33	U23	U13	U12
Fe(1)	14(1)	15(1)	21(1)	-2(1)	4(1)	1(1)
O(1)	36(1)	47(1)	41(1)	-11(1)	8(1)	-3(1)
N(1)	15(1)	19(1)	21(1)	-1(1)	3(1)	3(1)
N(2)	16(1)	22(1)	20(1)	2(1)	5(1)	2(1)
N(3)	14(1)	19(1)	22(1)	0(1)	3(1)	3(1)
N(4)	16(1)	19(1)	20(1)	-2(1)	4(1)	0(1)
N(5)	22(1)	24(1)	28(1)	7(1)	13(1)	8(1)
C(1)	17(1)	20(1)	23(1)	0(1)	3(1)	1(1)
C(2)	19(1)	22(1)	23(1)	3(1)	3(1)	3(1)
C(3)	17(1)	22(1)	22(1)	4(1)	2(1)	2(1)
C(4)	22(1)	22(1)	27(1)	5(1)	4(1)	6(1)
C(5)	16(1)	25(1)	29(1)	3(1)	6(1)	8(1)
C(6)	16(1)	22(1)	20(1)	1(1)	3(1)	4(1)
C(7)	15(1)	24(1)	19(1)	0(1)	3(1)	1(1)
C(8)	14(1)	23(1)	22(1)	0(1)	3(1)	0(1)
C(9)	17(1)	23(1)	23(1)	0(1)	6(1)	-1(1)
C(10)	21(1)	19(1)	22(1)	1(1)	4(1)	-4(1)
C(11)	18(1)	18(1)	19(1)	0(1)	1(1)	-2(1)
C(12)	20(1)	18(1)	20(1)	1(1)	1(1)	0(1)
C(13)	18(1)	19(1)	22(1)	-1(1)	2(1)	2(1)
C(14)	22(1)	19(1)	29(1)	0(1)	4(1)	5(1)
C(15)	20(1)	23(1)	28(1)	-2(1)	6(1)	8(1)
C(16)	16(1)	21(1)	22(1)	-3(1)	4(1)	3(1)
C(17)	16(1)	21(1)	20(1)	-4(1)	5(1)	2(1)
C(18)	15(1)	21(1)	21(1)	-4(1)	4(1)	0(1)
C(19)	17(1)	24(1)	24(1)	-2(1)	7(1)	0(1)
C(20)	20(1)	22(1)	26(1)	4(1)	7(1)	0(1)
C(21)	21(1)	22(1)	34(1)	7(1)	13(1)	7(1)
C(22)	23(1)	29(1)	63(2)	11(1)	9(1)	1(1)
C(23)	32(2)	30(2)	85(2)	20(2)	29(2)	4(1)
C(24)	42(2)	37(2)	54(2)	21(1)	32(1)	22(1)
C(25)	46(2)	35(1)	28(1)	8(1)	18(1)	23(1)
C(26)	35(1)	27(1)	23(1)	2(1)	11(1)	11(1)
C(27)	16(1)	21(1)	24(1)	2(1)	4(1)	2(1)
C(28)	17(1)	44(2)	23(1)	2(1)	1(1)	2(1)
C(29)	17(1)	53(2)	30(1)	5(1)	0(1)	7(1)

C(30)	18(1)	38(2)	36(1)	0(1)	9(1)	4(1)
C(31)	22(1)	30(1)	26(1)	-2(1)	8(1)	0(1)
C(32)	17(1)	23(1)	23(1)	0(1)	1(1)	0(1)
C(33)	23(1)	19(1)	23(1)	2(1)	6(1)	4(1)
C(34)	31(1)	22(1)	30(1)	1(1)	0(1)	-2(1)
C(35)	44(2)	22(1)	38(2)	4(1)	2(1)	-7(1)
C(36)	46(2)	22(1)	38(2)	10(1)	5(1)	3(1)
C(37)	33(1)	32(1)	35(1)	10(1)	-1(1)	6(1)
C(38)	27(1)	26(1)	33(1)	6(1)	3(1)	0(1)
C(39)	20(1)	19(1)	26(1)	2(1)	9(1)	4(1)
C(40)	29(1)	43(2)	30(1)	-10(1)	4(1)	10(1)
C(41)	37(2)	40(2)	33(1)	-7(1)	13(1)	10(1)
C(42)	23(1)	37(2)	46(2)	0(1)	15(1)	7(1)
C(43)	19(1)	61(2)	55(2)	-22(2)	9(1)	-2(1)
C(44)	21(1)	47(2)	42(2)	-18(1)	7(1)	-2(1)
C(45)	28(1)	59(2)	43(2)	-18(2)	2(1)	-1(1)
C(46)	69(2)	72(2)	63(2)	-31(2)	-31(2)	32(2)
C(47)	45(2)	66(2)	63(2)	-4(2)	0(2)	-28(2)
O(2)	22(1)	41(1)	33(1)	-3(1)	1(1)	7(1)
C(48)	41(2)	50(2)	42(2)	-6(2)	10(2)	17(2)
C(49)	40(2)	43(2)	45(2)	-16(2)	15(2)	3(2)
C(50)	34(2)	47(2)	36(2)	-14(2)	-7(1)	6(2)
C(51)	26(2)	40(2)	36(2)	-11(2)	-3(1)	2(2)
O(2A)	22(1)	41(1)	33(1)	-3(1)	1(1)	7(1)
C(48A)	38(1)	34(1)	48(2)	-4(2)	-11(2)	0(2)
C(49A)	43(2)	43(2)	62(3)	-6(2)	-20(1)	-4(2)
C(50A)	36(1)	46(2)	88(5)	-7(3)	-15(2)	-3(1)
C(51A)	26(2)	44(2)	62(5)	-3(2)	-14(3)	2(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for [Fe(TPP)(THF)(iPrNO)].

	x	y	z	U(eq)
H(4A)	4157	2539	3022	28
H(5A)	5244	3130	2149	28
H(9A)	5537	6143	942	25
H(10A)	4428	7390	780	25
H(14A)	980	8296	1746	28
H(15A)	-188	7627	2520	28
H(19A)	-232	4782	3977	26
H(20A)	962	3596	4212	27
H(22A)	1555	2158	3443	46
H(23A)	1770	1013	4227	58
H(24A)	3006	1052	5157	51
H(25A)	4061	2215	5296	43
H(26A)	3883	3350	4507	33
H(28A)	6615	4535	2389	34
H(29A)	8098	4102	1940	40
H(30A)	8165	3910	724	36
H(31A)	6727	4106	-38	31
H(32A)	5223	4471	416	25
H(34A)	3886	8670	1545	33
H(35A)	3778	9929	901	42
H(36A)	2475	10142	25	42
H(37A)	1275	9085	-208	40
H(38A)	1387	7818	423	34
H(40A)	-128	6802	4199	41
H(41A)	-1686	7216	4531	44
H(42A)	-3122	6950	3783	42
H(43A)	-2998	6202	2736	54
H(44A)	-1437	5746	2424	44
H(45A)	568	5130	1862	52
H(46A)	730	6077	966	105
H(46B)	-126	5423	688	105
H(46C)	975	5339	428	105
H(47A)	-166	3968	1333	88
H(47B)	911	3643	1646	88
H(47C)	714	3850	821	88
H(48A)	2401	6625	3837	53
H(48B)	2964	7214	3305	53
H(49A)	3560	6913	4686	51
H(49B)	4127	7501	4151	51
H(50A)	5327	6450	4258	47
H(50B)	4538	5747	4482	47
H(51A)	4773	6357	3083	41
H(51B)	4723	5381	3327	41
H(48C)	2511	6881	3670	49

H(48D)	3276	7246	3132	49
H(49C)	3854	6608	4552	61
H(49D)	4131	7538	4250	61
H(50C)	4896	6780	3216	69
H(50D)	5506	6479	3950	69
H(51C)	4634	5236	3348	54
H(51D)	4192	5417	4104	54

Table S12. Torsion angles [°] for [Fe(TPP)(THF)(iPrNO)].

N(5)-Fe(1)-N(1)-C(1)	94.0(2)
N(3)-Fe(1)-N(1)-C(1)	-87.6(11)
N(2)-Fe(1)-N(1)-C(1)	4.4(2)
N(4)-Fe(1)-N(1)-C(1)	-173.7(2)
O(2)-Fe(1)-N(1)-C(1)	-84.4(2)
N(5)-Fe(1)-N(1)-C(18)	-89.9(2)
N(3)-Fe(1)-N(1)-C(18)	88.5(11)
N(2)-Fe(1)-N(1)-C(18)	-179.47(19)
N(4)-Fe(1)-N(1)-C(18)	2.37(19)
O(2)-Fe(1)-N(1)-C(18)	91.69(19)
N(5)-Fe(1)-N(2)-C(3)	-94.3(2)
N(3)-Fe(1)-N(2)-C(3)	176.9(2)
N(4)-Fe(1)-N(2)-C(3)	78(3)
N(1)-Fe(1)-N(2)-C(3)	1.0(2)
O(2)-Fe(1)-N(2)-C(3)	88.1(2)
N(5)-Fe(1)-N(2)-C(6)	79.8(2)
N(3)-Fe(1)-N(2)-C(6)	-9.0(2)
N(4)-Fe(1)-N(2)-C(6)	-108(3)
N(1)-Fe(1)-N(2)-C(6)	175.0(2)
O(2)-Fe(1)-N(2)-C(6)	-97.8(2)
N(5)-Fe(1)-N(3)-C(11)	90.2(2)
N(2)-Fe(1)-N(3)-C(11)	179.77(19)
N(4)-Fe(1)-N(3)-C(11)	-2.10(19)
N(1)-Fe(1)-N(3)-C(11)	-88.2(11)
O(2)-Fe(1)-N(3)-C(11)	-91.41(19)
N(5)-Fe(1)-N(3)-C(8)	-86.4(2)
N(2)-Fe(1)-N(3)-C(8)	3.20(19)
N(4)-Fe(1)-N(3)-C(8)	-178.67(19)
N(1)-Fe(1)-N(3)-C(8)	95.2(11)
O(2)-Fe(1)-N(3)-C(8)	92.02(19)
N(5)-Fe(1)-N(4)-C(13)	-86.3(2)
N(3)-Fe(1)-N(4)-C(13)	2.46(19)
N(2)-Fe(1)-N(4)-C(13)	102(3)
N(1)-Fe(1)-N(4)-C(13)	178.43(19)
O(2)-Fe(1)-N(4)-C(13)	91.30(19)
N(5)-Fe(1)-N(4)-C(16)	92.2(2)
N(3)-Fe(1)-N(4)-C(16)	-179.04(19)
N(2)-Fe(1)-N(4)-C(16)	-80(3)
N(1)-Fe(1)-N(4)-C(16)	-3.07(19)
O(2)-Fe(1)-N(4)-C(16)	-90.20(19)
N(3)-Fe(1)-N(5)-O(1)	42.3(2)
N(2)-Fe(1)-N(5)-O(1)	-48.0(2)
N(4)-Fe(1)-N(5)-O(1)	132.2(2)
N(1)-Fe(1)-N(5)-O(1)	-137.8(2)
O(2)-Fe(1)-N(5)-O(1)	8.2(18)
N(3)-Fe(1)-N(5)-C(45)	-134.3(2)
N(2)-Fe(1)-N(5)-C(45)	135.4(2)

N(4)-Fe(1)-N(5)-C(45)	-44.3(2)
N(1)-Fe(1)-N(5)-C(45)	45.6(2)
O(2)-Fe(1)-N(5)-C(45)	-168.4(16)
C(18)-N(1)-C(1)-C(2)	178.9(2)
Fe(1)-N(1)-C(1)-C(2)	-4.3(3)
C(18)-N(1)-C(1)-C(20)	-0.6(3)
Fe(1)-N(1)-C(1)-C(20)	176.15(16)
N(1)-C(1)-C(2)-C(3)	-2.6(4)
C(20)-C(1)-C(2)-C(3)	176.9(2)
N(1)-C(1)-C(2)-C(21)	175.1(2)
C(20)-C(1)-C(2)-C(21)	-5.5(4)
C(6)-N(2)-C(3)-C(2)	177.7(2)
Fe(1)-N(2)-C(3)-C(2)	-7.2(4)
C(6)-N(2)-C(3)-C(4)	-2.4(3)
Fe(1)-N(2)-C(3)-C(4)	172.67(16)
C(1)-C(2)-C(3)-N(2)	8.7(4)
C(21)-C(2)-C(3)-N(2)	-169.0(2)
C(1)-C(2)-C(3)-C(4)	-171.2(2)
C(21)-C(2)-C(3)-C(4)	11.1(4)
N(2)-C(3)-C(4)-C(5)	0.9(3)
C(2)-C(3)-C(4)-C(5)	-179.2(2)
C(3)-C(4)-C(5)-C(6)	0.9(3)
C(3)-N(2)-C(6)-C(7)	-173.8(2)
Fe(1)-N(2)-C(6)-C(7)	11.1(3)
C(3)-N(2)-C(6)-C(5)	3.0(3)
Fe(1)-N(2)-C(6)-C(5)	-172.12(16)
C(4)-C(5)-C(6)-N(2)	-2.5(3)
C(4)-C(5)-C(6)-C(7)	174.3(2)
N(2)-C(6)-C(7)-C(8)	-4.4(4)
C(5)-C(6)-C(7)-C(8)	179.3(2)
N(2)-C(6)-C(7)-C(27)	174.8(2)
C(5)-C(6)-C(7)-C(27)	-1.5(4)
C(11)-N(3)-C(8)-C(7)	-175.8(2)
Fe(1)-N(3)-C(8)-C(7)	1.4(3)
C(11)-N(3)-C(8)-C(9)	2.4(3)
Fe(1)-N(3)-C(8)-C(9)	179.59(15)
C(6)-C(7)-C(8)-N(3)	-2.2(4)
C(27)-C(7)-C(8)-N(3)	178.7(2)
C(6)-C(7)-C(8)-C(9)	179.9(2)
C(27)-C(7)-C(8)-C(9)	0.7(3)
N(3)-C(8)-C(9)-C(10)	-2.6(3)
C(7)-C(8)-C(9)-C(10)	175.7(2)
C(8)-C(9)-C(10)-C(11)	1.7(3)
C(8)-N(3)-C(11)-C(12)	177.0(2)
Fe(1)-N(3)-C(11)-C(12)	-0.2(3)
C(8)-N(3)-C(11)-C(10)	-1.4(2)
Fe(1)-N(3)-C(11)-C(10)	-178.51(15)
C(9)-C(10)-C(11)-N(3)	-0.2(3)
C(9)-C(10)-C(11)-C(12)	-178.6(2)
N(3)-C(11)-C(12)-C(13)	3.2(4)

C(10)-C(11)-C(12)-C(13)	-178.7(2)
N(3)-C(11)-C(12)-C(33)	-175.3(2)
C(10)-C(11)-C(12)-C(33)	2.8(3)
C(16)-N(4)-C(13)-C(12)	-179.4(2)
Fe(1)-N(4)-C(13)-C(12)	-0.6(3)
C(16)-N(4)-C(13)-C(14)	0.9(3)
Fe(1)-N(4)-C(13)-C(14)	179.64(16)
C(11)-C(12)-C(13)-N(4)	-2.8(4)
C(33)-C(12)-C(13)-N(4)	175.7(2)
C(11)-C(12)-C(13)-C(14)	176.9(2)
C(33)-C(12)-C(13)-C(14)	-4.5(3)
N(4)-C(13)-C(14)-C(15)	-0.8(3)
C(12)-C(13)-C(14)-C(15)	179.4(2)
C(13)-C(14)-C(15)-C(16)	0.4(3)
C(13)-N(4)-C(16)-C(17)	-179.9(2)
Fe(1)-N(4)-C(16)-C(17)	1.3(3)
C(13)-N(4)-C(16)-C(15)	-0.6(3)
Fe(1)-N(4)-C(16)-C(15)	-179.41(16)
C(14)-C(15)-C(16)-N(4)	0.2(3)
C(14)-C(15)-C(16)-C(17)	179.5(2)
N(4)-C(16)-C(17)-C(18)	2.6(4)
C(15)-C(16)-C(17)-C(18)	-176.6(2)
N(4)-C(16)-C(17)-C(39)	-176.5(2)
C(15)-C(16)-C(17)-C(39)	4.3(3)
C(16)-C(17)-C(18)-N(1)	-3.4(4)
C(39)-C(17)-C(18)-N(1)	175.7(2)
C(16)-C(17)-C(18)-C(19)	174.2(2)
C(39)-C(17)-C(18)-C(19)	-6.8(4)
C(1)-N(1)-C(18)-C(17)	177.0(2)
Fe(1)-N(1)-C(18)-C(17)	0.2(3)
C(1)-N(1)-C(18)-C(19)	-0.8(3)
Fe(1)-N(1)-C(18)-C(19)	-177.60(16)
C(17)-C(18)-C(19)-C(20)	-175.8(2)
N(1)-C(18)-C(19)-C(20)	2.0(3)
C(18)-C(19)-C(20)-C(1)	-2.3(3)
N(1)-C(1)-C(20)-C(19)	1.9(3)
C(2)-C(1)-C(20)-C(19)	-177.6(2)
C(1)-C(2)-C(21)-C(22)	72.9(3)
C(3)-C(2)-C(21)-C(22)	-109.3(3)
C(1)-C(2)-C(21)-C(26)	-106.0(3)
C(3)-C(2)-C(21)-C(26)	71.8(3)
C(26)-C(21)-C(22)-C(23)	-1.6(4)
C(2)-C(21)-C(22)-C(23)	179.5(3)
C(21)-C(22)-C(23)-C(24)	1.5(5)
C(22)-C(23)-C(24)-C(25)	-0.7(5)
C(23)-C(24)-C(25)-C(26)	0.0(4)
C(24)-C(25)-C(26)-C(21)	-0.1(4)
C(22)-C(21)-C(26)-C(25)	0.9(4)
C(2)-C(21)-C(26)-C(25)	179.8(2)
C(6)-C(7)-C(27)-C(32)	111.9(3)

C(8)-C(7)-C(27)-C(32)	-68.8(3)
C(6)-C(7)-C(27)-C(28)	-68.1(3)
C(8)-C(7)-C(27)-C(28)	111.2(3)
C(32)-C(27)-C(28)-C(29)	-0.4(4)
C(7)-C(27)-C(28)-C(29)	179.6(3)
C(27)-C(28)-C(29)-C(30)	1.7(5)
C(28)-C(29)-C(30)-C(31)	-1.2(5)
C(29)-C(30)-C(31)-C(32)	-0.5(4)
C(30)-C(31)-C(32)-C(27)	1.8(4)
C(28)-C(27)-C(32)-C(31)	-1.4(4)
C(7)-C(27)-C(32)-C(31)	178.6(2)
C(13)-C(12)-C(33)-C(34)	116.1(3)
C(11)-C(12)-C(33)-C(34)	-65.3(3)
C(13)-C(12)-C(33)-C(38)	-61.6(3)
C(11)-C(12)-C(33)-C(38)	117.0(3)
C(38)-C(33)-C(34)-C(35)	0.7(4)
C(12)-C(33)-C(34)-C(35)	-177.1(3)
C(33)-C(34)-C(35)-C(36)	-0.1(5)
C(34)-C(35)-C(36)-C(37)	-0.2(5)
C(35)-C(36)-C(37)-C(38)	-0.2(5)
C(36)-C(37)-C(38)-C(33)	0.9(4)
C(34)-C(33)-C(38)-C(37)	-1.1(4)
C(12)-C(33)-C(38)-C(37)	176.7(2)
C(18)-C(17)-C(39)-C(44)	-93.6(3)
C(16)-C(17)-C(39)-C(44)	85.6(3)
C(18)-C(17)-C(39)-C(40)	87.6(3)
C(16)-C(17)-C(39)-C(40)	-93.3(3)
C(44)-C(39)-C(40)-C(41)	-1.6(4)
C(17)-C(39)-C(40)-C(41)	177.3(3)
C(39)-C(40)-C(41)-C(42)	-0.8(5)
C(40)-C(41)-C(42)-C(43)	2.0(5)
C(41)-C(42)-C(43)-C(44)	-0.8(5)
C(40)-C(39)-C(44)-C(43)	2.8(5)
C(17)-C(39)-C(44)-C(43)	-176.1(3)
C(42)-C(43)-C(44)-C(39)	-1.6(5)
O(1)-N(5)-C(45)-C(46)	-66.3(3)
Fe(1)-N(5)-C(45)-C(46)	110.4(3)
O(1)-N(5)-C(45)-C(47)	56.5(4)
Fe(1)-N(5)-C(45)-C(47)	-126.8(2)
N(5)-Fe(1)-O(2)-C(51)	-13.0(18)
N(3)-Fe(1)-O(2)-C(51)	-47.0(2)
N(2)-Fe(1)-O(2)-C(51)	43.3(2)
N(4)-Fe(1)-O(2)-C(51)	-137.0(2)
N(1)-Fe(1)-O(2)-C(51)	133.2(2)
N(5)-Fe(1)-O(2)-C(48)	135.4(17)
N(3)-Fe(1)-O(2)-C(48)	101.3(3)
N(2)-Fe(1)-O(2)-C(48)	-168.3(3)
N(4)-Fe(1)-O(2)-C(48)	11.3(3)
N(1)-Fe(1)-O(2)-C(48)	-78.5(3)
C(51)-O(2)-C(48)-C(49)	-24.4(4)

Fe(1)-O(2)-C(48)-C(49)	-177.4(2)
O(2)-C(48)-C(49)-C(50)	-0.2(4)
C(48)-C(49)-C(50)-C(51)	23.7(4)
C(48)-O(2)-C(51)-C(50)	40.0(4)
Fe(1)-O(2)-C(51)-C(50)	-166.4(2)
C(49)-C(50)-C(51)-O(2)	-39.0(4)
C(48A)-C(49A)-C(50A)-C(51A)	-63.2(13)

Table S13. Crystal data and structure refinement for [Fe(3,5-Me-BAFP)(iPrNO)$_2$].

CCDC number	
Empirical formula	$C_{120.25}H_{119.96}Cl_{0.19}FeN_{5.56}O_{10}$
Formula weight	1865.65
Temperature [K]	150(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	12.688(7)
b [Å]	14.426(7)
c [Å]	16.484(10)
α [°]	113.275(17)
β [°]	111.806(15)
γ [°]	91.44(2)
Volume [Å^3]	2521(2)
Z	1
ρ_{calc} [gcm^{-3}]	1.229
μ [mm^{-1}]	0.219
F(000)	989.6
Crystal size [mm^3]	0.320×0.290×0.040
Crystal colour	purple
Crystal shape	plate
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.22 to 56.88 (0.75 Å)
Index ranges	−16 ≤ h ≤ 16 −19 ≤ k ≤ 17 −21 ≤ l ≤ 22
Reflections collected	27632
Independent reflections	12279 R_{int} = 0.0940 R_{sigma} = 0.1347
Completeness to θ = 25.242°	98.6 %
Data / Restraints / Parameters	12279/222/705
Absorption correction	0.6727/0.7457
T_{min}/T_{max} (method)	(multi-scan)
Goodness-of-fit on F^2	1.003
Final R indexes	R_1 = 0.0634
[I≥2σ(I)]	wR_2 = 0.1379
Final R indexes	R_1 = 0.1440
[all data]	wR_2 = 0.1712
Largest peak/hole [eÅ^{-3}]	0.45/−0.42

Refinement details:
The iPrNO ligand was found to be disordered with a THF molecule. Bond distances of THF were restrained to expected target values (1.45(2) Å for C-O and 1.51(2) Å for C-C bonds) and the molecule was assumed to be 2-fold symmetric (SAME command). Uij 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 0.778(4) to 0.222(4). A solvate occupied area was refined as major hexanes and minor methylene chloride. The hexane molecule is inversion symmetric.

Bond distances of methylene chloride were restrained to expected target values (1.77(2) Å for C-Cl bonds and 2.90(2) Å for Cl...Cl).

Table S14. Atomic coordinates and U_{eq} [Å^2] for [Fe(3,5-Me-BAFP)(iPrNO)$_2$].

Atom	*x*	*y*	*z*	U_{eq}
Fe1	0.500000	0.500000	0.500000	0.01872(14)
O5	0.4214(2)	0.6401(2)	0.4255(2)	0.0369(8)
N3	0.4522(5)	0.5586(9)	0.4076(6)	0.0257(13)
C55	0.4510(4)	0.5048(3)	0.3089(3)	0.0338(9)
H55	0.476324	0.438058	0.302426	0.041
C56	0.3292(5)	0.4809(4)	0.2346(4)	0.0535(15)
H56A	0.326792	0.443945	0.169436	0.080
H56B	0.301810	0.545262	0.240752	0.080
H56C	0.279109	0.437904	0.244857	0.080
C57	0.5403(5)	0.5714(4)	0.3035(4)	0.0504(13)
H57A	0.548002	0.534766	0.242359	0.076
H57B	0.615222	0.586544	0.358169	0.076
H57C	0.515377	0.636022	0.306644	0.076
O6	0.4547(16)	0.553(3)	0.396(2)	0.033(3)
C58	0.3388(13)	0.5253(12)	0.3188(10)	0.045(3)
H58A	0.295409	0.580835	0.335505	0.054
H58B	0.295595	0.460968	0.309106	0.054
C59	0.3535(16)	0.511(2)	0.2280(12)	0.062(4)
H59A	0.328599	0.566094	0.208797	0.074
H59B	0.307855	0.443299	0.173613	0.074
C60	0.4819(15)	0.5148(16)	0.2554(12)	0.069(4)
H60A	0.509308	0.539842	0.217309	0.083
H60B	0.502789	0.447252	0.248412	0.083
C61	0.5271(14)	0.5931(11)	0.3614(10)	0.042(3)
H61A	0.610025	0.595345	0.397416	0.051
H61B	0.516514	0.662925	0.367441	0.051
O1	0.14173(16)	0.28073(15)	0.50210(14)	0.0306(5)
O2	0.05814(18)	0.33783(17)	0.22250(15)	0.0354(5)
O3	0.37185(19)	0.87454(15)	0.61011(15)	0.0342(5)
O4	0.4317(2)	0.72192(15)	0.82367(15)	0.0387(5)
N1	0.41209(18)	0.35989(15)	0.39776(15)	0.0189(5)
N2	0.35836(18)	0.53160(15)	0.52417(15)	0.0181(4)
C1	0.4544(2)	0.28381(19)	0.34391(19)	0.0201(5)
C2	0.3633(2)	0.1937(2)	0.2770(2)	0.0264(6)
H2	0.369999	0.130983	0.231584	0.032
C3	0.2671(2)	0.2154(2)	0.2912(2)	0.0256(6)
H3	0.192976	0.171061	0.257337	0.031
C4	0.2979(2)	0.31856(19)	0.36730(18)	0.0199(5)
C5	0.2217(2)	0.36752(19)	0.40443(18)	0.0194(5)
C6	0.2514(2)	0.46702(19)	0.47844(18)	0.0196(5)
C7	0.1729(2)	0.5172(2)	0.5172(2)	0.0252(6)
H7	0.094708	0.488217	0.498393	0.030
C8	0.2309(2)	0.6131(2)	0.5853(2)	0.0241(6)

H8	0.201421	0.664608	0.623164	0.029
C9	0.3462(2)	0.62208(19)	0.58942(19)	0.0193(5)
C10	0.4335(2)	0.70969(19)	0.65129(19)	0.0204(5)
C11	0.1010(2)	0.30737(19)	0.36127(19)	0.0209(5)
C12	0.0642(2)	0.2599(2)	0.4090(2)	0.0234(6)
C13	-0.0424(2)	0.1935(2)	0.3641(2)	0.0303(7)
H13	-0.064495	0.160503	0.396701	0.036
C14	-0.1159(2)	0.1761(2)	0.2707(2)	0.0326(7)
H14	-0.188628	0.130104	0.238898	0.039
C15	-0.0850(2)	0.2247(2)	0.2232(2)	0.0322(7)
H15	-0.136624	0.213329	0.159624	0.039
C16	0.0222(2)	0.2901(2)	0.2692(2)	0.0253(6)
C17	0.0940(2)	0.2602(2)	0.5594(2)	0.0289(6)
C18	0.0140(3)	0.3149(2)	0.5847(2)	0.0316(7)
H18	-0.006566	0.368196	0.565302	0.038
C19	-0.0362(3)	0.2921(2)	0.6384(2)	0.0354(7)
C20	-0.0033(3)	0.2134(3)	0.6656(2)	0.0389(8)
H20	-0.036842	0.197040	0.702290	0.047
C21	0.0769(3)	0.1582(2)	0.6408(2)	0.0364(7)
C22	0.1264(3)	0.1830(2)	0.5872(2)	0.0332(7)
H22	0.182151	0.146850	0.569945	0.040
C23	-0.1268(3)	0.3469(3)	0.6619(3)	0.0503(9)
H23A	-0.116023	0.415113	0.663225	0.075
H23B	-0.119973	0.354674	0.725527	0.075
H23C	-0.203745	0.306965	0.612301	0.075
C24	0.1055(4)	0.0677(3)	0.6640(3)	0.0583(11)
H24A	0.170960	0.045213	0.648830	0.088
H24B	0.037963	0.010792	0.625089	0.088
H24C	0.126246	0.088570	0.733137	0.088
H24D	0.052486	0.051171	0.689207	0.088
H24E	0.185483	0.085591	0.712948	0.088
H24F	0.097200	0.007813	0.604900	0.088
C25	-0.0241(3)	0.3742(2)	0.1658(2)	0.0349(7)
C26	-0.1003(3)	0.4290(2)	0.1977(3)	0.0424(8)
H26	-0.101000	0.438967	0.258013	0.051
C27	-0.1758(3)	0.4693(3)	0.1402(3)	0.0502(10)
C28	-0.1738(3)	0.4513(3)	0.0509(3)	0.0594(11)
H28	-0.225307	0.478402	0.011410	0.071
C29	-0.0989(3)	0.3952(3)	0.0185(3)	0.0553(10)
C30	-0.0228(3)	0.3571(3)	0.0773(2)	0.0414(8)
H30	0.030210	0.319348	0.056939	0.050
C31	-0.2573(4)	0.5306(3)	0.1748(4)	0.0752(14)
H31A	-0.325145	0.526458	0.118714	0.113
H31B	-0.217631	0.602753	0.216578	0.113
H31C	-0.282320	0.502636	0.211522	0.113
C32	-0.1010(4)	0.3744(4)	-0.0796(3)	0.0833(16)
H32A	-0.109250	0.300263	-0.117050	0.125
H32B	-0.028520	0.411136	-0.070629	0.125
H32C	-0.166535	0.398335	-0.114727	0.125
C33	0.4105(2)	0.80260(19)	0.72070(19)	0.0217(6)

C34	0.3896(2)	0.8885(2)	0.7018(2)	0.0240(6)
C35	0.3843(2)	0.9802(2)	0.7716(2)	0.0261(6)
H35	0.371090	1.038119	0.758182	0.031
C36	0.3986(2)	0.9858(2)	0.8614(2)	0.0272(6)
H36	0.396909	1.048621	0.909900	0.033
C37	0.4153(2)	0.9009(2)	0.8812(2)	0.0288(6)
H37	0.423518	0.904773	0.942192	0.035
C38	0.4199(2)	0.8102(2)	0.8101(2)	0.0248(6)
C39	0.3932(3)	0.9599(2)	0.5938(2)	0.0326(7)
C40	0.3089(3)	0.9670(2)	0.5158(2)	0.0350(7)
H40	0.237119	0.919027	0.479579	0.042
C41	0.3290(3)	1.0446(3)	0.4898(3)	0.0438(8)
C42	0.4330(3)	1.1149(3)	0.5455(3)	0.0461(9)
H42	0.446990	1.168356	0.528701	0.055
C43	0.5177(3)	1.1095(3)	0.6254(3)	0.0440(9)
C44	0.4974(3)	1.0298(2)	0.6491(2)	0.0382(8)
H44	0.554711	1.023860	0.702694	0.046
C45	0.2411(4)	1.0499(3)	0.4015(3)	0.0606(11)
H45A	0.268332	1.026895	0.349698	0.091
H45B	0.230365	1.120985	0.417636	0.091
H45C	0.167121	1.005113	0.379540	0.091
C46	0.6318(4)	1.1857(3)	0.6844(3)	0.0613(12)
H46A	0.645878	1.216753	0.645178	0.092
H46B	0.694447	1.150034	0.703763	0.092
H46C	0.629139	1.239709	0.742420	0.092
C47	0.5067(3)	0.7338(2)	0.9158(2)	0.0333(7)
C48	0.4611(3)	0.7185(3)	0.9745(2)	0.0430(8)
H48	0.379509	0.704550	0.954196	0.052
C49	0.5357(4)	0.7235(3)	1.0641(3)	0.0517(10)
C50	0.6532(4)	0.7436(3)	1.0902(3)	0.0569(11)
H50	0.704509	0.746036	1.150491	0.068
C51	0.6998(4)	0.7604(4)	1.0320(3)	0.0612(11)
C52	0.6241(3)	0.7553(3)	0.9437(3)	0.0492(9)
H52	0.653481	0.766590	0.902435	0.059
C53	0.4881(5)	0.7069(4)	1.1303(3)	0.0954(19)
H53A	0.459021	0.633139	1.105591	0.143
H53B	0.424792	0.743999	1.132003	0.143
H53C	0.549876	0.732742	1.195910	0.143
C54	0.8300(5)	0.7844(7)	1.0637(4)	0.132(3)
H54A	0.867043	0.743849	1.097922	0.197
H54B	0.860168	0.857958	1.107067	0.197
H54C	0.846615	0.766887	1.006451	0.197
C62	0.0386(5)	-0.0340(4)	0.0189(4)	0.0952(19)
H62A	0.039397	-0.023568	0.082238	0.114
H62B	0.004221	-0.107251	-0.027009	0.114
C63	0.1623(5)	-0.0109(4)	0.0313(4)	0.0861(17)
H63A	0.196020	0.062985	0.075136	0.103
H63B	0.162173	-0.024459	-0.032504	0.103
C64	0.2417(6)	-0.0790(5)	0.0749(5)	0.110(2)
H64A	0.214592	-0.151652	0.027880	0.165

H64B	0.236707	-0.070462	0.135295	0.165
H64C	0.322311	-0.056394	0.088259	0.165
C65	0.129(4)	-0.052(11)	0.028(6)	0.098(6)
H65A	0.095546	0.010373	0.035568	0.118
H65B	0.075538	-0.109908	-0.033663	0.118
Cl1	0.143(3)	-0.082(2)	0.126(2)	0.116(10)
Cl2	0.267(3)	-0.032(3)	0.028(2)	0.116(9)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S15. Anisotropic displacement parameters [Å^2] for [Fe(3,5-Me-BAFP)(iPrNO)$_2$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	0.0175(3)	0.0160(3)	0.0194(3)	0.0047(2)	0.0077(2)	0.0015(2)
O5	0.0453(17)	0.0341(16)	0.0382(16)	0.0198(12)	0.0194(14)	0.0174(13)
N3	0.0189(16)	0.023(2)	0.031(3)	0.005(2)	0.0122(16)	0.0043(15)
C55	0.044(2)	0.037(2)	0.0301(19)	0.0193(16)	0.0197(17)	0.0199(16)
C56	0.062(3)	0.049(3)	0.037(3)	0.017(2)	0.010(2)	0.001(3)
C57	0.060(3)	0.061(3)	0.050(3)	0.031(3)	0.035(3)	0.015(3)
O6	0.033(4)	0.034(5)	0.033(5)	0.013(4)	0.015(4)	0.007(4)
C58	0.045(4)	0.039(4)	0.035(4)	0.012(4)	0.005(4)	0.014(4)
C59	0.062(6)	0.055(6)	0.045(6)	0.017(5)	0.004(5)	0.013(5)
C60	0.065(5)	0.061(5)	0.057(5)	0.017(5)	0.010(5)	0.011(5)
C61	0.044(4)	0.045(4)	0.043(4)	0.027(4)	0.015(4)	0.011(4)
O1	0.0227(10)	0.0379(11)	0.0334(11)	0.0196(9)	0.0100(9)	0.0032(9)
O2	0.0262(11)	0.0485(13)	0.0329(12)	0.0223(10)	0.0091(10)	0.0041(9)
O3	0.0498(13)	0.0239(10)	0.0310(11)	0.0133(9)	0.0172(10)	0.0081(9)
O4	0.0601(15)	0.0200(10)	0.0249(11)	0.0077(8)	0.0086(11)	0.0044(10)
N1	0.0181(11)	0.0160(10)	0.0203(11)	0.0063(9)	0.0074(9)	0.0029(8)
N2	0.0171(11)	0.0156(10)	0.0202(11)	0.0066(8)	0.0078(9)	0.0018(8)
C1	0.0198(13)	0.0153(12)	0.0219(13)	0.0064(10)	0.0072(11)	0.0035(10)
C2	0.0246(14)	0.0175(13)	0.0270(15)	0.0023(11)	0.0084(12)	0.0022(11)
C3	0.0188(13)	0.0185(13)	0.0287(15)	0.0034(11)	0.0067(12)	0.0001(10)
C4	0.0175(12)	0.0167(12)	0.0210(13)	0.0056(10)	0.0065(11)	−0.0003(10)
C5	0.0154(12)	0.0176(12)	0.0206(13)	0.0065(10)	0.0050(11)	0.0002(9)
C6	0.0162(12)	0.0188(12)	0.0212(13)	0.0069(10)	0.0072(11)	0.0026(10)
C7	0.0187(13)	0.0246(14)	0.0306(15)	0.0092(11)	0.0115(12)	0.0057(11)
C8	0.0177(13)	0.0203(13)	0.0312(15)	0.0074(11)	0.0112(12)	0.0045(10)
C9	0.0177(12)	0.0172(12)	0.0235(13)	0.0079(10)	0.0098(11)	0.0066(10)
C10	0.0243(13)	0.0155(12)	0.0201(13)	0.0068(10)	0.0089(11)	0.0059(10)
C11	0.0159(12)	0.0183(13)	0.0252(14)	0.0065(10)	0.0086(11)	0.0023(10)
C12	0.0214(13)	0.0206(13)	0.0267(14)	0.0091(11)	0.0098(12)	0.0057(10)
C13	0.0263(15)	0.0241(14)	0.0426(18)	0.0139(13)	0.0173(14)	0.0025(12)
C14	0.0215(14)	0.0244(15)	0.0385(17)	0.0047(13)	0.0088(14)	−0.0020(12)
C15	0.0196(14)	0.0372(17)	0.0270(15)	0.0073(13)	0.0041(12)	0.0006(12)
C16	0.0231(14)	0.0253(14)	0.0250(14)	0.0081(11)	0.0105(12)	0.0032(11)
C17	0.0260(15)	0.0308(15)	0.0291(15)	0.0149(12)	0.0089(13)	0.0008(12)
C18	0.0324(16)	0.0303(15)	0.0348(17)	0.0171(13)	0.0136(14)	0.0065(12)

C19	0.0334(17)	0.0365(17)	0.0354(17)	0.0144(14)	0.0148(15)	0.0036(13)
C20	0.0376(18)	0.0419(18)	0.0405(18)	0.0209(15)	0.0168(16)	0.0031(15)
C21	0.0369(18)	0.0360(17)	0.0393(18)	0.0241(15)	0.0107(15)	0.0049(14)
C22	0.0294(16)	0.0326(16)	0.0384(17)	0.0175(14)	0.0127(14)	0.0074(13)
C23	0.046(2)	0.054(2)	0.061(2)	0.0258(19)	0.032(2)	0.0120(17)
C24	0.065(3)	0.057(2)	0.076(3)	0.047(2)	0.033(2)	0.018(2)
C25	0.0277(16)	0.0340(16)	0.0355(17)	0.0160(14)	0.0049(14)	0.0004(13)
C26	0.0367(18)	0.0375(18)	0.045(2)	0.0134(15)	0.0138(16)	0.0065(15)
C27	0.0339(19)	0.0332(18)	0.070(3)	0.0190(18)	0.0109(18)	0.0035(15)
C28	0.043(2)	0.060(2)	0.070(3)	0.042(2)	0.003(2)	0.0024(19)
C29	0.048(2)	0.065(3)	0.047(2)	0.034(2)	0.0054(19)	−0.003(2)
C30	0.0355(18)	0.050(2)	0.0356(18)	0.0192(15)	0.0114(15)	0.0031(15)
C31	0.054(3)	0.050(2)	0.103(4)	0.025(2)	0.022(3)	0.022(2)
C32	0.079(3)	0.118(4)	0.053(3)	0.056(3)	0.008(2)	−0.002(3)
C33	0.0159(12)	0.0178(13)	0.0261(14)	0.0047(10)	0.0087(11)	0.0025(10)
C34	0.0222(13)	0.0222(14)	0.0246(14)	0.0077(11)	0.0094(12)	0.0035(11)
C35	0.0212(14)	0.0181(13)	0.0339(16)	0.0077(11)	0.0100(12)	0.0054(10)
C36	0.0202(13)	0.0223(14)	0.0257(14)	0.0014(11)	0.0054(12)	0.0032(11)
C37	0.0287(15)	0.0268(15)	0.0216(14)	0.0025(11)	0.0098(13)	0.0006(12)
C38	0.0226(14)	0.0216(13)	0.0248(14)	0.0073(11)	0.0074(12)	0.0038(11)
C39	0.0429(18)	0.0251(15)	0.0374(17)	0.0143(13)	0.0233(15)	0.0110(13)
C40	0.0397(18)	0.0345(17)	0.0390(18)	0.0198(14)	0.0205(16)	0.0133(14)
C41	0.059(2)	0.0418(19)	0.051(2)	0.0286(16)	0.0335(19)	0.0248(17)
C42	0.066(2)	0.0345(18)	0.062(2)	0.0294(17)	0.042(2)	0.0196(17)
C43	0.052(2)	0.0337(18)	0.058(2)	0.0189(16)	0.036(2)	0.0081(15)
C44	0.0401(18)	0.0356(17)	0.0429(19)	0.0175(15)	0.0206(16)	0.0120(14)
C45	0.080(3)	0.067(3)	0.063(3)	0.046(2)	0.038(2)	0.040(2)
C46	0.064(3)	0.038(2)	0.089(3)	0.022(2)	0.046(3)	0.0036(18)
C47	0.0493(19)	0.0216(14)	0.0266(15)	0.0110(12)	0.0125(15)	0.0121(13)
C48	0.052(2)	0.0387(18)	0.0368(18)	0.0163(15)	0.0170(17)	0.0010(16)
C49	0.079(3)	0.040(2)	0.037(2)	0.0208(16)	0.021(2)	0.0055(19)
C50	0.079(3)	0.050(2)	0.036(2)	0.0234(17)	0.012(2)	0.027(2)
C51	0.054(2)	0.080(3)	0.045(2)	0.023(2)	0.019(2)	0.033(2)
C52	0.055(2)	0.059(2)	0.0378(19)	0.0198(17)	0.0244(18)	0.0226(19)
C53	0.126(5)	0.109(4)	0.053(3)	0.045(3)	0.032(3)	−0.018(4)
C54	0.059(3)	0.237(8)	0.087(4)	0.061(5)	0.027(3)	0.058(4)
C62	0.086(4)	0.073(3)	0.079(3)	0.014(3)	0.007(3)	−0.002(3)
C63	0.071(3)	0.066(3)	0.067(3)	−0.001(3)	0.007(3)	−0.002(3)
C64	0.108(5)	0.068(4)	0.085(4)	0.009(3)	−0.001(4)	−0.005(3)
C65	0.087(7)	0.072(7)	0.078(7)	0.004(7)	0.007(7)	−0.001(7)
Cl1	0.125(14)	0.076(12)	0.085(12)	0.000(11)	0.018(12)	−0.007(12)
Cl2	0.103(11)	0.084(11)	0.094(11)	0.012(10)	0.004(10)	−0.003(10)

Table S16. Bond lengths and angles for [Fe(3,5-Me-BAFP)(iPrNO)$_2$].

.Atom–Atom	Length [Å]
Fe1–N3	1.940(10)
Fe1–N3$^{\#1}$	1.940(10)
Fe1–N1	1.992(2)
Fe1–N1$^{\#1}$	1.992(2)
Fe1–N2$^{\#1}$	2.007(2)
Fe1–N2	2.007(2)
Fe1–O6	2.05(3)
Fe1–O6$^{\#1}$	2.05(3)
O5–N3	1.207(13)
N3–C55	1.494(10)
C55–C56	1.498(7)
C55–C57	1.517(6)
C55–H55	1.0000
C56–H56A	0.9800
C56–H56B	0.9800
C56–H56C	0.9800
C57–H57A	0.9800
C57–H57B	0.9800
C57–H57C	0.9800
O6–C58	1.454(16)
O6–C61	1.455(16)
C58–C59	1.509(14)
C58–H58A	0.9900
C58–H58B	0.9900
C59–C60	1.512(18)
C59–H59A	0.9900
C59–H59B	0.9900
C60–C61	1.524(14)
C60–H60A	0.9900
C60–H60B	0.9900
C61–H61A	0.9900
C61–H61B	0.9900
O1–C12	1.383(3)
O1–C17	1.409(3)
O2–C25	1.389(4)
O2–C16	1.392(3)
O3–C34	1.371(3)
O3–C39	1.400(4)
O4–C38	1.380(4)
O4–C47	1.398(4)
N1–C4	1.373(3)
N1–C1	1.377(3)
N2–C6	1.378(3)
N2–C9	1.381(3)
C1–C10$^{\#1}$	1.393(4)
C1–C2	1.444(4)
C2–C3	1.348(4)
C2–H2	0.9500

C3–C4	1.440(3)
C3–H3	0.9500
C4–C5	1.394(4)
C5–C6	1.392(3)
C5–C11	1.496(3)
C6–C7	1.439(4)
C7–C8	1.351(4)
C7–H7	0.9500
C8–C9	1.439(4)
C8–H8	0.9500
C9–C10	1.392(4)
C10–C33	1.499(3)
C11–C16	1.388(4)
C11–C12	1.411(4)
C12–C13	1.387(4)
C13–C14	1.385(4)
C13–H13	0.9500
C14–C15	1.381(4)
C14–H14	0.9500
C15–C16	1.385(4)
C15–H15	0.9500
C17–C22	1.380(4)
C17–C18	1.386(4)
C18–C19	1.391(4)
C18–H18	0.9500
C19–C20	1.398(5)
C19–C23	1.493(5)
C20–C21	1.388(5)
C20–H20	0.9500
C21–C22	1.398(4)
C21–C24	1.516(5)
C22–H22	0.9500
C23–H23A	0.9800
C23–H23B	0.9800
C23–H23C	0.9800
C24–H24A	0.9800
C24–H24B	0.9800
C24–H24C	0.9800
C24–H24D	0.9800
C24–H24E	0.9800
C24–H24F	0.9800
C25–C30	1.387(5)
C25–C26	1.387(5)
C26–C27	1.394(5)
C26–H26	0.9500
C27–C28	1.400(6)
C27–C31	1.504(5)
C28–C29	1.384(6)
C28–H28	0.9500

C29–C30	1.388(5)
C29–C32	1.514(6)
C30–H30	0.9500
C31–H31A	0.9800
C31–H31B	0.9800
C31–H31C	0.9800
C32–H32A	0.9800
C32–H32B	0.9800
C32–H32C	0.9800
C33–C38	1.392(4)
C33–C34	1.402(4)
C34–C35	1.392(4)
C35–C36	1.391(4)
C35–H35	0.9500
C36–C37	1.389(4)
C36–H36	0.9500
C37–C38	1.390(4)
C37–H37	0.9500
C39–C40	1.377(5)
C39–C44	1.382(5)
C40–C41	1.395(5)
C40–H40	0.9500
C41–C42	1.382(5)
C41–C45	1.502(5)
C42–C43	1.388(5)
C42–H42	0.9500
C43–C44	1.399(5)
C43–C46	1.509(5)
C44–H44	0.9500
C45–H45A	0.9800
C45–H45B	0.9800
C45–H45C	0.9800
C46–H46A	0.9800
C46–H46B	0.9800
C46–H46C	0.9800
C47–C52	1.372(5)
C47–C48	1.377(5)
C48–C49	1.399(5)
C48–H48	0.9500
C49–C50	1.377(6)
C49–C53	1.516(6)
C50–C51	1.389(6)
C50–H50	0.9500
C51–C52	1.384(5)
C51–C54	1.519(7)
C52–H52	0.9500
C53–H53A	0.9800
C53–H53B	0.9800
C53–H53C	0.9800
C54–H54A	0.9800

C54–H54B	0.9800
C54–H54C	0.9800
C62–C63	1.516(8)
C62–C62$^{\#2}$	1.545(11)
C62–H62A	0.9900
C62–H62B	0.9900
C63–C64	1.601(8)
C63–H63A	0.9900
C63–H63B	0.9900
C64–H64A	0.9800
C64–H64B	0.9800
C64–H64C	0.9800
C65–Cl1	1.76(2)
C65–Cl2	1.77(2)
C65–H65A	0.9900
C65–H65B	0.9900

Atom–Atom–Atom	**Angle [°]**
N3–Fe1–N3	180.0
N3–Fe1–N1	92.0(3)
N3–Fe1–N1	88.0(3)
N3–Fe1–N1	88.0(3)
N3–Fe1–N1	92.0(3)
N1–Fe1–N1	180.0
N3–Fe1–N2	91.9(2)
N3–Fe1–N2	88.1(2)
N1–Fe1–N2	89.93(9)
N1–Fe1–N2	90.07(9)
N3–Fe1–N2	88.1(2)
N3–Fe1–N2	91.9(2)
N1–Fe1–N2	90.07(9)
N1–Fe1–N2	89.93(9)
N2–Fe1–N2	180.0
N1–Fe1–O6	89.3(10)
N1–Fe1–O6	90.7(10)
N2–Fe1–O6	88.1(8)
N2–Fe1–O6	91.9(8)
N3–Fe1–O6	175.3(14)
N3–Fe1–O6	4.7(14)
N1–Fe1–O6	90.7(10)
N1–Fe1–O6	89.3(10)
N2–Fe1–O6	91.9(8)
N2–Fe1–O6	88.1(8)
O5–N3–C55	115.7(8)
O5–N3–Fe1	122.6(6)
C55–N3–Fe1	121.6(8)
N3–C55–C56	108.6(5)
N3–C55–C57	107.4(5)
C56–C55–C57	116.4(4)

N3–C55–H55	108.1
C56–C55–H55	108.1
C57–C55–H55	108.1
C55–C56–H56A	109.5
C55–C56–H56B	109.5
H56A–C56–H56B	109.5
C55–C56–H56C	109.5
H56A–C56–H56C	109.5
H56B–C56–H56C	109.5
C55–C57–H57A	109.5
C55–C57–H57B	109.5
H57A–C57–H57B	109.5
C55–C57–H57C	109.5
H57A–C57–H57C	109.5
H57B–C57–H57C	109.5
C58–O6–C61	104.0(19)
C58–O6–Fe1	123.6(16)
C61–O6–Fe1	129.8(16)
O6–C58–C59	106.6(15)
O6–C58–H58A	110.4
C59–C58–H58A	110.4
O6–C58–H58B	110.4
C59–C58–H58B	110.4
H58A–C58–H58B	108.6
C58–C59–C60	104.6(11)
C58–C59–H59A	110.8
C60–C59–H59A	110.8
C58–C59–H59B	110.8
C60–C59–H59B	110.8
H59A–C59–H59B	108.9
C59–C60–C61	98.6(11)
C59–C60–H60A	112.0
C61–C60–H60A	112.0
C59–C60–H60B	112.0
C61–C60–H60B	112.0
H60A–C60–H60B	109.7
O6–C61–C60	102.1(17)
O6–C61–H61A	111.4
C60–C61–H61A	111.4
O6–C61–H61B	111.4
C60–C61–H61B	111.4
H61A–C61–H61B	109.2
C12–O1–C17	115.7(2)
C25–O2–C16	117.4(2)
C34–O3–C39	119.6(2)
C38–O4–C47	117.1(2)
C4–N1–C1	105.8(2)
C4–N1–Fe1	127.47(17)
C1–N1–Fe1	126.74(17)
C6–N2–C9	105.0(2)

C6–N2–Fe1	127.07(16)
C9–N2–Fe1	127.92(16)
N1–C1–C10	126.8(2)
N1–C1–C2	109.8(2)
C10–C1–C2	123.3(2)
C3–C2–C1	107.1(2)
C3–C2–H2	126.4
C1–C2–H2	126.4
C2–C3–C4	107.0(2)
C2–C3–H3	126.5
C4–C3–H3	126.5
N1–C4–C5	125.7(2)
N1–C4–C3	110.3(2)
C5–C4–C3	124.0(2)
C6–C5–C4	124.1(2)
C6–C5–C11	119.1(2)
C4–C5–C11	116.8(2)
N2–C6–C5	125.5(2)
N2–C6–C7	110.4(2)
C5–C6–C7	124.1(2)
C8–C7–C6	107.2(2)
C8–C7–H7	126.4
C6–C7–H7	126.4
C7–C8–C9	106.6(2)
C7–C8–H8	126.7
C9–C8–H8	126.7
N2–C9–C10	124.8(2)
N2–C9–C8	110.7(2)
C10–C9–C8	124.5(2)
C9–C10–C1	123.8(2)
C9–C10–C33	119.8(2)
C1–C10–C33	116.3(2)
C16–C11–C12	116.7(2)
C16–C11–C5	121.3(2)
C12–C11–C5	121.9(2)
O1–C12–C13	121.8(3)
O1–C12–C11	116.3(2)
C13–C12–C11	121.9(3)
C14–C13–C12	118.8(3)
C14–C13–H13	120.6
C12–C13–H13	120.6
C15–C14–C13	121.0(3)
C15–C14–H14	119.5
C13–C14–H14	119.5
C14–C15–C16	119.2(3)
C14–C15–H15	120.4
C16–C15–H15	120.4
C15–C16–C11	122.2(3)
C15–C16–O2	121.0(3)
C11–C16–O2	116.7(2)

C22–C17–C18	121.3(3)
C22–C17–O1	118.5(3)
C18–C17–O1	120.2(3)
C17–C18–C19	120.2(3)
C17–C18–H18	119.9
C19–C18–H18	119.9
C18–C19–C20	118.0(3)
C18–C19–C23	120.7(3)
C20–C19–C23	121.2(3)
C21–C20–C19	122.2(3)
C21–C20–H20	118.9
C19–C20–H20	118.9
C20–C21–C22	118.6(3)
C20–C21–C24	121.9(3)
C22–C21–C24	119.3(3)
C17–C22–C21	119.6(3)
C17–C22–H22	120.2
C21–C22–H22	120.2
C19–C23–H23A	109.5
C19–C23–H23B	109.5
H23A–C23–H23B	109.5
C19–C23–H23C	109.5
H23A–C23–H23C	109.5
H23B–C23–H23C	109.5
C21–C24–H24A	109.5
C21–C24–H24B	109.5
H24A–C24–H24B	109.5
C21–C24–H24C	109.5
H24A–C24–H24C	109.5
H24B–C24–H24C	109.5
C21–C24–H24D	109.5
H24A–C24–H24D	141.1
H24B–C24–H24D	56.3
H24C–C24–H24D	56.3
C21–C24–H24E	109.5
H24A–C24–H24E	56.3
H24B–C24–H24E	141.1
H24C–C24–H24E	56.3
H24D–C24–H24E	109.5
C21–C24–H24F	109.5
H24A–C24–H24F	56.3
H24B–C24–H24F	56.3
H24C–C24–H24F	141.1
H24D–C24–H24F	109.5
H24E–C24–H24F	109.5
C30–C25–C26	121.6(3)
C30–C25–O2	116.5(3)
C26–C25–O2	121.8(3)
C25–C26–C27	119.1(3)
C25–C26–H26	120.4

C27–C26–H26	120.4
C26–C27–C28	118.8(4)
C26–C27–C31	119.7(4)
C28–C27–C31	121.5(4)
C29–C28–C27	122.0(4)
C29–C28–H28	119.0
C27–C28–H28	119.0
C28–C29–C30	118.7(4)
C28–C29–C32	120.8(4)
C30–C29–C32	120.5(4)
C25–C30–C29	119.9(3)
C25–C30–H30	120.1
C29–C30–H30	120.1
C27–C31–H31A	109.5
C27–C31–H31B	109.5
H31A–C31–H31B	109.5
C27–C31–H31C	109.5
H31A–C31–H31C	109.5
H31B–C31–H31C	109.5
C29–C32–H32A	109.5
C29–C32–H32B	109.5
H32A–C32–H32B	109.5
C29–C32–H32C	109.5
H32A–C32–H32C	109.5
H32B–C32–H32C	109.5
C38–C33–C34	117.7(2)
C38–C33–C10	121.0(2)
C34–C33–C10	121.1(2)
O3–C34–C35	123.2(3)
O3–C34–C33	115.5(2)
C35–C34–C33	121.3(3)
C36–C35–C34	119.1(3)
C36–C35–H35	120.4
C34–C35–H35	120.4
C37–C36–C35	121.0(2)
C37–C36–H36	119.5
C35–C36–H36	119.5
C36–C37–C38	118.7(3)
C36–C37–H37	120.6
C38–C37–H37	120.6
O4–C38–C37	121.6(3)
O4–C38–C33	116.3(2)
C37–C38–C33	122.1(3)
C40–C39–C44	121.3(3)
C40–C39–O3	117.0(3)
C44–C39–O3	121.5(3)
C39–C40–C41	120.0(3)
C39–C40–H40	120.0
C41–C40–H40	120.0
C42–C41–C40	118.6(3)

C42–C41–C45	120.6(3)
C40–C41–C45	120.8(4)
C41–C42–C43	121.9(3)
C41–C42–H42	119.1
C43–C42–H42	119.1
C42–C43–C44	118.8(3)
C42–C43–C46	121.2(3)
C44–C43–C46	119.9(4)
C39–C44–C43	119.3(3)
C39–C44–H44	120.3
C43–C44–H44	120.3
C41–C45–H45A	109.5
C41–C45–H45B	109.5
H45A–C45–H45B	109.5
C41–C45–H45C	109.5
H45A–C45–H45C	109.5
H45B–C45–H45C	109.5
C43–C46–H46A	109.5
C43–C46–H46B	109.5
H46A–C46–H46B	109.5
C43–C46–H46C	109.5
H46A–C46–H46C	109.5
H46B–C46–H46C	109.5
C52–C47–C48	121.5(3)
C52–C47–O4	119.2(3)
C48–C47–O4	119.2(3)
C47–C48–C49	119.5(4)
C47–C48–H48	120.2
C49–C48–H48	120.2
C50–C49–C48	118.1(3)
C50–C49–C53	121.1(4)
C48–C49–C53	120.8(4)
C49–C50–C51	122.6(4)
C49–C50–H50	118.7
C51–C50–H50	118.7
C52–C51–C50	118.1(4)
C52–C51–C54	120.5(4)
C50–C51–C54	121.4(4)
C47–C52–C51	120.1(4)
C47–C52–H52	120.0
C51–C52–H52	120.0
C49–C53–H53A	109.5
C49–C53–H53B	109.5
H53A–C53–H53B	109.5
C49–C53–H53C	109.5
H53A–C53–H53C	109.5
H53B–C53–H53C	109.5
C51–C54–H54A	109.5
C51–C54–H54B	109.5
H54A–C54–H54B	109.5

C51–C54–H54C	109.5
H54A–C54–H54C	109.5
H54B–C54–H54C	109.5
C63–C62–C62	113.4(7)
C63–C62–H62A	108.9
C62–C62–H62A	108.9
C63–C62–H62B	108.9
C62–C62–H62B	108.9
H62A–C62–H62B	107.7
C62–C63–C64	112.3(6)
C62–C63–H63A	109.2
C64–C63–H63A	109.2
C62–C63–H63B	109.2
C64–C63–H63B	109.2
H63A–C63–H63B	107.9
C63–C64–H64A	109.5
C63–C64–H64B	109.5
H64A–C64–H64B	109.5
C63–C64–H64C	109.5
H64A–C64–H64C	109.5
H64B–C64–H64C	109.5
Cl1–C65–Cl2	109.1(17)
Cl1–C65–H65A	109.9
Cl2–C65–H65A	109.9
Cl1–C65–H65B	109.9
Cl2–C65–H65B	109.9
H65A–C65–H65B	108.3

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 1-Y, 1-Z; #2: -X, -Y, -Z;

Table S17. Crystal data and structure refinement for the second crystal of [Fe(3,5-Me-BAFP)(iPrNO)$_2$].

CCDC number	
Empirical formula	$C_{118.53}H_{118.37}Cl_{0.67}FeN_6O_{9.04}$
Formula weight	1851.13
Temperature [K]	150(2)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	12.6436(4)
b [Å]	14.3552(4)
c [Å]	16.4422(5)
α [°]	113.0869(14)
β [°]	111.5479(12)
γ [°]	91.5369(13)
Volume [Å^3]	2501.99(13)
Z	1
ρ_{calc} [gcm^{-3}]	1.229
μ [mm^{-1}]	1.866
F(000)	981.2
Crystal size [mm^3]	0.430×0.170×0.140
Crystal colour	purple
Crystal shape	rod
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	6.41 to 160.12 (0.78 Å)
Index ranges	−15 ≤ h ≤ 14 −18 ≤ k ≤ 17 −20 ≤ l ≤ 20
Reflections collected	25304
Independent reflections	9876 R_{int} = 0.0372 R_{sigma} = 0.0428
Completeness to θ = 67.679°	98.0 %
Data / Restraints / Parameters	9876/146/689
Absorption correction	0.5494/0.7543
T_{min}/T_{max} (method)	(multi-scan)
Goodness-of-fit on F^2	1.091
Final *R* indexes	R_1 = 0.0436
[$I \geq 2\sigma(I)$]	wR_2 = 0.1194
Final *R* indexes	R_1 = 0.0465
[all data]	wR_2 = 0.1220
Largest peak/hole [eÅ^{-3}]	0.29/−0.44

Refinement Details:
A second crystal was very similar with slightly different iPrNO/THF ratios and solvate molecules. This structure was solved by isomorphous replacement from the first crystal of the same compound (grown under slightly different conditions). The disorder model was adjusted (two methylene chloride moieties). The iPrNO ligand was again found to be disordered with a THF molecule. Bond distances of THF were restrained to expected target values (1.45(2) Å for C-O and 1.51(2) Å for C-

C bonds) and the molecule was assumed to be 2-fold symmetric (SAME command). Uij 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 0.917(3) to 0.083(3). A solvate occupied area was refined as major hexanes and minor methylene chloride (two moieties). The hexane molecule is inversion symmetric. Bond distances of methylene chloride were restrained to expected target values (1.77(2) Å for C-Cl bonds and 2.90(2) Å for Cl...Cl). C-C bond distances of the hexane were restrained to 1.51(2) and 1.55(2) Å for CH_2-CH_2 and CH_2-CH_3 moieties, respectively. Uij components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Occupancies were not constrained to unity. Subject to these conditions, occupancy ratios refined to 0.667(7), 0.168(4) and 0.062(3), respectively, for hexane and the two CH_2Cl_2 moieties.

Table S18. Atomic coordinates and U_{eq} [Å^2] for the second crystal structure of [Fe(3,5-Me-BAFP)(iPrNO)$_2$].

Atom	***x***	***y***	***z***	U_{eq}
Fe1	0.500000	0.500000	0.500000	0.01836(10)
O5	0.4200(2)	0.64059(16)	0.42644(16)	0.0301(8)
N3	0.44796(13)	0.55638(10)	0.40418(10)	0.0284(3)
H3A	0.373346	0.562853	0.394112	0.043
H3B	0.490492	0.621667	0.433529	0.043
C55	0.44973(17)	0.50662(14)	0.30612(12)	0.0324(4)
H55	0.470825	0.437597	0.296460	0.039
C56	0.3297(2)	0.4895(2)	0.23005(17)	0.0691(8)
H56A	0.329652	0.454834	0.165468	0.104
H56B	0.306652	0.556180	0.238866	0.104
H56C	0.274690	0.446179	0.236363	0.104
C57	0.5433(2)	0.5721(2)	0.3040(2)	0.0613(7)
H57A	0.548260	0.538565	0.241288	0.092
H57B	0.617933	0.580077	0.356059	0.092
H57C	0.524329	0.640330	0.313432	0.092
O1	0.14065(10)	0.28088(9)	0.50370(9)	0.0306(3)
O2	0.06054(10)	0.33581(11)	0.22328(9)	0.0361(3)
O3	0.37252(12)	0.87543(9)	0.61094(9)	0.0345(3)
O4	0.42915(13)	0.72077(9)	0.82327(9)	0.0377(3)
N1	0.41307(10)	0.35869(9)	0.39831(9)	0.0190(2)
N2	0.35837(11)	0.53086(9)	0.52542(9)	0.0191(2)
C1	0.45498(13)	0.28260(11)	0.34372(11)	0.0206(3)
C2	0.36390(14)	0.19262(12)	0.27703(12)	0.0260(3)
H2	0.370535	0.129886	0.231315	0.031
C3	0.26774(14)	0.21426(11)	0.29174(12)	0.0257(3)
H3	0.193580	0.169811	0.258152	0.031
C4	0.29856(13)	0.31785(11)	0.36826(11)	0.0204(3)
C5	0.22228(13)	0.36647(11)	0.40568(11)	0.0206(3)
C6	0.25179(13)	0.46599(11)	0.47994(11)	0.0201(3)
C7	0.17317(14)	0.51600(12)	0.51918(12)	0.0247(3)
H7	0.094855	0.487049	0.500586	0.030
C8	0.23146(13)	0.61176(12)	0.58736(12)	0.0244(3)
H8	0.202035	0.662999	0.625845	0.029
C9	0.34636(13)	0.62145(11)	0.59067(11)	0.0209(3)
C10	0.43268(13)	0.70962(11)	0.65158(11)	0.0209(3)

C11	0.10146(13)	0.30614(11)	0.36267(11)	0.0224(3)
C12	0.06406(14)	0.25967(12)	0.41032(12)	0.0245(3)
C13	-0.04331(15)	0.19324(12)	0.36499(13)	0.0298(4)
H13	-0.066679	0.161156	0.398073	0.036
C14	-0.11559(15)	0.17451(13)	0.27109(13)	0.0325(4)
H14	-0.187844	0.127466	0.239012	0.039
C15	-0.08430(15)	0.22305(14)	0.22359(13)	0.0335(4)
H15	-0.135620	0.211708	0.160033	0.040
C16	0.02321(14)	0.28881(13)	0.26966(12)	0.0273(3)
C17	0.09180(15)	0.26079(13)	0.56043(12)	0.0299(4)
C18	0.01110(16)	0.31607(14)	0.58460(13)	0.0330(4)
H18	-0.009404	0.368952	0.564200	0.040
C19	-0.03966(16)	0.29420(14)	0.63851(14)	0.0351(4)
C20	-0.00627(17)	0.21633(15)	0.66777(14)	0.0385(4)
H20	-0.039878	0.200892	0.705201	0.046
C21	0.07438(17)	0.16111(15)	0.64373(15)	0.0387(4)
C22	0.12506(16)	0.18468(14)	0.59000(14)	0.0344(4)
H22	0.181793	0.148709	0.573981	0.041
C23	-0.1316(2)	0.35021(18)	0.66116(18)	0.0484(5)
H23A	-0.122926	0.416844	0.658447	0.073
H23B	-0.123192	0.361812	0.726267	0.073
H23C	-0.208566	0.308416	0.613509	0.073
C24	0.1037(2)	0.0722(2)	0.6698(2)	0.0593(6)
H24A	0.169485	0.049186	0.655073	0.089
H24B	0.036353	0.014913	0.632112	0.089
H24C	0.124177	0.094946	0.739164	0.089
H24D	0.050526	0.056844	0.695827	0.089
H24E	0.183657	0.091117	0.718787	0.089
H24F	0.095833	0.011084	0.611736	0.089
C25	-0.02080(15)	0.37256(14)	0.16608(13)	0.0340(4)
C26	-0.09686(17)	0.42820(15)	0.19789(15)	0.0415(4)
H26	-0.097475	0.438851	0.258489	0.050
C27	-0.17239(19)	0.46836(16)	0.14012(18)	0.0497(5)
C28	-0.1706(2)	0.4496(2)	0.05115(19)	0.0565(6)
H28	-0.222320	0.476579	0.011426	0.068
C29	-0.0955(2)	0.3925(2)	0.01836(18)	0.0558(6)
C30	-0.01950(18)	0.35426(17)	0.07782(15)	0.0425(5)
H30	0.033211	0.315573	0.057466	0.051
C31	-0.2541(2)	0.5305(2)	0.1744(2)	0.0713(8)
H31A	-0.320030	0.528836	0.118409	0.107
H31B	-0.213242	0.602146	0.218039	0.107
H31C	-0.282286	0.500952	0.208974	0.107
C32	-0.0967(3)	0.3712(3)	-0.0794(2)	0.0824(9)
H32A	-0.120503	0.296726	-0.121125	0.124
H32B	-0.018765	0.395747	-0.071320	0.124
H32C	-0.151497	0.407360	-0.109321	0.124
C33	0.40900(13)	0.80252(11)	0.72074(11)	0.0219(3)
C34	0.38966(14)	0.88932(12)	0.70259(12)	0.0249(3)
C35	0.38514(14)	0.98160(12)	0.77285(12)	0.0277(3)
H35	0.372980	1.040165	0.759680	0.033

C36	0.39860(14)	0.98670(12)	0.86182(12)	0.0291(4)
H36	0.397085	1.049799	0.910320	0.035
C37	0.41426(15)	0.90156(13)	0.88168(12)	0.0305(4)
H37	0.421923	0.905338	0.942637	0.037
C38	0.41854(14)	0.81002(12)	0.81018(11)	0.0254(3)
C39	0.39289(17)	0.96076(13)	0.59452(14)	0.0335(4)
C40	0.30769(18)	0.96752(15)	0.51664(15)	0.0385(4)
H40	0.235873	0.919450	0.480999	0.046
C41	0.3280(2)	1.04573(17)	0.49059(17)	0.0474(5)
C42	0.4327(2)	1.11606(16)	0.54635(19)	0.0513(6)
H42	0.445989	1.170485	0.529971	0.062
C43	0.5178(2)	1.11017(15)	0.62427(18)	0.0483(5)
C44	0.49749(18)	1.03038(14)	0.64852(15)	0.0399(4)
H44	0.555206	1.024102	0.701729	0.048
C45	0.2392(3)	1.0514(2)	0.40300(19)	0.0602(7)
H45A	0.263808	1.024897	0.349492	0.090
H45B	0.231535	1.123394	0.418293	0.090
H45C	0.164262	1.009583	0.383976	0.090
C46	0.6318(3)	1.18585(18)	0.6817(2)	0.0669(8)
H46A	0.695446	1.148374	0.691846	0.100
H46B	0.634424	1.233877	0.744576	0.100
H46C	0.639733	1.224621	0.645992	0.100
C47	0.50308(18)	0.73168(13)	0.91469(13)	0.0352(4)
C48	0.4569(2)	0.71712(16)	0.97323(15)	0.0460(5)
H48	0.375132	0.704253	0.953165	0.055
C49	0.5302(3)	0.72127(18)	1.06231(16)	0.0592(7)
C50	0.6486(3)	0.7402(2)	1.08865(17)	0.0649(8)
H50	0.699409	0.743108	1.149213	0.078
C51	0.6953(2)	0.7551(3)	1.02982(18)	0.0716(9)
C52	0.6204(2)	0.7515(2)	0.94158(16)	0.0543(6)
H52	0.650471	0.762667	0.900289	0.065
C53	0.4832(4)	0.7073(3)	1.1290(2)	0.1086(15)
H53A	0.467290	0.633633	1.113202	0.163
H53B	0.411250	0.733772	1.121119	0.163
H53C	0.540336	0.745207	1.196182	0.163
C54	0.8253(3)	0.7767(6)	1.0594(3)	0.160(3)
H54A	0.863396	0.745360	1.102976	0.240
H54B	0.854876	0.851582	1.092770	0.240
H54C	0.841560	0.747308	1.001469	0.240
C65	0.145(2)	-0.071(3)	0.031(2)	0.116(5)
H65A	0.143859	-0.008216	0.018470	0.139
H65B	0.095704	-0.130167	-0.031314	0.139
Cl1	0.2885(10)	-0.0910(13)	0.0697(9)	0.100(4)
Cl2	0.0860(11)	-0.0548(9)	0.1136(10)	0.122(4)
C66	0.116(4)	-0.034(7)	0.049(5)	0.114(5)
H66A	0.091984	0.033685	0.068130	0.137
H66B	0.052371	-0.084431	-0.011661	0.137
Cl3	0.244(2)	-0.0214(17)	0.0271(14)	0.116(6)
Cl4	0.147(2)	-0.0751(19)	0.1410(16)	0.120(7)
C62	0.0397(5)	-0.0332(4)	0.0181(5)	0.110(2)

H62A	0.040495	-0.024196	0.081232	0.132
H62B	0.005780	-0.106620	-0.028060	0.132
C63	0.1625(6)	-0.0109(5)	0.0308(4)	0.102(2)
H63A	0.196426	0.063066	0.074751	0.123
H63B	0.163175	-0.024108	-0.032831	0.123
C64	0.2411(9)	-0.0800(8)	0.0742(7)	0.133(4)
H64A	0.215584	-0.152436	0.026191	0.200
H64B	0.233260	-0.073652	0.133184	0.200
H64C	0.322464	-0.056050	0.089817	0.200

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S19. Anisotropic displacement parameters [Å^2] for the second crystal of [Fe(3,5-Me-BAFP)(iPrNO)$_2$].
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	0.01539(17)	0.01686(15)	0.02072(17)	0.00594(12)	0.00757(13)	0.00361(12)
O5	0.0349(14)	0.0241(12)	0.0350(13)	0.0158(10)	0.0144(10)	0.0128(9)
N3	0.0320(8)	0.0225(6)	0.0345(7)	0.0117(6)	0.0179(6)	0.0107(5)
C55	0.0408(10)	0.0354(9)	0.0294(8)	0.0173(7)	0.0188(8)	0.0188(8)
C56	0.0593(16)	0.0666(15)	0.0402(12)	0.0021(11)	−0.0012(11)	0.0314(13)
C57	0.0707(17)	0.0782(17)	0.0809(18)	0.0547(15)	0.0558(15)	0.0326(14)
O1	0.0225(6)	0.0390(6)	0.0341(6)	0.0203(5)	0.0107(5)	0.0049(5)
O2	0.0238(6)	0.0525(8)	0.0357(6)	0.0254(6)	0.0092(5)	0.0064(5)
O3	0.0521(8)	0.0225(5)	0.0316(6)	0.0134(5)	0.0181(6)	0.0094(5)
O4	0.0582(9)	0.0238(6)	0.0258(6)	0.0105(5)	0.0119(6)	0.0068(5)
N1	0.0166(6)	0.0181(6)	0.0222(6)	0.0084(5)	0.0080(5)	0.0049(5)
N2	0.0174(6)	0.0165(5)	0.0213(6)	0.0074(5)	0.0065(5)	0.0043(4)
C1	0.0197(7)	0.0182(6)	0.0220(7)	0.0070(5)	0.0083(6)	0.0052(5)
C2	0.0240(8)	0.0189(7)	0.0286(8)	0.0045(6)	0.0102(6)	0.0038(6)
C3	0.0214(8)	0.0194(7)	0.0287(8)	0.0043(6)	0.0089(6)	0.0013(6)
C4	0.0187(7)	0.0165(6)	0.0229(7)	0.0075(5)	0.0066(6)	0.0024(5)
C5	0.0173(7)	0.0200(7)	0.0240(7)	0.0096(6)	0.0079(6)	0.0037(5)
C6	0.0174(7)	0.0197(7)	0.0237(7)	0.0102(6)	0.0079(6)	0.0050(5)
C7	0.0181(7)	0.0232(7)	0.0327(8)	0.0102(6)	0.0124(6)	0.0056(6)
C8	0.0202(8)	0.0236(7)	0.0289(8)	0.0080(6)	0.0129(6)	0.0072(6)
C9	0.0203(7)	0.0196(7)	0.0243(7)	0.0102(6)	0.0098(6)	0.0082(6)
C10	0.0216(7)	0.0179(6)	0.0238(7)	0.0091(6)	0.0094(6)	0.0063(5)
C11	0.0177(7)	0.0183(6)	0.0274(7)	0.0063(6)	0.0091(6)	0.0046(5)
C12	0.0207(8)	0.0223(7)	0.0307(8)	0.0111(6)	0.0111(6)	0.0072(6)
C13	0.0258(8)	0.0240(7)	0.0418(9)	0.0137(7)	0.0165(7)	0.0055(6)
C14	0.0203(8)	0.0266(8)	0.0399(9)	0.0063(7)	0.0102(7)	0.0003(6)
C15	0.0219(8)	0.0368(9)	0.0302(8)	0.0079(7)	0.0060(7)	0.0025(7)
C16	0.0216(8)	0.0285(8)	0.0288(8)	0.0099(6)	0.0098(6)	0.0053(6)
C17	0.0264(8)	0.0327(8)	0.0328(8)	0.0165(7)	0.0120(7)	0.0048(7)
C18	0.0316(9)	0.0320(8)	0.0409(9)	0.0205(7)	0.0153(8)	0.0091(7)
C19	0.0310(9)	0.0373(9)	0.0392(10)	0.0170(8)	0.0162(8)	0.0068(7)
C20	0.0392(10)	0.0420(10)	0.0420(10)	0.0229(8)	0.0198(9)	0.0063(8)
C21	0.0384(10)	0.0384(10)	0.0455(10)	0.0253(8)	0.0156(9)	0.0084(8)
C22	0.0316(9)	0.0346(9)	0.0417(10)	0.0202(8)	0.0158(8)	0.0111(7)

C23	0.0457(12)	0.0497(12)	0.0642(14)	0.0271(11)	0.0342(11)	0.0166(10)
C24	0.0698(16)	0.0565(13)	0.0809(17)	0.0498(13)	0.0389(14)	0.0256(12)
C25	0.0256(9)	0.0374(9)	0.0339(9)	0.0161(7)	0.0064(7)	0.0031(7)
C26	0.0345(10)	0.0402(10)	0.0425(10)	0.0146(8)	0.0119(8)	0.0054(8)
C27	0.0349(11)	0.0384(10)	0.0679(14)	0.0236(10)	0.0122(10)	0.0065(8)
C28	0.0402(12)	0.0634(14)	0.0702(15)	0.0463(13)	0.0085(11)	0.0100(10)
C29	0.0468(13)	0.0736(16)	0.0504(13)	0.0386(12)	0.0109(10)	0.0062(11)
C30	0.0364(10)	0.0540(12)	0.0397(10)	0.0236(9)	0.0146(8)	0.0091(9)
C31	0.0501(15)	0.0527(14)	0.098(2)	0.0255(14)	0.0234(15)	0.0229(12)
C32	0.074(2)	0.127(3)	0.0568(16)	0.0595(18)	0.0163(14)	0.0156(18)
C33	0.0172(7)	0.0187(7)	0.0252(7)	0.0053(6)	0.0084(6)	0.0041(5)
C34	0.0217(7)	0.0215(7)	0.0283(8)	0.0087(6)	0.0093(6)	0.0048(6)
C35	0.0238(8)	0.0197(7)	0.0352(9)	0.0088(6)	0.0107(7)	0.0066(6)
C36	0.0233(8)	0.0212(7)	0.0318(8)	0.0019(6)	0.0101(7)	0.0053(6)
C37	0.0313(9)	0.0277(8)	0.0246(8)	0.0046(6)	0.0105(7)	0.0051(7)
C38	0.0246(8)	0.0210(7)	0.0265(8)	0.0079(6)	0.0089(6)	0.0050(6)
C39	0.0456(11)	0.0255(8)	0.0414(10)	0.0175(7)	0.0265(8)	0.0145(7)
C40	0.0450(11)	0.0384(9)	0.0432(10)	0.0220(8)	0.0243(9)	0.0189(8)
C41	0.0668(15)	0.0453(11)	0.0570(13)	0.0328(10)	0.0405(12)	0.0327(11)
C42	0.0764(16)	0.0362(10)	0.0749(15)	0.0338(11)	0.0543(14)	0.0274(11)
C43	0.0617(14)	0.0319(9)	0.0649(14)	0.0173(9)	0.0439(12)	0.0119(9)
C44	0.0443(11)	0.0309(9)	0.0497(11)	0.0166(8)	0.0251(9)	0.0128(8)
C45	0.0849(19)	0.0645(15)	0.0630(14)	0.0457(13)	0.0420(14)	0.0426(14)
C46	0.0740(18)	0.0388(11)	0.092(2)	0.0160(12)	0.0529(16)	0.0011(11)
C47	0.0512(12)	0.0267(8)	0.0273(8)	0.0112(7)	0.0157(8)	0.0149(8)
C48	0.0610(14)	0.0387(10)	0.0353(10)	0.0150(8)	0.0184(9)	0.0003(9)
C49	0.096(2)	0.0427(11)	0.0372(11)	0.0219(9)	0.0215(12)	0.0067(12)
C50	0.089(2)	0.0571(14)	0.0381(11)	0.0222(10)	0.0119(13)	0.0374(14)
C51	0.0592(16)	0.097(2)	0.0447(13)	0.0193(13)	0.0169(12)	0.0480(15)
C52	0.0541(14)	0.0705(15)	0.0387(11)	0.0165(10)	0.0261(10)	0.0267(12)
C53	0.154(4)	0.111(3)	0.0513(16)	0.0402(18)	0.030(2)	−0.032(3)
C54	0.061(2)	0.309(8)	0.081(3)	0.055(4)	0.027(2)	0.085(4)
C65	0.101(6)	0.082(5)	0.092(5)	−0.004(5)	0.010(5)	−0.001(6)
Cl1	0.088(6)	0.122(7)	0.058(4)	0.004(4)	0.034(4)	0.019(5)
Cl2	0.108(7)	0.094(6)	0.112(7)	−0.010(5)	0.053(6)	−0.021(5)
C66	0.101(6)	0.078(6)	0.091(6)	−0.006(6)	0.011(6)	−0.003(6)
Cl3	0.114(9)	0.096(8)	0.077(7)	−0.012(7)	0.030(7)	−0.011(8)
Cl4	0.112(10)	0.088(8)	0.097(9)	0.014(7)	0.005(8)	−0.005(8)
C62	0.096(4)	0.070(3)	0.097(4)	0.003(3)	0.007(3)	−0.003(3)
C63	0.089(4)	0.067(3)	0.079(3)	−0.013(2)	0.008(3)	0.002(3)
C64	0.135(7)	0.087(4)	0.093(5)	0.007(4)	−0.005(5)	−0.003(5)

Table S20. Bond lengths and angles for second crystal of [Fe(3,5-Me-BAFP)(iPrNO)$_2$].

Atom–Atom	**Length [Å]**		
Fe1–N3	1.9589(14)	Fe1–N2	2.0061(13)
Fe1–N3$^{\#1}$	1.9590(14)	O5–N3	1.221(2)
Fe1–N1$^{\#1}$	1.9973(12)	N3–C55	1.495(2)
Fe1–N1	1.9973(12)	N3–H3A	0.9100
Fe1–N2$^{\#1}$	2.0061(13)	N3–H3B	0.9100
		C55–C56	1.508(3)

C55–C57	1.510(3)	C19–C23	1.507(3)
C55–H55	1.0000	C20–C21	1.385(3)
C56–H56A	0.9800	C20–H20	0.9500
C56–H56B	0.9800	C21–C22	1.394(3)
C56–H56C	0.9800	C21–C24	1.512(3)
C57–H57A	0.9800	C22–H22	0.9500
C57–H57B	0.9800	C23–H23A	0.9800
C57–H57C	0.9800	C23–H23B	0.9800
O1–C12	1.3832(19)	C23–H23C	0.9800
O1–C17	1.400(2)	C24–H24A	0.9800
O2–C16	1.382(2)	C24–H24B	0.9800
O2–C25	1.389(2)	C24–H24C	0.9800
O3–C34	1.371(2)	C24–H24D	0.9800
O3–C39	1.390(2)	C24–H24E	0.9800
O4–C38	1.3820(19)	C24–H24F	0.9800
O4–C47	1.390(2)	C25–C30	1.376(3)
N1–C4	1.3733(19)	C25–C26	1.385(3)
N1–C1	1.3751(19)	C26–C27	1.393(3)
N2–C6	1.3744(19)	C26–H26	0.9500
N2–C9	1.3789(19)	C27–C28	1.389(4)
C1–C10$^{\#1}$	1.393(2)	C27–C31	1.504(4)
C1–C2	1.442(2)	C28–C29	1.391(4)
C2–C3	1.346(2)	C28–H28	0.9500
C2–H2	0.9500	C29–C30	1.393(3)
C3–C4	1.445(2)	C29–C32	1.508(4)
C3–H3	0.9500	C30–H30	0.9500
C4–C5	1.390(2)	C31–H31A	0.9800
C5–C6	1.393(2)	C31–H31B	0.9800
C5–C11	1.496(2)	C31–H31C	0.9800
C6–C7	1.437(2)	C32–H32A	0.9800
C7–C8	1.349(2)	C32–H32B	0.9800
C7–H7	0.9500	C32–H32C	0.9800
C8–C9	1.435(2)	C33–C38	1.390(2)
C8–H8	0.9500	C33–C34	1.399(2)
C9–C10	1.387(2)	C34–C35	1.395(2)
C10–C33	1.498(2)	C35–C36	1.381(2)
C11–C12	1.396(2)	C35–H35	0.9500
C11–C16	1.399(2)	C36–C37	1.385(2)
C12–C13	1.392(2)	C36–H36	0.9500
C13–C14	1.384(3)	C37–C38	1.397(2)
C13–H13	0.9500	C37–H37	0.9500
C14–C15	1.375(3)	C39–C40	1.378(3)
C14–H14	0.9500	C39–C44	1.381(3)
C15–C16	1.388(2)	C40–C41	1.397(3)
C15–H15	0.9500	C40–H40	0.9500
C17–C22	1.378(2)	C41–C42	1.387(4)
C17–C18	1.387(3)	C41–C45	1.500(3)
C18–C19	1.386(3)	C42–C43	1.373(4)
C18–H18	0.9500	C42–H42	0.9500
C19–C20	1.399(3)	C43–C44	1.398(3)

C43–C46	1.503(3)
C44–H44	0.9500
C45–H45A	0.9800
C45–H45B	0.9800
C45–H45C	0.9800
C46–H46A	0.9800
C46–H46B	0.9800
C46–H46C	0.9800
C47–C52	1.369(3)
C47–C48	1.370(3)
C48–C49	1.393(3)
C48–H48	0.9500
C49–C50	1.382(4)
C49–C53	1.496(4)
C50–C51	1.380(4)
C50–H50	0.9500
C51–C52	1.391(3)
C51–C54	1.517(5)
C52–H52	0.9500
C53–H53A	0.9800
C53–H53B	0.9800
C53–H53C	0.9800
C54–H54A	0.9800
C54–H54B	0.9800
C54–H54C	0.9800
C65–Cl2	1.724(19)
C65–Cl1	1.767(19)
C65–H65A	0.9900
C65–H65B	0.9900
C66–Cl4	1.76(2)
C66–Cl3	1.79(2)
C66–H66A	0.9900
C66–H66B	0.9900
C62–C63	1.497(9)
C62–C62$^{\#2}$	1.526(13)
C62–H62A	0.9900
C62–H62B	0.9900
C63–C64	1.602(11)
C63–H63A	0.9900
C63–H63B	0.9900
C64–H64A	0.9800
C64–H64B	0.9800
C64–H64C	0.9800

Atom–Atom–Atom	**Angle [°]**
N3–Fe1–N3	180.00(12)
N3–Fe1–N1	89.14(5)
N3–Fe1–N1	90.86(5)
N3–Fe1–N1	90.86(5)
N3–Fe1–N1	89.14(5)
N1–Fe1–N1	180.00(7)
N3–Fe1–N2	91.91(5)
N3–Fe1–N2	88.09(5)
N1–Fe1–N2	90.31(5)
N1–Fe1–N2	89.69(5)
N3–Fe1–N2	88.09(5)
N3–Fe1–N2	91.91(5)
N1–Fe1–N2	89.69(5)
N1–Fe1–N2	90.31(5)
N2–Fe1–N2	180.0
O5–N3–C55	116.51(16)
O5–N3–Fe1	119.49(14)
C55–N3–Fe1	123.78(10)
C55–N3–H3A	106.4
Fe1–N3–H3A	106.4
C55–N3–H3B	106.4
Fe1–N3–H3B	106.4
H3A–N3–H3B	106.5
N3–C55–C56	109.04(17)
N3–C55–C57	108.53(17)
C56–C55–C57	114.8(2)
N3–C55–H55	108.1
C56–C55–H55	108.1
C57–C55–H55	108.1
C55–C56–H56A	109.5
C55–C56–H56B	109.5
H56A–C56–H56B	109.5
C55–C56–H56C	109.5
H56A–C56–H56C	109.5
H56B–C56–H56C	109.5
C55–C57–H57A	109.5
C55–C57–H57B	109.5
H57A–C57–H57B	109.5
C55–C57–H57C	109.5
H57A–C57–H57C	109.5
H57B–C57–H57C	109.5
C12–O1–C17	115.63(13)
C16–O2–C25	117.34(14)
C34–O3–C39	119.51(13)
C38–O4–C47	117.05(13)
C4–N1–C1	105.87(12)
C4–N1–Fe1	126.84(10)
C1–N1–Fe1	127.28(10)
C6–N2–C9	105.39(12)
C6–N2–Fe1	126.94(10)
C9–N2–Fe1	127.66(10)
N1–C1–C10	126.04(13)
N1–C1–C2	110.03(13)
C10–C1–C2	123.90(14)

C3–C2–C1	107.08(13)	C17–C18–H18	120.0
C3–C2–H2	126.5	C18–C19–C20	118.13(17)
C1–C2–H2	126.5	C18–C19–C23	120.53(17)
C2–C3–C4	107.07(14)	C20–C19–C23	121.30(18)
C2–C3–H3	126.5	C21–C20–C19	121.88(18)
C4–C3–H3	126.5	C21–C20–H20	119.1
N1–C4–C5	126.08(13)	C19–C20–H20	119.1
N1–C4–C3	109.94(13)	C20–C21–C22	119.15(17)
C5–C4–C3	123.97(14)	C20–C21–C24	121.40(19)
C4–C5–C6	124.20(14)	C22–C21–C24	119.38(19)
C4–C5–C11	116.79(13)	C17–C22–C21	119.15(17)
C6–C5–C11	119.01(14)	C17–C22–H22	120.4
N2–C6–C5	125.58(14)	C21–C22–H22	120.4
N2–C6–C7	110.20(13)	C19–C23–H23A	109.5
C5–C6–C7	124.22(14)	C19–C23–H23B	109.5
C8–C7–C6	107.13(14)	H23A–C23–H23B	109.5
C8–C7–H7	126.4	C19–C23–H23C	109.5
C6–C7–H7	126.4	H23A–C23–H23C	109.5
C7–C8–C9	106.92(14)	H23B–C23–H23C	109.5
C7–C8–H8	126.5	C21–C24–H24A	109.5
C9–C8–H8	126.5	C21–C24–H24B	109.5
N2–C9–C10	125.26(14)	H24A–C24–H24B	109.5
N2–C9–C8	110.32(13)	C21–C24–H24C	109.5
C10–C9–C8	124.41(14)	H24A–C24–H24C	109.5
C9–C10–C1	124.04(14)	H24B–C24–H24C	109.5
C9–C10–C33	119.95(14)	C21–C24–H24D	109.5
C1–C10–C33	115.96(13)	H24A–C24–H24D	141.1
C12–C11–C16	117.12(14)	H24B–C24–H24D	56.3
C12–C11–C5	121.97(14)	H24C–C24–H24D	56.3
C16–C11–C5	120.80(14)	C21–C24–H24E	109.5
O1–C12–C13	121.98(15)	H24A–C24–H24E	56.3
O1–C12–C11	116.43(14)	H24B–C24–H24E	141.1
C13–C12–C11	121.57(15)	H24C–C24–H24E	56.3
C14–C13–C12	119.16(16)	H24D–C24–H24E	109.5
C14–C13–H13	120.4	C21–C24–H24F	109.5
C12–C13–H13	120.4	H24A–C24–H24F	56.3
C15–C14–C13	120.94(16)	H24B–C24–H24F	56.3
C15–C14–H14	119.5	H24C–C24–H24F	141.1
C13–C14–H14	119.5	H24D–C24–H24F	109.5
C14–C15–C16	119.18(16)	H24E–C24–H24F	109.5
C14–C15–H15	120.4	C30–C25–C26	121.60(18)
C16–C15–H15	120.4	C30–C25–O2	116.84(17)
O2–C16–C15	121.26(15)	C26–C25–O2	121.52(17)
O2–C16–C11	116.77(14)	C25–C26–C27	119.3(2)
C15–C16–C11	121.87(16)	C25–C26–H26	120.3
C22–C17–C18	121.64(17)	C27–C26–H26	120.3
C22–C17–O1	118.32(16)	C28–C27–C26	118.8(2)
C18–C17–O1	120.04(15)	C28–C27–C31	121.3(2)
C19–C18–C17	120.04(16)	C26–C27–C31	120.0(2)
C19–C18–H18	120.0	C27–C28–C29	122.1(2)

C27–C28–H28	119.0	C42–C43–C44	118.5(2)
C29–C28–H28	119.0	C42–C43–C46	121.4(2)
C28–C29–C30	118.3(2)	C44–C43–C46	120.1(2)
C28–C29–C32	121.2(2)	C39–C44–C43	119.5(2)
C30–C29–C32	120.5(3)	C39–C44–H44	120.3
C25–C30–C29	119.9(2)	C43–C44–H44	120.3
C25–C30–H30	120.0	C41–C45–H45A	109.5
C29–C30–H30	120.0	C41–C45–H45B	109.5
C27–C31–H31A	109.5	H45A–C45–H45B	109.5
C27–C31–H31B	109.5	C41–C45–H45C	109.5
H31A–C31–H31B	109.5	H45A–C45–H45C	109.5
C27–C31–H31C	109.5	H45B–C45–H45C	109.5
H31A–C31–H31C	109.5	C43–C46–H46A	109.5
H31B–C31–H31C	109.5	C43–C46–H46B	109.5
C29–C32–H32A	109.5	H46A–C46–H46B	109.5
C29–C32–H32B	109.5	C43–C46–H46C	109.5
H32A–C32–H32B	109.5	H46A–C46–H46C	109.5
C29–C32–H32C	109.5	H46B–C46–H46C	109.5
H32A–C32–H32C	109.5	C52–C47–C48	121.81(19)
H32B–C32–H32C	109.5	C52–C47–O4	118.80(18)
C38–C33–C34	117.50(14)	C48–C47–O4	119.30(19)
C38–C33–C10	120.93(13)	C47–C48–C49	119.7(2)
C34–C33–C10	121.17(14)	C47–C48–H48	120.1
O3–C34–C35	123.37(14)	C49–C48–H48	120.1
O3–C34–C33	115.12(13)	C50–C49–C48	118.2(2)
C35–C34–C33	121.49(15)	C50–C49–C53	120.4(3)
C36–C35–C34	119.10(15)	C48–C49–C53	121.3(3)
C36–C35–H35	120.5	C51–C50–C49	122.1(2)
C34–C35–H35	120.5	C51–C50–H50	118.9
C35–C36–C37	121.25(15)	C49–C50–H50	118.9
C35–C36–H36	119.4	C50–C51–C52	118.6(3)
C37–C36–H36	119.4	C50–C51–C54	122.0(3)
C36–C37–C38	118.58(16)	C52–C51–C54	119.4(3)
C36–C37–H37	120.7	C47–C52–C51	119.5(2)
C38–C37–H37	120.7	C47–C52–H52	120.3
O4–C38–C33	116.13(13)	C51–C52–H52	120.3
O4–C38–C37	121.83(15)	C49–C53–H53A	109.5
C33–C38–C37	122.01(15)	C49–C53–H53B	109.5
C40–C39–C44	121.61(17)	H53A–C53–H53B	109.5
C40–C39–O3	116.72(17)	C49–C53–H53C	109.5
C44–C39–O3	121.44(17)	H53A–C53–H53C	109.5
C39–C40–C41	119.4(2)	H53B–C53–H53C	109.5
C39–C40–H40	120.3	C51–C54–H54A	109.5
C41–C40–H40	120.3	C51–C54–H54B	109.5
C42–C41–C40	118.4(2)	H54A–C54–H54B	109.5
C42–C41–C45	121.2(2)	C51–C54–H54C	109.5
C40–C41–C45	120.4(2)	H54A–C54–H54C	109.5
C43–C42–C41	122.61(19)	H54B–C54–H54C	109.5
C43–C42–H42	118.7	Cl2–C65–Cl1	113.1(15)
C41–C42–H42	118.7	Cl2–C65–H65A	109.0

Cl1–C65–H65A	109.0
Cl2–C65–H65B	109.0
Cl1–C65–H65B	109.0
H65A–C65–H65B	107.8
Cl4–C66–Cl3	109.3(17)
Cl4–C66–H66A	109.8
Cl3–C66–H66A	109.8
Cl4–C66–H66B	109.8
Cl3–C66–H66B	109.8
H66A–C66–H66B	108.3
C63–C62–C62	115.8(7)
C63–C62–H62A	108.3
C62–C62–H62A	108.3
C63–C62–H62B	108.3
C62–C62–H62B	108.3
H62A–C62–H62B	107.4
C62–C63–C64	112.4(8)
C62–C63–H63A	109.1
C64–C63–H63A	109.1
C62–C63–H63B	109.1
C64–C63–H63B	109.1
H63A–C63–H63B	107.9
C63–C64–H64A	109.5
C63–C64–H64B	109.5
H64A–C64–H64B	109.5
C63–C64–H64C	109.5
H64A–C64–H64C	109.5
H64B–C64–H64C	109.5

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 1-Y, 1-Z; #2: -X, -Y, -Z;

Table S21. Torsion angles for second crystal of [Fe(3,5-Me-BAFP)(iPrNO)$_2$].

Atom–Atom–Atom–Atom	Torsion Angle [°]
O5–N3–C55–C56	−60.5(2)
Fe1–N3–C55–C56	124.88(17)
O5–N3–C55–C57	65.2(2)
Fe1–N3–C55–C57	−109.37(16)
C4–N1–C1–C10$^{\#1}$	178.89(14)
Fe1–N1–C1–C10$^{\#1}$	−0.8(2)
C4–N1–C1–C2	0.83(16)
Fe1–N1–C1–C2	−178.86(10)
N1–C1–C2–C3	−0.30(18)
C10$^{\#1}$–C1–C2–C3	−178.41(15)
C1–C2–C3–C4	−0.34(18)
C1–N1–C4–C5	177.94(14)
Fe1–N1–C4–C5	−2.4(2)
C1–N1–C4–C3	−1.04(16)
Fe1–N1–C4–C3	178.65(10)
C2–C3–C4–N1	0.88(18)
C2–C3–C4–C5	−178.13(15)
N1–C4–C5–C6	0.6(2)
C3–C4–C5–C6	179.48(15)
N1–C4–C5–C11	−178.94(14)
C3–C4–C5–C11	−0.1(2)
C9–N2–C6–C5	177.80(14)
Fe1–N2–C6–C5	−1.3(2)
C9–N2–C6–C7	−1.48(16)
Fe1–N2–C6–C7	179.39(10)
C4–C5–C6–N2	1.3(2)
C11–C5–C6–N2	−179.11(13)
C4–C5–C6–C7	−179.50(15)
C11–C5–C6–C7	0.1(2)
N2–C6–C7–C8	0.95(18)
C5–C6–C7–C8	−178.34(15)
C6–C7–C8–C9	−0.02(18)
C6–N2–C9–C10	−178.90(14)
Fe1–N2–C9–C10	0.2(2)
C6–N2–C9–C8	1.47(16)
Fe1–N2–C9–C8	−179.41(10)
C7–C8–C9–N2	−0.92(18)
C7–C8–C9–C10	179.45(15)
N2–C9–C10–C1$^{\#1}$	−1.5(2)
C8–C9–C10–C1$^{\#1}$	178.11(15)
N2–C9–C10–C33	−178.78(14)
C8–C9–C10–C33	0.8(2)
C4–C5–C11–C12	103.08(17)
C6–C5–C11–C12	−76.52(19)
C4–C5–C11–C16	−72.97(19)
C6–C5–C11–C16	107.44(17)

C17–O1–C12–C13	−20.2(2)
C17–O1–C12–C11	161.63(14)
C16–C11–C12–O1	−177.49(13)
C5–C11–C12–O1	6.3(2)
C16–C11–C12–C13	4.3(2)
C5–C11–C12–C13	−171.90(14)
O1–C12–C13–C14	−179.44(15)
C11–C12–C13–C14	−1.3(2)
C12–C13–C14–C15	−2.1(3)
C13–C14–C15–C16	2.3(3)
C25–O2–C16–C15	40.2(2)
C25–O2–C16–C11	−143.30(15)
C14–C15–C16–O2	177.17(16)
C14–C15–C16–C11	0.9(3)
C12–C11–C16–O2	179.46(14)
C5–C11–C16–O2	−4.3(2)
C12–C11–C16–C15	−4.1(2)
C5–C11–C16–C15	172.16(15)
C12–O1–C17–C22	115.22(17)
C12–O1–C17–C18	−64.0(2)
C22–C17–C18–C19	−1.0(3)
O1–C17–C18–C19	178.21(16)
C17–C18–C19–C20	0.5(3)
C17–C18–C19–C23	−177.07(18)
C18–C19–C20–C21	−0.5(3)
C23–C19–C20–C21	177.1(2)
C19–C20–C21–C22	0.9(3)
C19–C20–C21–C24	−175.7(2)
C18–C17–C22–C21	1.4(3)
O1–C17–C22–C21	−177.81(16)
C20–C21–C22–C17	−1.4(3)
C24–C21–C22–C17	175.4(2)
C16–O2–C25–C30	−137.26(17)
C16–O2–C25–C26	45.0(2)
C30–C25–C26–C27	−1.3(3)
O2–C25–C26–C27	176.41(17)
C25–C26–C27–C28	1.2(3)
C25–C26–C27–C31	−179.0(2)
C26–C27–C28–C29	−0.3(3)
C31–C27–C28–C29	179.9(2)
C27–C28–C29–C30	−0.6(4)
C27–C28–C29–C32	178.8(3)
C26–C25–C30–C29	0.3(3)
O2–C25–C30–C29	−177.44(19)
C28–C29–C30–C25	0.6(3)
C32–C29–C30–C25	−178.8(2)
C9–C10–C33–C38	83.30(19)
C1$^{\#1}$–C10–C33–C38	−94.22(18)
C9–C10–C33–C34	−104.08(18)
C1$^{\#1}$–C10–C33–C34	78.40(19)

C39–O3–C34–C35	24.3(2)
C39–O3–C34–C33	−157.54(15)
C38–C33–C34–O3	−175.46(14)
C10–C33–C34–O3	11.7(2)
C38–C33–C34–C35	2.8(2)
C10–C33–C34–C35	−170.09(15)
O3–C34–C35–C36	177.22(15)
C33–C34–C35–C36	−0.9(2)
C34–C35–C36–C37	−1.2(3)
C35–C36–C37–C38	1.2(3)
C47–O4–C38–C33	142.38(16)
C47–O4–C38–C37	−39.4(2)
C34–C33–C38–O4	175.45(14)
C10–C33–C38–O4	−11.7(2)
C34–C33–C38–C37	−2.7(2)
C10–C33–C38–C37	170.14(15)
C36–C37–C38–O4	−177.29(15)
C36–C37–C38–C33	0.8(3)
C34–O3–C39–C40	−131.81(17)
C34–O3–C39–C44	53.6(2)
C44–C39–C40–C41	0.9(3)
O3–C39–C40–C41	−173.66(17)
C39–C40–C41–C42	−1.9(3)
C39–C40–C41–C45	176.76(19)
C40–C41–C42–C43	1.7(3)
C45–C41–C42–C43	−177.0(2)
C41–C42–C43–C44	−0.4(3)
C41–C42–C43–C46	178.3(2)
C40–C39–C44–C43	0.3(3)
O3–C39–C44–C43	174.66(17)
C42–C43–C44–C39	−0.6(3)
C46–C43–C44–C39	−179.3(2)
C38–O4–C47–C52	−75.3(2)
C38–O4–C47–C48	108.1(2)
C52–C47–C48–C49	−0.7(3)
O4–C47–C48–C49	175.85(18)
C47–C48–C49–C50	0.0(3)
C47–C48–C49–C53	179.1(3)
C48–C49–C50–C51	0.1(4)
C53–C49–C50–C51	−179.0(3)
C49–C50–C51–C52	0.5(4)
C49–C50–C51–C54	179.5(4)
C48–C47–C52–C51	1.3(3)
O4–C47–C52–C51	−175.3(2)
C50–C51–C52–C47	−1.1(4)
C54–C51–C52–C47	179.8(4)
C62$^{\#2}$–C62–C63–C64	177.0(7)

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 1-Y, 1-Z; #2: -X, -Y, -Z;

Table S22. Crystal data and structure refinement for [Fe(3,5-Me-BAFP)(iPrNH$_2$)(iPrNO)].

CCDC number	
Empirical formula	$C_{118.53}H_{118.38}Cl_{0.67}FeN_6O_{9.05}$
Formula weight	1851.32
Temperature [K]	150(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	12.6436(4)
b [Å]	14.3552(4)
c [Å]	16.4422(5)
α [°]	113.0869(14)
β [°]	111.5479(12)
γ [°]	91.5369(13)
Volume [Å^3]	2501.99(13)
Z	1
ρ_{calc} [gcm^{-3}]	1.229
μ [mm^{-1}]	1.867
F(000)	981
Crystal size [mm^3]	0.430×0.170×0.140
Crystal colour	?
Crystal shape	?
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	6.41 to 160.12 (0.78 Å)
Index ranges	−15 ≤ h ≤ 14
	−18 ≤ k ≤ 17
	−20 ≤ l ≤ 20
Reflections collected	25304
Independent reflections	9876
	R_{int} = 0.0372
	R_{sigma} = 0.0428
Completeness to θ = 67.679°	98.0 %
Data / Restraints / Parameters	9876/146/689
Absorption correction	0.5494/0.7543
T_{min}/T_{max} (method)	(multi-scan)
Goodness-of-fit on F^2	1.091
Final *R* indexes	R_1 = 0.0436
[$I \geq 2\sigma(I)$]	wR_2 = 0.1194
Final *R* indexes	R_1 = 0.0465
[all data]	wR_2 = 0.1220
Largest peak/hole [eÅ^{-3}]	0.29/−0.44

Refinement Details:

A crystal structure was obtained of [Fe(3,5-Me-BAFP)(iPrNO)$_2$] reacted with B$_2$(pin)$_2$. The structure was solved by isomorphous replacement from the [Fe(3,5-Me-BAFP)(iPrNO)$_2$] crystal. The disorder model was adjusted (two methylene chloride moieties, no THF molecule, partial oxygen loss).The isopropyl nitrosyl ligand was found to be disordered with an isopropyl amine ligand, i.e. the oxygen atom at the nitrogen was partially replaced by two hydrogen atoms. No disorder was refined for the N atom or the isopropyl group. The occupancy ratio refined to 0.522(6)

to 0.478(6) iPrNO:iPrNH$_2$. A solvate occupied area was refined as major hexanes and minor methylene chloride (two moieties). The hexane molecule is inversion symmetric. Bond distances of methylene chloride were restrained to expected target values (1.77(2) Å for C-Cl bonds and 2.90(2) Å for Cl...Cl). C-C bond distances of the hexane were restrained to 1.51(2) and 1.55(2) Å for CH_2-CH_2 and CH_2-CH_3 moieties, respectively. Uij components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar. Occupancies were not constrained to unity. Subject to these conditions, occupancy rates refined to 0.699(7), 0.113(3) and 0.054(3), respectively, for hexane and the two CH_2Cl_2 moieties.

Table S23. Atomic coordinates and U_{eq} [Å^2] for [Fe(3,5-Me-BAFP)(iPrNH$_2$)(iPrNO)].

Atom	***x***	***y***	***z***	U_{eq}
Fe1	0.500000	0.500000	0.500000	0.01836(10)
O5	0.4200(2)	0.64059(16)	0.42644(16)	0.0301(8)
N3	0.44796(13)	0.55638(10)	0.40418(10)	0.0284(3)
H3A	0.373346	0.562853	0.394112	0.043
H3B	0.490492	0.621667	0.433529	0.043
C55	0.44973(17)	0.50662(14)	0.30612(12)	0.0324(4)
H55	0.470825	0.437597	0.296460	0.039
C56	0.3297(2)	0.4895(2)	0.23005(17)	0.0691(8)
H56A	0.329652	0.454834	0.165468	0.104
H56B	0.306652	0.556180	0.238866	0.104
H56C	0.274690	0.446179	0.236363	0.104
C57	0.5433(2)	0.5721(2)	0.3040(2)	0.0613(7)
H57A	0.548260	0.538565	0.241288	0.092
H57B	0.617933	0.580077	0.356059	0.092
H57C	0.524329	0.640330	0.313432	0.092
O1	0.14065(10)	0.28088(9)	0.50370(9)	0.0306(3)
O2	0.06054(10)	0.33581(11)	0.22328(9)	0.0361(3)
O3	0.37252(12)	0.87543(9)	0.61094(9)	0.0345(3)
O4	0.42915(13)	0.72077(9)	0.82327(9)	0.0377(3)
N1	0.41307(10)	0.35869(9)	0.39831(9)	0.0190(2)
N2	0.35837(11)	0.53086(9)	0.52542(9)	0.0191(2)
C1	0.45498(13)	0.28260(11)	0.34372(11)	0.0206(3)
C2	0.36390(14)	0.19262(12)	0.27703(12)	0.0260(3)
H2	0.370535	0.129886	0.231315	0.031
C3	0.26774(14)	0.21426(11)	0.29174(12)	0.0257(3)
H3	0.193580	0.169811	0.258152	0.031
C4	0.29856(13)	0.31785(11)	0.36826(11)	0.0204(3)
C5	0.22228(13)	0.36647(11)	0.40568(11)	0.0206(3)
C6	0.25179(13)	0.46599(11)	0.47994(11)	0.0201(3)
C7	0.17317(14)	0.51600(12)	0.51918(12)	0.0247(3)
H7	0.094855	0.487049	0.500586	0.030
C8	0.23146(13)	0.61176(12)	0.58736(12)	0.0244(3)
H8	0.202035	0.662999	0.625845	0.029
C9	0.34636(13)	0.62145(11)	0.59067(11)	0.0209(3)
C10	0.43268(13)	0.70962(11)	0.65158(11)	0.0209(3)
C11	0.10146(13)	0.30614(11)	0.36267(11)	0.0224(3)

C12	0.06406(14)	0.25967(12)	0.41032(12)	0.0245(3)
C13	-0.04331(15)	0.19324(12)	0.36499(13)	0.0298(4)
H13	-0.066679	0.161156	0.398073	0.036
C14	-0.11559(15)	0.17451(13)	0.27109(13)	0.0325(4)
H14	-0.187844	0.127466	0.239012	0.039
C15	-0.08430(15)	0.22305(14)	0.22359(13)	0.0335(4)
H15	-0.135620	0.211708	0.160033	0.040
C16	0.02321(14)	0.28881(13)	0.26966(12)	0.0273(3)
C17	0.09180(15)	0.26079(13)	0.56043(12)	0.0299(4)
C18	0.01110(16)	0.31607(14)	0.58460(13)	0.0330(4)
H18	-0.009404	0.368952	0.564200	0.040
C19	-0.03966(16)	0.29420(14)	0.63851(14)	0.0351(4)
C20	-0.00627(17)	0.21633(15)	0.66777(14)	0.0385(4)
H20	-0.039878	0.200892	0.705201	0.046
C21	0.07438(17)	0.16111(15)	0.64373(15)	0.0387(4)
C22	0.12506(16)	0.18468(14)	0.59000(14)	0.0344(4)
H22	0.181793	0.148709	0.573981	0.041
C23	-0.1316(2)	0.35021(18)	0.66116(18)	0.0484(5)
H23A	-0.122926	0.416844	0.658447	0.073
H23B	-0.123192	0.361812	0.726267	0.073
H23C	-0.208566	0.308416	0.613509	0.073
C24	0.1037(2)	0.0722(2)	0.6698(2)	0.0593(6)
H24A	0.169485	0.049186	0.655073	0.089
H24B	0.036353	0.014913	0.632112	0.089
H24C	0.124177	0.094946	0.739164	0.089
H24D	0.050526	0.056844	0.695827	0.089
H24E	0.183657	0.091117	0.718787	0.089
H24F	0.095833	0.011084	0.611736	0.089
C25	-0.02080(15)	0.37256(14)	0.16608(13)	0.0340(4)
C26	-0.09686(17)	0.42820(15)	0.19789(15)	0.0415(4)
H26	-0.097475	0.438851	0.258489	0.050
C27	-0.17239(19)	0.46836(16)	0.14012(18)	0.0497(5)
C28	-0.1706(2)	0.4496(2)	0.05115(19)	0.0565(6)
H28	-0.222320	0.476579	0.011426	0.068
C29	-0.0955(2)	0.3925(2)	0.01836(18)	0.0558(6)
C30	-0.01950(18)	0.35426(17)	0.07782(15)	0.0425(5)
H30	0.033211	0.315573	0.057466	0.051
C31	-0.2541(2)	0.5305(2)	0.1744(2)	0.0713(8)
H31A	-0.320030	0.528836	0.118409	0.107
H31B	-0.213242	0.602146	0.218039	0.107
H31C	-0.282286	0.500952	0.208974	0.107
C32	-0.0967(3)	0.3712(3)	-0.0794(2)	0.0824(9)
H32A	-0.120503	0.296726	-0.121125	0.124
H32B	-0.018765	0.395747	-0.071320	0.124
H32C	-0.151497	0.407360	-0.109321	0.124
C33	0.40900(13)	0.80252(11)	0.72074(11)	0.0219(3)
C34	0.38966(14)	0.88932(12)	0.70259(12)	0.0249(3)
C35	0.38514(14)	0.98160(12)	0.77285(12)	0.0277(3)
H35	0.372980	1.040165	0.759680	0.033
C36	0.39860(14)	0.98670(12)	0.86182(12)	0.0291(4)

H36	0.397085	1.049799	0.910320	0.035
C37	0.41426(15)	0.90156(13)	0.88168(12)	0.0305(4)
H37	0.421923	0.905338	0.942637	0.037
C38	0.41854(14)	0.81002(12)	0.81018(11)	0.0254(3)
C39	0.39289(17)	0.96076(13)	0.59452(14)	0.0335(4)
C40	0.30769(18)	0.96752(15)	0.51664(15)	0.0385(4)
H40	0.235873	0.919450	0.480999	0.046
C41	0.3280(2)	1.04573(17)	0.49059(17)	0.0474(5)
C42	0.4327(2)	1.11606(16)	0.54635(19)	0.0513(6)
H42	0.445989	1.170485	0.529971	0.062
C43	0.5178(2)	1.11017(15)	0.62427(18)	0.0483(5)
C44	0.49749(18)	1.03038(14)	0.64852(15)	0.0399(4)
H44	0.555206	1.024102	0.701729	0.048
C45	0.2392(3)	1.0514(2)	0.40300(19)	0.0602(7)
H45A	0.263808	1.024897	0.349492	0.090
H45B	0.231535	1.123394	0.418293	0.090
H45C	0.164262	1.009583	0.383976	0.090
C46	0.6318(3)	1.18585(18)	0.6817(2)	0.0669(8)
H46A	0.695446	1.148374	0.691846	0.100
H46B	0.634424	1.233877	0.744576	0.100
H46C	0.639733	1.224621	0.645992	0.100
C47	0.50308(18)	0.73168(13)	0.91469(13)	0.0352(4)
C48	0.4569(2)	0.71712(16)	0.97323(15)	0.0460(5)
H48	0.375132	0.704253	0.953165	0.055
C49	0.5302(3)	0.72127(18)	1.06231(16)	0.0592(7)
C50	0.6486(3)	0.7402(2)	1.08865(17)	0.0649(8)
H50	0.699409	0.743108	1.149213	0.078
C51	0.6953(2)	0.7551(3)	1.02982(18)	0.0716(9)
C52	0.6204(2)	0.7515(2)	0.94158(16)	0.0543(6)
H52	0.650471	0.762667	0.900289	0.065
C53	0.4832(4)	0.7073(3)	1.1290(2)	0.1086(15)
H53A	0.467290	0.633633	1.113202	0.163
H53B	0.411250	0.733772	1.121119	0.163
H53C	0.540336	0.745207	1.196182	0.163
C54	0.8253(3)	0.7767(6)	1.0594(3)	0.160(3)
H54A	0.863396	0.745360	1.102976	0.240
H54B	0.854876	0.851582	1.092770	0.240
H54C	0.841560	0.747308	1.001469	0.240
C65	0.145(2)	-0.071(3)	0.031(2)	0.116(5)
H65A	0.143859	-0.008216	0.018470	0.139
H65B	0.095704	-0.130167	-0.031314	0.139
Cl1	0.2885(10)	-0.0910(13)	0.0697(9)	0.100(4)
Cl2	0.0860(11)	-0.0548(9)	0.1136(10)	0.122(4)
C66	0.116(4)	-0.034(7)	0.049(5)	0.114(5)
H66A	0.091984	0.033685	0.068130	0.137
H66B	0.052371	-0.084431	-0.011661	0.137
Cl3	0.244(2)	-0.0214(17)	0.0271(14)	0.116(6)
Cl4	0.147(2)	-0.0751(19)	0.1410(16)	0.120(7)
C62	0.0397(5)	-0.0332(4)	0.0181(5)	0.110(2)
H62A	0.040495	-0.024196	0.081232	0.132

H62B	0.005780	-0.106620	-0.028060	0.132
C63	0.1625(6)	-0.0109(5)	0.0308(4)	0.102(2)
H63A	0.196426	0.063066	0.074751	0.123
H63B	0.163175	-0.024108	-0.032831	0.123
C64	0.2411(9)	-0.0800(8)	0.0742(7)	0.133(4)
H64A	0.215584	-0.152436	0.026191	0.200
H64B	0.233260	-0.073652	0.133184	0.200
H64C	0.322464	-0.056050	0.089817	0.200

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S24. Anisotropic displacement parameters [Å^2] fo [Fe(3,5-Me-BAFP)(iPrNH$_2$)(iPrNO)]. The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	0.01539(17)	0.01686(15)	0.02072(17)	0.00594(12)	0.00757(13)	0.00361(12)
O5	0.0349(14)	0.0241(12)	0.0350(13)	0.0158(10)	0.0144(10)	0.0128(9)
N3	0.0320(8)	0.0225(6)	0.0345(7)	0.0117(6)	0.0179(6)	0.0107(5)
C55	0.0408(10)	0.0354(9)	0.0294(8)	0.0173(7)	0.0188(8)	0.0188(8)
C56	0.0593(16)	0.0666(15)	0.0402(12)	0.0021(11)	−0.0012(11)	0.0314(13)
C57	0.0707(17)	0.0782(17)	0.0809(18)	0.0547(15)	0.0558(15)	0.0326(14)
O1	0.0225(6)	0.0390(6)	0.0341(6)	0.0203(5)	0.0107(5)	0.0049(5)
O2	0.0238(6)	0.0525(8)	0.0357(6)	0.0254(6)	0.0092(5)	0.0064(5)
O3	0.0521(8)	0.0225(5)	0.0316(6)	0.0134(5)	0.0181(6)	0.0094(5)
O4	0.0582(9)	0.0238(6)	0.0258(6)	0.0105(5)	0.0119(6)	0.0068(5)
N1	0.0166(6)	0.0181(6)	0.0222(6)	0.0084(5)	0.0080(5)	0.0049(5)
N2	0.0174(6)	0.0165(5)	0.0213(6)	0.0074(5)	0.0065(5)	0.0043(4)
C1	0.0197(7)	0.0182(6)	0.0220(7)	0.0070(5)	0.0083(6)	0.0052(5)
C2	0.0240(8)	0.0189(7)	0.0286(8)	0.0045(6)	0.0102(6)	0.0038(6)
C3	0.0214(8)	0.0194(7)	0.0287(8)	0.0043(6)	0.0089(6)	0.0013(6)
C4	0.0187(7)	0.0165(6)	0.0229(7)	0.0075(5)	0.0066(6)	0.0024(5)
C5	0.0173(7)	0.0200(7)	0.0240(7)	0.0096(6)	0.0079(6)	0.0037(5)
C6	0.0174(7)	0.0197(7)	0.0237(7)	0.0102(6)	0.0079(6)	0.0050(5)
C7	0.0181(7)	0.0232(7)	0.0327(8)	0.0102(6)	0.0124(6)	0.0056(6)
C8	0.0202(8)	0.0236(7)	0.0289(8)	0.0080(6)	0.0129(6)	0.0072(6)
C9	0.0203(7)	0.0196(7)	0.0243(7)	0.0102(6)	0.0098(6)	0.0082(6)
C10	0.0216(7)	0.0179(6)	0.0238(7)	0.0091(6)	0.0094(6)	0.0063(5)
C11	0.0177(7)	0.0183(6)	0.0274(7)	0.0063(6)	0.0091(6)	0.0046(5)
C12	0.0207(8)	0.0223(7)	0.0307(8)	0.0111(6)	0.0111(6)	0.0072(6)
C13	0.0258(8)	0.0240(7)	0.0418(9)	0.0137(7)	0.0165(7)	0.0055(6)
C14	0.0203(8)	0.0266(8)	0.0399(9)	0.0063(7)	0.0102(7)	0.0003(6)
C15	0.0219(8)	0.0368(9)	0.0302(8)	0.0079(7)	0.0060(7)	0.0025(7)
C16	0.0216(8)	0.0285(8)	0.0288(8)	0.0099(6)	0.0098(6)	0.0053(6)
C17	0.0264(8)	0.0327(8)	0.0328(8)	0.0165(7)	0.0120(7)	0.0048(7)
C18	0.0316(9)	0.0320(8)	0.0409(9)	0.0205(7)	0.0153(8)	0.0091(7)
C19	0.0310(9)	0.0373(9)	0.0392(10)	0.0170(8)	0.0162(8)	0.0068(7)
C20	0.0392(10)	0.0420(10)	0.0420(10)	0.0229(8)	0.0198(9)	0.0063(8)
C21	0.0384(10)	0.0384(10)	0.0455(10)	0.0253(8)	0.0156(9)	0.0084(8)
C22	0.0316(9)	0.0346(9)	0.0417(10)	0.0202(8)	0.0158(8)	0.0111(7)
C23	0.0457(12)	0.0497(12)	0.0642(14)	0.0271(11)	0.0342(11)	0.0166(10)
C24	0.0698(16)	0.0565(13)	0.0809(17)	0.0498(13)	0.0389(14)	0.0256(12)

C25	0.0256(9)	0.0374(9)	0.0339(9)	0.0161(7)	0.0064(7)	0.0031(7)
C26	0.0345(10)	0.0402(10)	0.0425(10)	0.0146(8)	0.0119(8)	0.0054(8)
C27	0.0349(11)	0.0384(10)	0.0679(14)	0.0236(10)	0.0122(10)	0.0065(8)
C28	0.0402(12)	0.0634(14)	0.0702(15)	0.0463(13)	0.0085(11)	0.0100(10)
C29	0.0468(13)	0.0736(16)	0.0504(13)	0.0386(12)	0.0109(10)	0.0062(11)
C30	0.0364(10)	0.0540(12)	0.0397(10)	0.0236(9)	0.0146(8)	0.0091(9)
C31	0.0501(15)	0.0527(14)	0.098(2)	0.0255(14)	0.0234(15)	0.0229(12)
C32	0.074(2)	0.127(3)	0.0568(16)	0.0595(18)	0.0163(14)	0.0156(18)
C33	0.0172(7)	0.0187(7)	0.0252(7)	0.0053(6)	0.0084(6)	0.0041(5)
C34	0.0217(7)	0.0215(7)	0.0283(8)	0.0087(6)	0.0093(6)	0.0048(6)
C35	0.0238(8)	0.0197(7)	0.0352(9)	0.0088(6)	0.0107(7)	0.0066(6)
C36	0.0233(8)	0.0212(7)	0.0318(8)	0.0019(6)	0.0101(7)	0.0053(6)
C37	0.0313(9)	0.0277(8)	0.0246(8)	0.0046(6)	0.0105(7)	0.0051(7)
C38	0.0246(8)	0.0210(7)	0.0265(8)	0.0079(6)	0.0089(6)	0.0050(6)
C39	0.0456(11)	0.0255(8)	0.0414(10)	0.0175(7)	0.0265(8)	0.0145(7)
C40	0.0450(11)	0.0384(9)	0.0432(10)	0.0220(8)	0.0243(9)	0.0189(8)
C41	0.0668(15)	0.0453(11)	0.0570(13)	0.0328(10)	0.0405(12)	0.0327(11)
C42	0.0764(16)	0.0362(10)	0.0749(15)	0.0338(11)	0.0543(14)	0.0274(11)
C43	0.0617(14)	0.0319(9)	0.0649(14)	0.0173(9)	0.0439(12)	0.0119(9)
C44	0.0443(11)	0.0309(9)	0.0497(11)	0.0166(8)	0.0251(9)	0.0128(8)
C45	0.0849(19)	0.0645(15)	0.0630(14)	0.0457(13)	0.0420(14)	0.0426(14)
C46	0.0740(18)	0.0388(11)	0.092(2)	0.0160(12)	0.0529(16)	0.0011(11)
C47	0.0512(12)	0.0267(8)	0.0273(8)	0.0112(7)	0.0157(8)	0.0149(8)
C48	0.0610(14)	0.0387(10)	0.0353(10)	0.0150(8)	0.0184(9)	0.0003(9)
C49	0.096(2)	0.0427(11)	0.0372(11)	0.0219(9)	0.0215(12)	0.0067(12)
C50	0.089(2)	0.0571(14)	0.0381(11)	0.0222(10)	0.0119(13)	0.0374(14)
C51	0.0592(16)	0.097(2)	0.0447(13)	0.0193(13)	0.0169(12)	0.0480(15)
C52	0.0541(14)	0.0705(15)	0.0387(11)	0.0165(10)	0.0261(10)	0.0267(12)
C53	0.154(4)	0.111(3)	0.0513(16)	0.0402(18)	0.030(2)	−0.032(3)
C54	0.061(2)	0.309(8)	0.081(3)	0.055(4)	0.027(2)	0.085(4)
C65	0.101(6)	0.082(5)	0.092(5)	−0.004(5)	0.010(5)	−0.001(6)
Cl1	0.088(6)	0.122(7)	0.058(4)	0.004(4)	0.034(4)	0.019(5)
Cl2	0.108(7)	0.094(6)	0.112(7)	−0.010(5)	0.053(6)	−0.021(5)
C66	0.101(6)	0.078(6)	0.091(6)	−0.006(6)	0.011(6)	−0.003(6)
Cl3	0.114(9)	0.096(8)	0.077(7)	−0.012(7)	0.030(7)	−0.011(8)
Cl4	0.112(10)	0.088(8)	0.097(9)	0.014(7)	0.005(8)	−0.005(8)
C62	0.096(4)	0.070(3)	0.097(4)	0.003(3)	0.007(3)	−0.003(3)
C63	0.089(4)	0.067(3)	0.079(3)	−0.013(2)	0.008(3)	0.002(3)
C64	0.135(7)	0.087(4)	0.093(5)	0.007(4)	−0.005(5)	−0.003(5)

Table S25. Bond lengths and angles for [Fe(3,5-Me-BAFP)(iPrNH$_2$)(iPrNO)].

Atom–Atom	**Length [Å]**
Fe1–N3	1.9589(14)
Fe1–N3$^{\#1}$	1.9590(14)
Fe1–N1$^{\#1}$	1.9973(12)
Fe1–N1	1.9973(12)
Fe1–N2$^{\#1}$	2.0061(13)
Fe1–N2	2.0061(13)
O5–N3	1.221(2)
N3–C55	1.495(2)
N3–H3A	0.9100
N3–H3B	0.9100
C55–C56	1.508(3)
C55–C57	1.510(3)
C55–H55	1.0000
C56–H56A	0.9800
C56–H56B	0.9800

C56–H56C	0.9800	C21–C24	1.512(3)
C57–H57A	0.9800	C22–H22	0.9500
C57–H57B	0.9800	C23–H23A	0.9800
C57–H57C	0.9800	C23–H23B	0.9800
O1–C12	1.3832(19)	C23–H23C	0.9800
O1–C17	1.400(2)	C24–H24A	0.9800
O2–C16	1.382(2)	C24–H24B	0.9800
O2–C25	1.389(2)	C24–H24C	0.9800
O3–C34	1.371(2)	C24–H24D	0.9800
O3–C39	1.390(2)	C24–H24E	0.9800
O4–C38	1.3820(19)	C24–H24F	0.9800
O4–C47	1.390(2)	C25–C30	1.376(3)
N1–C4	1.3733(19)	C25–C26	1.385(3)
N1–C1	1.3751(19)	C26–C27	1.393(3)
N2–C6	1.3744(19)	C26–H26	0.9500
N2–C9	1.3789(19)	C27–C28	1.389(4)
C1–C10$^{\#1}$	1.393(2)	C27–C31	1.504(4)
C1–C2	1.442(2)	C28–C29	1.391(4)
C2–C3	1.346(2)	C28–H28	0.9500
C2–H2	0.9500	C29–C30	1.393(3)
C3–C4	1.445(2)	C29–C32	1.508(4)
C3–H3	0.9500	C30–H30	0.9500
C4–C5	1.390(2)	C31–H31A	0.9800
C5–C6	1.393(2)	C31–H31B	0.9800
C5–C11	1.496(2)	C31–H31C	0.9800
C6–C7	1.437(2)	C32–H32A	0.9800
C7–C8	1.349(2)	C32–H32B	0.9800
C7–H7	0.9500	C32–H32C	0.9800
C8–C9	1.435(2)	C33–C38	1.390(2)
C8–H8	0.9500	C33–C34	1.399(2)
C9–C10	1.387(2)	C34–C35	1.395(2)
C10–C33	1.498(2)	C35–C36	1.381(2)
C11–C12	1.396(2)	C35–H35	0.9500
C11–C16	1.399(2)	C36–C37	1.385(2)
C12–C13	1.392(2)	C36–H36	0.9500
C13–C14	1.384(3)	C37–C38	1.397(2)
C13–H13	0.9500	C37–H37	0.9500
C14–C15	1.375(3)	C39–C40	1.378(3)
C14–H14	0.9500	C39–C44	1.381(3)
C15–C16	1.388(2)	C40–C41	1.397(3)
C15–H15	0.9500	C40–H40	0.9500
C17–C22	1.378(2)	C41–C42	1.387(4)
C17–C18	1.387(3)	C41–C45	1.500(3)
C18–C19	1.386(3)	C42–C43	1.373(4)
C18–H18	0.9500	C42–H42	0.9500
C19–C20	1.399(3)	C43–C44	1.398(3)
C19–C23	1.507(3)	C43–C46	1.503(3)
C20–C21	1.385(3)	C44–H44	0.9500
C20–H20	0.9500	C45–H45A	0.9800
C21–C22	1.394(3)	C45–H45B	0.9800

C45–H45C	0.9800
C46–H46A	0.9800
C46–H46B	0.9800
C46–H46C	0.9800
C47–C52	1.369(3)
C47–C48	1.370(3)
C48–C49	1.393(3)
C48–H48	0.9500
C49–C50	1.382(4)
C49–C53	1.496(4)
C50–C51	1.380(4)
C50–H50	0.9500
C51–C52	1.391(3)
C51–C54	1.517(5)
C52–H52	0.9500
C53–H53A	0.9800
C53–H53B	0.9800
C53–H53C	0.9800
C54–H54A	0.9800
C54–H54B	0.9800
C54–H54C	0.9800
C65–Cl2	1.724(19)
C65–Cl1	1.767(19)
C65–H65A	0.9900
C65–H65B	0.9900
C66–Cl4	1.76(2)
C66–Cl3	1.79(2)
C66–H66A	0.9900
C66–H66B	0.9900
C62–C63	1.497(9)
C62–C62$^{\#2}$	1.526(13)
C62–H62A	0.9900
C62–H62B	0.9900
C63–C64	1.602(11)
C63–H63A	0.9900
C63–H63B	0.9900
C64–H64A	0.9800
C64–H64B	0.9800
C64–H64C	0.9800

Atom–Atom–Atom	**Angle [°]**
N3–Fe1–N3	180.00(12)
N3–Fe1–N1	89.14(5)
N3–Fe1–N1	90.86(5)
N3–Fe1–N1	90.86(5)
N3–Fe1–N1	89.14(5)
N1–Fe1–N1	180.00(7)
N3–Fe1–N2	91.91(5)
N3–Fe1–N2	88.09(5)
N1–Fe1–N2	90.31(5)
N1–Fe1–N2	89.69(5)
N3–Fe1–N2	88.09(5)
N3–Fe1–N2	91.91(5)
N1–Fe1–N2	89.69(5)
N1–Fe1–N2	90.31(5)
N2–Fe1–N2	180.0
O5–N3–C55	116.51(16)
O5–N3–Fe1	119.49(14)
C55–N3–Fe1	123.78(10)
C55–N3–H3A	106.4
Fe1–N3–H3A	106.4
C55–N3–H3B	106.4
Fe1–N3–H3B	106.4
H3A–N3–H3B	106.5
N3–C55–C56	109.04(17)
N3–C55–C57	108.53(17)
C56–C55–C57	114.8(2)
N3–C55–H55	108.1
C56–C55–H55	108.1
C57–C55–H55	108.1
C55–C56–H56A	109.5
C55–C56–H56B	109.5
H56A–C56–H56B	109.5
C55–C56–H56C	109.5
H56A–C56–H56C	109.5
H56B–C56–H56C	109.5
C55–C57–H57A	109.5
C55–C57–H57B	109.5
H57A–C57–H57B	109.5
C55–C57–H57C	109.5
H57A–C57–H57C	109.5
H57B–C57–H57C	109.5
C12–O1–C17	115.63(13)
C16–O2–C25	117.34(14)
C34–O3–C39	119.51(13)
C38–O4–C47	117.05(13)
C4–N1–C1	105.87(12)
C4–N1–Fe1	126.84(10)
C1–N1–Fe1	127.28(10)
C6–N2–C9	105.39(12)
C6–N2–Fe1	126.94(10)
C9–N2–Fe1	127.66(10)
N1–C1–C10	126.04(13)
N1–C1–C2	110.03(13)
C10–C1–C2	123.90(14)
C3–C2–C1	107.08(13)
C3–C2–H2	126.5
C1–C2–H2	126.5
C2–C3–C4	107.07(14)

C2–C3–H3	126.5	C21–C20–C19	121.88(18)
C4–C3–H3	126.5	C21–C20–H20	119.1
N1–C4–C5	126.08(13)	C19–C20–H20	119.1
N1–C4–C3	109.94(13)	C20–C21–C22	119.15(17)
C5–C4–C3	123.97(14)	C20–C21–C24	121.40(19)
C4–C5–C6	124.20(14)	C22–C21–C24	119.38(19)
C4–C5–C11	116.79(13)	C17–C22–C21	119.15(17)
C6–C5–C11	119.01(14)	C17–C22–H22	120.4
N2–C6–C5	125.58(14)	C21–C22–H22	120.4
N2–C6–C7	110.20(13)	C19–C23–H23A	109.5
C5–C6–C7	124.22(14)	C19–C23–H23B	109.5
C8–C7–C6	107.13(14)	H23A–C23–H23B	109.5
C8–C7–H7	126.4	C19–C23–H23C	109.5
C6–C7–H7	126.4	H23A–C23–H23C	109.5
C7–C8–C9	106.92(14)	H23B–C23–H23C	109.5
C7–C8–H8	126.5	C21–C24–H24A	109.5
C9–C8–H8	126.5	C21–C24–H24B	109.5
N2–C9–C10	125.26(14)	H24A–C24–H24B	109.5
N2–C9–C8	110.32(13)	C21–C24–H24C	109.5
C10–C9–C8	124.41(14)	H24A–C24–H24C	109.5
C9–C10–C1	124.04(14)	H24B–C24–H24C	109.5
C9–C10–C33	119.95(14)	C21–C24–H24D	109.5
C1–C10–C33	115.96(13)	H24A–C24–H24D	141.1
C12–C11–C16	117.12(14)	H24B–C24–H24D	56.3
C12–C11–C5	121.97(14)	H24C–C24–H24D	56.3
C16–C11–C5	120.80(14)	C21–C24–H24E	109.5
O1–C12–C13	121.98(15)	H24A–C24–H24E	56.3
O1–C12–C11	116.43(14)	H24B–C24–H24E	141.1
C13–C12–C11	121.57(15)	H24C–C24–H24E	56.3
C14–C13–C12	119.16(16)	H24D–C24–H24E	109.5
C14–C13–H13	120.4	C21–C24–H24F	109.5
C12–C13–H13	120.4	H24A–C24–H24F	56.3
C15–C14–C13	120.94(16)	H24B–C24–H24F	56.3
C15–C14–H14	119.5	H24C–C24–H24F	141.1
C13–C14–H14	119.5	H24D–C24–H24F	109.5
C14–C15–C16	119.18(16)	H24E–C24–H24F	109.5
C14–C15–H15	120.4	C30–C25–C26	121.60(18)
C16–C15–H15	120.4	C30–C25–O2	116.84(17)
O2–C16–C15	121.26(15)	C26–C25–O2	121.52(17)
O2–C16–C11	116.77(14)	C25–C26–C27	119.3(2)
C15–C16–C11	121.87(16)	C25–C26–H26	120.3
C22–C17–C18	121.64(17)	C27–C26–H26	120.3
C22–C17–O1	118.32(16)	C28–C27–C26	118.8(2)
C18–C17–O1	120.04(15)	C28–C27–C31	121.3(2)
C19–C18–C17	120.04(16)	C26–C27–C31	120.0(2)
C19–C18–H18	120.0	C27–C28–C29	122.1(2)
C17–C18–H18	120.0	C27–C28–H28	119.0
C18–C19–C20	118.13(17)	C29–C28–H28	119.0
C18–C19–C23	120.53(17)	C28–C29–C30	118.3(2)
C20–C19–C23	121.30(18)	C28–C29–C32	121.2(2)

C30–C29–C32	120.5(3)	C39–C44–H44	120.3
C25–C30–C29	119.9(2)	C43–C44–H44	120.3
C25–C30–H30	120.0	C41–C45–H45A	109.5
C29–C30–H30	120.0	C41–C45–H45B	109.5
C27–C31–H31A	109.5	H45A–C45–H45B	109.5
C27–C31–H31B	109.5	C41–C45–H45C	109.5
H31A–C31–H31B	109.5	H45A–C45–H45C	109.5
C27–C31–H31C	109.5	H45B–C45–H45C	109.5
H31A–C31–H31C	109.5	C43–C46–H46A	109.5
H31B–C31–H31C	109.5	C43–C46–H46B	109.5
C29–C32–H32A	109.5	H46A–C46–H46B	109.5
C29–C32–H32B	109.5	C43–C46–H46C	109.5
H32A–C32–H32B	109.5	H46A–C46–H46C	109.5
C29–C32–H32C	109.5	H46B–C46–H46C	109.5
H32A–C32–H32C	109.5	C52–C47–C48	121.81(19)
H32B–C32–H32C	109.5	C52–C47–O4	118.80(18)
C38–C33–C34	117.50(14)	C48–C47–O4	119.30(19)
C38–C33–C10	120.93(13)	C47–C48–C49	119.7(2)
C34–C33–C10	121.17(14)	C47–C48–H48	120.1
O3–C34–C35	123.37(14)	C49–C48–H48	120.1
O3–C34–C33	115.12(13)	C50–C49–C48	118.2(2)
C35–C34–C33	121.49(15)	C50–C49–C53	120.4(3)
C36–C35–C34	119.10(15)	C48–C49–C53	121.3(3)
C36–C35–H35	120.5	C51–C50–C49	122.1(2)
C34–C35–H35	120.5	C51–C50–H50	118.9
C35–C36–C37	121.25(15)	C49–C50–H50	118.9
C35–C36–H36	119.4	C50–C51–C52	118.6(3)
C37–C36–H36	119.4	C50–C51–C54	122.0(3)
C36–C37–C38	118.58(16)	C52–C51–C54	119.4(3)
C36–C37–H37	120.7	C47–C52–C51	119.5(2)
C38–C37–H37	120.7	C47–C52–H52	120.3
O4–C38–C33	116.13(13)	C51–C52–H52	120.3
O4–C38–C37	121.83(15)	C49–C53–H53A	109.5
C33–C38–C37	122.01(15)	C49–C53–H53B	109.5
C40–C39–C44	121.61(17)	H53A–C53–H53B	109.5
C40–C39–O3	116.72(17)	C49–C53–H53C	109.5
C44–C39–O3	121.44(17)	H53A–C53–H53C	109.5
C39–C40–C41	119.4(2)	H53B–C53–H53C	109.5
C39–C40–H40	120.3	C51–C54–H54A	109.5
C41–C40–H40	120.3	C51–C54–H54B	109.5
C42–C41–C40	118.4(2)	H54A–C54–H54B	109.5
C42–C41–C45	121.2(2)	C51–C54–H54C	109.5
C40–C41–C45	120.4(2)	H54A–C54–H54C	109.5
C43–C42–C41	122.61(19)	H54B–C54–H54C	109.5
C43–C42–H42	118.7	Cl2–C65–Cl1	113.1(15)
C41–C42–H42	118.7	Cl2–C65–H65A	109.0
C42–C43–C44	118.5(2)	Cl1–C65–H65A	109.0
C42–C43–C46	121.4(2)	Cl2–C65–H65B	109.0
C44–C43–C46	120.1(2)	Cl1–C65–H65B	109.0
C39–C44–C43	119.5(2)	H65A–C65–H65B	107.8

Cl4–C66–Cl3	109.3(17)
Cl4–C66–H66A	109.8
Cl3–C66–H66A	109.8
Cl4–C66–H66B	109.8
Cl3–C66–H66B	109.8
H66A–C66–H66B	108.3
C63–C62–C62	115.8(7)
C63–C62–H62A	108.3
C62–C62–H62A	108.3
C63–C62–H62B	108.3
C62–C62–H62B	108.3
H62A–C62–H62B	107.4
C62–C63–C64	112.4(8)
C62–C63–H63A	109.1
C64–C63–H63A	109.1
C62–C63–H63B	109.1
C64–C63–H63B	109.1
H63A–C63–H63B	107.9
C63–C64–H64A	109.5
C63–C64–H64B	109.5
H64A–C64–H64B	109.5
C63–C64–H64C	109.5
H64A–C64–H64C	109.5
H64B–C64–H64C	109.5

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 1-Y, 1-Z; #2: -X, -Y, -Z;

Table S26. Torsion angles for [Fe(3,5-Me-BAFP)(iPrNH$_2$)(iPrNO)].

Atom–Atom–Atom–Atom	Torsion Angle [°]
O5–N3–C55–C56	−60.5(2)
Fe1–N3–C55–C56	124.88(17)
O5–N3–C55–C57	65.2(2)
Fe1–N3–C55–C57	−109.37(16)
C4–N1–C1–C10$^{\#1}$	178.89(14)
Fe1–N1–C1–C10$^{\#1}$	−0.8(2)
C4–N1–C1–C2	0.83(16)
Fe1–N1–C1–C2	−178.86(10)
N1–C1–C2–C3	−0.30(18)
C10$^{\#1}$–C1–C2–C3	−178.41(15)
C1–C2–C3–C4	−0.34(18)
C1–N1–C4–C5	177.94(14)
Fe1–N1–C4–C5	−2.4(2)
C1–N1–C4–C3	−1.04(16)
Fe1–N1–C4–C3	178.65(10)
C2–C3–C4–N1	0.88(18)
C2–C3–C4–C5	−178.13(15)
N1–C4–C5–C6	0.6(2)
C3–C4–C5–C6	179.48(15)
N1–C4–C5–C11	−178.94(14)
C3–C4–C5–C11	−0.1(2)
C9–N2–C6–C5	177.80(14)
Fe1–N2–C6–C5	−1.3(2)
C9–N2–C6–C7	−1.48(16)
Fe1–N2–C6–C7	179.39(10)
C4–C5–C6–N2	1.3(2)
C11–C5–C6–N2	−179.11(13)
C4–C5–C6–C7	−179.50(15)
C11–C5–C6–C7	0.1(2)
N2–C6–C7–C8	0.95(18)
C5–C6–C7–C8	−178.34(15)
C6–C7–C8–C9	−0.02(18)
C6–N2–C9–C10	−178.90(14)
Fe1–N2–C9–C10	0.2(2)
C6–N2–C9–C8	1.47(16)
Fe1–N2–C9–C8	−179.41(10)
C7–C8–C9–N2	−0.92(18)
C7–C8–C9–C10	179.45(15)

N2–C9–C10–C1$^{\#1}$	−1.5(2)
C8–C9–C10–C1$^{\#1}$	178.11(15)
N2–C9–C10–C33	−178.78(14)
C8–C9–C10–C33	0.8(2)
C4–C5–C11–C12	103.08(17)
C6–C5–C11–C12	−76.52(19)
C4–C5–C11–C16	−72.97(19)
C6–C5–C11–C16	107.44(17)
C17–O1–C12–C13	−20.2(2)
C17–O1–C12–C11	161.63(14)
C16–C11–C12–O1	−177.49(13)
C5–C11–C12–O1	6.3(2)
C16–C11–C12–C13	4.3(2)
C5–C11–C12–C13	−171.90(14)
O1–C12–C13–C14	−179.44(15)
C11–C12–C13–C14	−1.3(2)
C12–C13–C14–C15	−2.1(3)
C13–C14–C15–C16	2.3(3)
C25–O2–C16–C15	40.2(2)
C25–O2–C16–C11	−143.30(15)
C14–C15–C16–O2	177.17(16)
C14–C15–C16–C11	0.9(3)
C12–C11–C16–O2	179.46(14)
C5–C11–C16–O2	−4.3(2)
C12–C11–C16–C15	−4.1(2)
C5–C11–C16–C15	172.16(15)
C12–O1–C17–C22	115.22(17)
C12–O1–C17–C18	−64.0(2)
C22–C17–C18–C19	−1.0(3)
O1–C17–C18–C19	178.21(16)
C17–C18–C19–C20	0.5(3)
C17–C18–C19–C23	−177.07(18)
C18–C19–C20–C21	−0.5(3)
C23–C19–C20–C21	177.1(2)
C19–C20–C21–C22	0.9(3)
C19–C20–C21–C24	−175.7(2)
C18–C17–C22–C21	1.4(3)
O1–C17–C22–C21	−177.81(16)
C20–C21–C22–C17	−1.4(3)
C24–C21–C22–C17	175.4(2)
C16–O2–C25–C30	−137.26(17)
C16–O2–C25–C26	45.0(2)

C30–C25–C26–C27	−1.3(3)
O2–C25–C26–C27	176.41(17)
C25–C26–C27–C28	1.2(3)
C25–C26–C27–C31	−179.0(2)
C26–C27–C28–C29	−0.3(3)
C31–C27–C28–C29	179.9(2)
C27–C28–C29–C30	−0.6(4)
C27–C28–C29–C32	178.8(3)
C26–C25–C30–C29	0.3(3)
O2–C25–C30–C29	−177.44(19)
C28–C29–C30–C25	0.6(3)
C32–C29–C30–C25	−178.8(2)
C9–C10–C33–C38	83.30(19)
C1$^{\#1}$–C10–C33–C38	−94.22(18)
C9–C10–C33–C34	−104.08(18)
C1$^{\#1}$–C10–C33–C34	78.40(19)
C39–O3–C34–C35	24.3(2)
C39–O3–C34–C33	−157.54(15)
C38–C33–C34–O3	−175.46(14)
C10–C33–C34–O3	11.7(2)
C38–C33–C34–C35	2.8(2)
C10–C33–C34–C35	−170.09(15)
O3–C34–C35–C36	177.22(15)
C33–C34–C35–C36	−0.9(2)
C34–C35–C36–C37	−1.2(3)
C35–C36–C37–C38	1.2(3)
C47–O4–C38–C33	142.38(16)
C47–O4–C38–C37	−39.4(2)
C34–C33–C38–O4	175.45(14)
C10–C33–C38–O4	−11.7(2)
C34–C33–C38–C37	−2.7(2)
C10–C33–C38–C37	170.14(15)
C36–C37–C38–O4	−177.29(15)
C36–C37–C38–C33	0.8(3)
C34–O3–C39–C40	−131.81(17)
C34–O3–C39–C44	53.6(2)
C44–C39–C40–C41	0.9(3)
O3–C39–C40–C41	−173.66(17)
C39–C40–C41–C42	−1.9(3)
C39–C40–C41–C45	176.76(19)
C40–C41–C42–C43	1.7(3)
C45–C41–C42–C43	−177.0(2)

C41–C42–C43–C44	−0.4(3)
C41–C42–C43–C46	178.3(2)
C40–C39–C44–C43	0.3(3)
O3–C39–C44–C43	174.66(17)
C42–C43–C44–C39	−0.6(3)
C46–C43–C44–C39	−179.3(2)
C38–O4–C47–C52	−75.3(2)
C38–O4–C47–C48	108.1(2)
C52–C47–C48–C49	−0.7(3)
O4–C47–C48–C49	175.85(18)
C47–C48–C49–C50	0.0(3)
C47–C48–C49–C53	179.1(3)
C48–C49–C50–C51	0.1(4)
C53–C49–C50–C51	−179.0(3)
C49–C50–C51–C52	0.5(4)
C49–C50–C51–C54	179.5(4)
C48–C47–C52–C51	1.3(3)
O4–C47–C52–C51	−175.3(2)
C50–C51–C52–C47	−1.1(4)
C54–C51–C52–C47	179.8(4)
C62[#2]–C62–C63–C64	177.0(7)

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 1-Y, 1-Z; #2: -X, -Y, -Z;

Table S27. Crystal data and structure refinement for [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)].

Empirical formula	$C_{119}H_{107}FeN_5O_{10}$
Formula weight	1822.94
Temperature	85(2)
Wavelength	1.54187
Crystal system, space group	Monoclinic, P_{21}/c
Unit cell dimensions	a = 12.7311(2) Å alpha = 90 deg. b = 23.0067(4) Å beta = 93.621(7) deg. c = 15.9989(11) Å gamma = 90 deg.
Volume	4673.8(3) $Å^3$
Z, Calculated density	2, 1.295 Mg/m^3
Absorption coefficient	1.826 mm^{-1}
F(000)	1924
Crystal size	0.12 x 0.12 x 0.10
Theta range for data collection	3.371 to 68.235 deg
Reflections collected / unique	127495/8513
Completeness to theta = 67.687	99.4%
Absorption correction	Empirical
Max. and min. transmission	0.8106/0.8385
Refinement method	Full Matrix Least Squares on F^2
Data / restraints / parameters	8513 / 114 / 682
Goodness-of-fit on F^2	1.079
Final R indices [I>2sigma(I)]	R_1 = 0.0429, wR_2 = 0.1113
R indices (all data)	R_1 = 0.0442, wR_2 = 0.1124
Extinction coefficient	N/A
Largest diff. peak and hole	0.546 and -0.530 $Å^3$

Table S28. Atomic coordinates and U_{eq} [Å^2] for [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)].

Atom	*x*	*y*	*z*	U_{eq}
Fe	0.000000	0.000000	1.000000	0.02144(11)
O1	-0.23621(10)	0.02341(5)	0.69939(7)	0.0276(3)
O2	-0.21823(9)	0.18603(5)	0.88201(7)	0.0243(3)
O3	0.33168(9)	-0.03508(5)	0.77757(8)	0.0250(3)
O4	0.28315(9)	0.14582(5)	0.91014(8)	0.0278(3)
O5	-0.1038(3)	-0.10707(16)	0.9685(2)	0.0301(8)
O6A	-0.0145(7)	-0.0773(5)	0.9317(7)	0.0277(17)
N1	0.02398(10)	0.03978(6)	0.89230(8)	0.0174(3)
N2	-0.15547(10)	0.01639(6)	0.98500(8)	0.0177(3)
N3	-0.0363(7)	-0.0715(5)	0.9453(7)	0.0166(13)
C1	0.11812(12)	0.04883(7)	0.85646(10)	0.0190(3)
C2	0.10085(13)	0.07912(8)	0.77808(10)	0.0225(3)
H2	0.152957	0.090109	0.741136	0.027
C3	-0.00344(13)	0.08889(8)	0.76716(10)	0.0217(3)
H3	-0.038751	0.107820	0.720656	0.026
C4	-0.05144(12)	0.06545(7)	0.83868(10)	0.0186(3)
C5	-0.15826(12)	0.06987(7)	0.85209(10)	0.0178(3)
C6	-0.20624(12)	0.04612(7)	0.91961(10)	0.0183(3)
C7	-0.31789(12)	0.04717(7)	0.92959(10)	0.0212(3)
H7	-0.369823	0.065526	0.893373	0.025
C8	-0.33493(13)	0.01719(8)	1.00004(10)	0.0210(3)
H8	-0.401128	0.009920	1.022276	0.025
C9	-0.23343(13)	-0.00172(7)	1.03513(11)	0.0182(3)
C10	-0.22192(12)	0.10487(7)	0.78822(10)	0.0182(3)
C11	-0.25339(12)	0.08215(7)	0.70943(11)	0.0204(3)
C12	-0.29860(12)	0.11714(8)	0.64617(10)	0.0213(3)
H12	-0.318919	0.101103	0.592837	0.026
C13	-0.31379(13)	0.17592(8)	0.66176(11)	0.0235(4)
H13	-0.343083	0.200215	0.618261	0.028
C14	-0.28684(13)	0.19944(8)	0.73972(11)	0.0248(4)
H14	-0.299156	0.239385	0.750553	0.030
C15	-0.24140(12)	0.16365(7)	0.80195(10)	0.0199(3)
C16	-0.25063(15)	0.00196(7)	0.61730(12)	0.0266(4)
C17	-0.17781(15)	0.01520(9)	0.55987(12)	0.0310(4)
H17	-0.117088	0.037390	0.576438	0.037
C18	-0.19371(16)	-0.00407(9)	0.47764(14)	0.0323(4)
C19	-0.28313(15)	-0.03695(8)	0.45623(12)	0.0301(4)
H19	-0.294986	-0.050010	0.400055	0.036
C20	-0.35548(15)	-0.05130(8)	0.51407(12)	0.0292(4)

C21	-0.33863(15)	-0.03100(8)	0.59633(11)	0.0276(4)
H21	-0.387286	-0.039856	0.637161	0.033
C22	-0.13274(13)	0.22327(7)	0.89416(11)	0.0244(4)
C23	-0.05145(14)	0.22562(8)	0.84071(12)	0.0271(4)
H23	-0.054486	0.202775	0.791124	0.033
C24	0.03446(15)	0.26142(8)	0.85969(13)	0.0312(4)
C25	0.03598(16)	0.29553(10)	0.93162(15)	0.0416(5)
H25	0.093661	0.320969	0.943988	0.050
C26	-0.04501(16)	0.29316(11)	0.98564(16)	0.0485(6)
C27	-0.13018(15)	0.25658(10)	0.96631(14)	0.0389(5)
H27	-0.186390	0.254487	1.002543	0.047
C28	-0.11806(18)	0.01123(12)	0.41265(15)	0.0469(6)
H28A	-0.071292	0.042440	0.433947	0.070
H28B	-0.157435	0.024279	0.361429	0.070
H28C	-0.076110	-0.023053	0.400203	0.070
C29	-0.45141(18)	-0.08706(10)	0.48940(13)	0.0411(5)
H29A	-0.469966	-0.082006	0.429418	0.062
H29B	-0.510235	-0.074313	0.521581	0.062
H29C	-0.436508	-0.128151	0.501117	0.062
C30	0.12527(16)	0.26197(10)	0.80381(14)	0.0403(5)
H30A	0.159580	0.223825	0.805543	0.060
H30B	0.176085	0.291772	0.823317	0.060
H30C	0.099255	0.270684	0.746174	0.060
C31	-0.0395(2)	0.32807(17)	1.0659(2)	0.0843(12)
H31A	-0.016767	0.302845	1.112979	0.126
H31B	-0.109168	0.344079	1.075072	0.126
H31C	0.010987	0.359915	1.061570	0.126
C32	0.21705(12)	0.03262(7)	0.89068(10)	0.0189(3)
C33	0.30953(12)	0.05462(7)	0.84612(10)	0.0191(3)
C34	0.36418(13)	0.02165(7)	0.78962(10)	0.0204(3)
C35	0.44347(13)	0.04612(8)	0.74497(11)	0.0237(4)
H35	0.479521	0.023139	0.706582	0.028
C36	0.46957(13)	0.10404(8)	0.75670(11)	0.0250(4)
H36	0.523502	0.120689	0.725954	0.030
C37	0.41838(14)	0.13786(8)	0.81237(11)	0.0258(4)
H37	0.436768	0.177563	0.820575	0.031
C38	0.33943(13)	0.11280(8)	0.85623(11)	0.0225(3)
C39	0.40579(13)	-0.07514(7)	0.75213(11)	0.0231(4)
C40	0.37363(14)	-0.11367(8)	0.68927(11)	0.0253(4)
H40	0.304851	-0.111020	0.662822	0.030
C41	0.44336(15)	-0.15660(8)	0.66500(12)	0.0298(4)
C42	0.54397(15)	-0.15854(8)	0.70373(12)	0.0315(4)

H42	0.591732	-0.187376	0.686949	0.038
C43	0.57697(14)	-0.11941(8)	0.76654(12)	0.0292(4)
C44	0.50611(13)	-0.07778(8)	0.79151(11)	0.0252(4)
H44	0.526217	-0.051311	0.835232	0.030
C45	0.41019(19)	-0.19906(9)	0.59653(14)	0.0410(5)
H45A	0.371038	-0.231133	0.620224	0.062
H45B	0.472738	-0.214402	0.571421	0.062
H45C	0.365224	-0.179233	0.553451	0.062
C46	0.68775(15)	-0.12038(10)	0.80610(14)	0.0378(5)
H46A	0.708655	-0.160615	0.818480	0.057
H46B	0.690726	-0.097815	0.858189	0.057
H46C	0.735813	-0.103327	0.767336	0.057
C47	0.33981(14)	0.17745(7)	0.97136(11)	0.0237(4)
C48	0.44201(14)	0.16345(8)	0.99984(11)	0.0255(4)
H48	0.477256	0.131712	0.975906	0.031
C49	0.49243(14)	0.19609(8)	1.06351(11)	0.0250(4)
C50	0.43820(15)	0.24183(8)	1.09875(12)	0.0280(4)
H50	0.472224	0.264145	1.142520	0.034
C51	0.33494(14)	0.25542(8)	1.07089(12)	0.0282(4)
C52	0.28601(14)	0.22302(8)	1.00610(11)	0.0259(4)
H52	0.216185	0.232052	0.985767	0.031
C53	0.60440(15)	0.18163(8)	1.09184(12)	0.0294(4)
H53A	0.617715	0.140387	1.081399	0.044
H53B	0.615931	0.189689	1.151901	0.044
H53C	0.652454	0.205395	1.060652	0.044
C54	0.27527(17)	0.30362(9)	1.11057(14)	0.0401(5)
H54A	0.212765	0.287566	1.134914	0.060
H54B	0.253670	0.332544	1.067884	0.060
H54C	0.320577	0.322115	1.154712	0.060
C55	0.0171(7)	-0.0903(5)	0.8730(7)	0.0191(15)
C56	0.1105(3)	-0.12214(17)	0.8795(2)	0.0291(8)
H56	0.146797	-0.129510	0.932149	0.035
C57	0.1475(3)	-0.14231(18)	0.8059(3)	0.0368(9)
H57	0.210459	-0.164574	0.808271	0.044
C58	0.0967(3)	-0.13144(18)	0.7293(3)	0.0344(9)
H58	0.124775	-0.146171	0.679916	0.041
C59	0.0046(3)	-0.09908(18)	0.7236(3)	0.0311(8)
H59	-0.029339	-0.090826	0.670291	0.037
C60	-0.0381(7)	-0.0786(6)	0.7966(7)	0.0314(17)
H60	-0.102340	-0.057517	0.794267	0.038
C61A	0.0462(8)	-0.0947(6)	0.8618(8)	0.030(2)
H61A	0.116631	-0.075321	0.866506	0.036

C62A	0.0591(3)	-0.15941(19)	0.8765(3)	0.0398(9)
H62A	0.117318	-0.167784	0.918772	0.048
H62B	0.071801	-0.180249	0.823874	0.048
C63A	-0.0493(3)	-0.17548(18)	0.9091(3)	0.0402(10)
H63A	-0.105054	-0.176681	0.863121	0.048
H63B	-0.046752	-0.213280	0.938797	0.048
C64A	-0.0655(4)	-0.1260(2)	0.9681(4)	0.0331(12)
H64A	-0.141390	-0.118171	0.972467	0.040
H64B	-0.033140	-0.134645	1.024654	0.040
C65A	-0.0091(8)	-0.0801(6)	0.7792(7)	0.038(2)
H65A	0.038960	-0.086104	0.734441	0.057
H65B	-0.031766	-0.039440	0.779369	0.057
H65C	-0.070706	-0.105369	0.769609	0.057

Table S29. Anisotropic displacement parameters [Å^2] for [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)].
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	0.01722(19)	0.0350(2)	0.0120(2)	0.00087(15)	-0.00037(14)	0.00934(15)
O1	0.0377(7)	0.0259(6)	0.0179(6)	-0.0033(5)	-0.0082(5)	0.0066(5)
O2	0.0272(6)	0.0265(6)	0.0193(6)	-0.0015(5)	0.0018(5)	-0.0021(5)
O3	0.0196(6)	0.0273(6)	0.0290(7)	-0.0050(5)	0.0077(5)	0.0008(5)
O4	0.0211(6)	0.0320(7)	0.0303(7)	-0.0121(5)	0.0013(5)	0.0000(5)
O5	0.0254(19)	0.036(2)	0.0294(16)	0.0004(15)	0.0055(15)	-0.0105(14)
O6A	0.016(3)	0.031(3)	0.037(4)	0.003(2)	0.009(2)	0.005(2)
N1	0.0141(6)	0.0231(7)	0.0146(7)	-0.0029(5)	-0.0017(5)	0.0029(5)
N2	0.0169(7)	0.0226(6)	0.0135(7)	-0.0002(5)	-0.0010(5)	0.0008(5)
N3	0.005(3)	0.021(2)	0.024(3)	0.001(2)	0.001(2)	0.002(2)
C1	0.0178(8)	0.0267(8)	0.0124(8)	-0.0022(6)	0.0003(6)	0.0028(6)
C2	0.0207(8)	0.0325(9)	0.0145(8)	0.0007(7)	0.0032(6)	0.0025(7)
C3	0.0214(8)	0.0298(9)	0.0137(8)	0.0013(6)	-0.0007(6)	0.0053(7)
C4	0.0180(8)	0.0239(8)	0.0133(8)	-0.0017(6)	-0.0030(6)	0.0032(6)
C5	0.0168(7)	0.0220(8)	0.0142(8)	-0.0014(6)	-0.0023(6)	0.0009(6)
C6	0.0165(7)	0.0217(8)	0.0161(8)	-0.0021(6)	-0.0032(6)	0.0019(6)
C7	0.0161(8)	0.0285(8)	0.0187(8)	0.0007(7)	-0.0021(6)	0.0032(6)
C8	0.0150(8)	0.0289(8)	0.0188(8)	-0.0001(7)	-0.0004(6)	0.0030(7)
C9	0.0155(8)	0.0228(8)	0.0163(8)	-0.0024(6)	0.0006(6)	0.0018(6)
C10	0.0133(7)	0.0245(8)	0.0165(8)	0.0013(6)	-0.0003(6)	0.0010(6)
C11	0.0163(7)	0.0245(8)	0.0203(8)	0.0007(6)	-0.0002(6)	0.0019(6)
C12	0.0154(7)	0.0319(9)	0.0163(8)	0.0013(7)	-0.0014(6)	0.0009(6)
C13	0.0184(8)	0.0298(9)	0.0221(9)	0.0081(7)	-0.0001(7)	0.0015(7)
C14	0.0251(8)	0.0246(8)	0.0246(9)	0.0038(7)	0.0014(7)	0.0031(7)
C15	0.0176(7)	0.0250(8)	0.0171(8)	-0.0001(6)	0.0012(6)	-0.0006(6)
C16	0.0298(10)	0.0298(9)	0.0191(9)	-0.0046(7)	-0.0064(8)	0.0068(7)
C17	0.0230(9)	0.0394(10)	0.0300(10)	-0.0083(8)	-0.0045(8)	0.0006(8)
C18	0.0255(10)	0.0408(11)	0.0305(11)	-0.0075(8)	0.0019(8)	0.0028(7)
C19	0.0335(10)	0.0365(10)	0.0200(9)	-0.0067(7)	-0.0008(7)	-0.0013(8)
C20	0.0329(10)	0.0315(9)	0.0227(9)	-0.0016(7)	-0.0021(7)	-0.0031(8)
C21	0.0317(9)	0.0302(9)	0.0207(9)	0.0011(7)	0.0001(7)	0.0015(7)
C22	0.0231(8)	0.0237(8)	0.0261(9)	-0.0012(7)	-0.0022(7)	0.0020(7)
C23	0.0292(9)	0.0279(9)	0.0241(9)	0.0002(7)	0.0008(7)	0.0013(7)
C24	0.0265(9)	0.0315(9)	0.0354(11)	0.0018(8)	0.0007(8)	0.0019(7)
C25	0.0249(10)	0.0424(11)	0.0572(14)	-0.0183(10)	0.0001(9)	-0.0018(8)
C26	0.0268(10)	0.0601(14)	0.0585(15)	-0.0358(12)	0.0024(10)	-0.0003(10)
C27	0.0235(9)	0.0534(13)	0.0402(12)	-0.0200(10)	0.0053(8)	0.0014(9)

C28	0.0325(11)	0.0699(15)	0.0392(13)	-0.0154(11)	0.0101(10)	-0.0094(11)
C29	0.0474(12)	0.0498(12)	0.0260(11)	-0.0052(9)	0.0014(9)	-0.0192(10)
C30	0.0336(10)	0.0477(12)	0.0400(12)	0.0046(10)	0.0045(9)	-0.0058(9)
C31	0.0353(13)	0.122(3)	0.097(2)	-0.083(2)	0.0146(14)	-0.0130(15)
C32	0.0157(7)	0.0254(8)	0.0155(8)	-0.0030(6)	0.0013(6)	0.0023(6)
C33	0.0149(7)	0.0268(8)	0.0153(8)	0.0012(6)	-0.0009(6)	0.0023(6)
C34	0.0165(8)	0.0264(8)	0.0181(8)	-0.0012(7)	-0.0007(6)	0.0013(6)
C35	0.0200(8)	0.0331(9)	0.0185(9)	0.0012(7)	0.0039(6)	0.0037(7)
C36	0.0189(8)	0.0338(9)	0.0223(9)	0.0061(7)	0.0007(7)	-0.0011(7)
C37	0.0242(8)	0.0278(9)	0.0252(9)	0.0015(7)	-0.0005(7)	-0.0015(7)
C38	0.0178(8)	0.0297(9)	0.0198(9)	-0.0017(7)	-0.0015(6)	0.0025(6)
C39	0.0224(8)	0.0267(8)	0.0212(9)	0.0012(7)	0.0088(7)	0.0012(7)
C40	0.0257(9)	0.0291(9)	0.0215(9)	0.0005(7)	0.0061(7)	-0.0026(7)
C41	0.0381(10)	0.0266(9)	0.0259(10)	-0.0012(7)	0.0127(8)	-0.0041(8)
C42	0.0336(10)	0.0277(9)	0.0349(11)	0.0034(8)	0.0155(8)	0.0066(8)
C43	0.0258(9)	0.0322(9)	0.0306(10)	0.0087(8)	0.0098(8)	0.0029(7)
C44	0.0241(8)	0.0285(9)	0.0235(9)	0.0014(7)	0.0048(7)	-0.0003(7)
C45	0.0522(13)	0.0350(11)	0.0375(12)	-0.0101(9)	0.0156(10)	-0.0070(9)
C46	0.0250(9)	0.0426(11)	0.0465(13)	0.0115(9)	0.0066(9)	0.0059(8)
C47	0.0247(8)	0.0249(8)	0.0218(9)	-0.0007(7)	0.0031(7)	-0.0042(7)
C48	0.0255(9)	0.0254(8)	0.0259(9)	-0.0010(7)	0.0033(7)	-0.0008(7)
C49	0.0265(9)	0.0261(8)	0.0224(9)	0.0038(7)	0.0026(7)	-0.0059(7)
C50	0.0309(9)	0.0292(9)	0.0243(9)	-0.0027(7)	0.0037(7)	-0.0073(7)
C51	0.0290(9)	0.0282(9)	0.0282(10)	-0.0027(7)	0.0068(7)	-0.0048(7)
C52	0.0238(8)	0.0275(9)	0.0269(9)	-0.0008(7)	0.0050(7)	-0.0019(7)
C53	0.0306(10)	0.0291(9)	0.0280(10)	0.0000(7)	-0.0018(8)	-0.0036(7)
C54	0.0344(11)	0.0413(11)	0.0448(13)	-0.0172(10)	0.0044(9)	-0.0008(9)
C55	0.025(4)	0.020(2)	0.013(3)	-0.007(2)	0.004(3)	-0.001(3)
C56	0.037(2)	0.0229(18)	0.027(2)	-0.0039(15)	-0.0003(16)	0.0012(18)
C57	0.0239(18)	0.042(2)	0.045(2)	-0.0146(18)	0.0047(16)	0.0031(16)
C58	0.0327(19)	0.042(2)	0.030(2)	-0.0127(17)	0.0128(16)	-0.0074(16)
C59	0.037(2)	0.038(2)	0.018(2)	-0.0051(17)	0.0033(16)	-0.0045(16)
C60	0.031(4)	0.033(3)	0.030(4)	-0.003(3)	0.004(3)	0.003(3)
C61A	0.035(5)	0.034(3)	0.023(4)	-0.007(2)	0.012(3)	-0.001(4)
C62A	0.039(2)	0.040(2)	0.041(2)	-0.0023(18)	0.0055(18)	0.004(2)
C63A	0.042(2)	0.035(2)	0.046(3)	-0.0072(18)	0.0170(19)	-0.0102(18)
C64A	0.030(3)	0.036(3)	0.035(3)	0.001(2)	0.008(2)	-0.010(2)
C65A	0.044(6)	0.037(3)	0.033(5)	-0.002(3)	0.000(3)	-0.009(4)

Table S30. Bond lengths and angles for [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)].

.Atom–Atom	Length [Å]
Fe1 N3	1.906(11)
Fe1 N3	1.906(11)
Fe1 N1	1.9905(14)
Fe1 N1	1.9906(14)
Fe1 N2	2.0143(13)
Fe1 N2	2.0143(13)
Fe1 O6A	2.088(10)
Fe1 O6A	2.088(10)
O1 C11	1.380(2)
O1 C16	1.403(2)
O2 C22	1.389(2)
O2 C15	1.394(2)
O3 C34	1.379(2)
O3 C39	1.398(2)
O4 C38	1.383(2)
O4 C47	1.385(2)
O5 N3	1.259(12)
O6A C64A	1.436(12)
O6A C61A	1.455(9)
N1 C1	1.377(2)
N1 C4	1.379(2)
N2 C6	1.376(2)
N2 C9	1.379(2)
N3 C55	1.446(8)
C1 C32	1.392(2)
C1 C2	1.439(2)
C2 C3	1.347(2)
C3 C4	1.435(2)
C4 C5	1.394(2)
C5 C6	1.386(2)
C5 C10	1.498(2)
C6 C7	1.441(2)
C7 C8	1.350(2)
C8 C9	1.443(2)
C9 C32	1.387(2)
C10 C15	1.395(2)
C10 C11	1.399(2)
C11 C12	1.389(2)
C12 C13	1.391(2)

C13 C14	1.382(3)
C14 C15	1.389(2)
C16 C21	1.377(3)
C16 C17	1.379(3)
C17 C18	1.390(3)
C18 C19	1.392(3)
C18 C28	1.502(3)
C19 C20	1.386(3)
C20 C21	1.399(3)
C20 C29	1.504(3)
C22 C27	1.384(3)
C22 C23	1.384(3)
C23 C24	1.387(3)
C24 C25	1.391(3)
C24 C30	1.505(3)
C25 C26	1.387(3)
C26 C27	1.392(3)
C26 C31	1.511(3)
C32 C33	1.502(2)
C33 C34	1.398(2)
C33 C38	1.398(2)
C34 C35	1.392(2)
C35 C36	1.383(3)
C36 C37	1.377(3)
C37 C38	1.387(2)
C39 C40	1.383(2)
C39 C44	1.389(2)
C40 C41	1.399(3)
C41 C42	1.388(3)
C41 C45	1.507(3)
C42 C43	1.394(3)
C43 C44	1.391(3)
C43 C46	1.509(3)
C47 C52	1.388(2)
C47 C48	1.389(2)
C48 C49	1.389(2)
C49 C50	1.397(3)
C49 C53	1.505(3)
C50 C51	1.397(3)
C51 C52	1.391(3)
C51 C54	1.507(3)
C55 C56	1.394(9)

C55 C60	1.396(15)
C56 C57	1.374(6)
C57 C58	1.371(6)
C58 C59	1.387(6)
C59 C60	1.400(9)
C61A C65A	1.494(17)
C61A C62A	1.515(14)
C62A C63A	1.551(6)
C63A C64A	1.501(7)

Atom–Atom–Atom	**Angle [°]**
N3 Fe1 N3	180.0
N3 Fe1 N1	92.6(4)
N3 Fe1 N1	87.4(4)
N3 Fe1 N1	87.4(4)
N3 Fe1 N1	92.6(4)
N1 Fe1 N1	180.0
N3 Fe1 N2	84.2(3)
N3 Fe1 N2	95.8(3)
N1 Fe1 N2	90.81(5)
N1 Fe1 N2	89.19(5)
N3 Fe1 N2	95.8(3)
N3 Fe1 N2	84.2(3)
N1 Fe1 N2	89.19(5)
N1 Fe1 N2	90.81(5)
N2 Fe1 N2	180.0
N3 Fe1 O6A	9.8(4)
N3 Fe1 O6A	170.2(4)
N1 Fe1 O6A	87.3(3)
N1 Fe1 O6A	92.7(3)
N2 Fe1 O6A	92.5(2)
N2 Fe1 O6A	87.5(2)
N1 Fe1 O6A	92.7(3)
N1 Fe1 O6A	87.3(3)
N2 Fe1 O6A	87.5(2)
N2 Fe1 O6A	92.5(2)
O6A Fe1 O6A	180.0
C11 O1 C16	116.16(13)
C22 O2 C15	118.35(13)
C34 O3 C39	117.55(13)
C38 O4 C47	117.51(13)

C64A O6A C61A	111.8(8)
C64A O6A Fe1	118.7(6)
C61A O6A Fe1	127.0(8)
C1 N1 C4	105.47(13)
C1 N1 Fe1	127.94(10)
C4 N1 Fe1	126.58(11)
C6 N2 C9	105.73(13)
C6 N2 Fe1	126.47(11)
C9 N2 Fe1	127.74(11)
O5 N3 C55	113.9(9)
O5 N3 Fe1	125.2(7)
C55 N3 Fe1	120.8(8)
N1 C1 C32	125.86(15)
N1 C1 C2	110.29(14)
C32 C1 C2	123.84(15)
C3 C2 C1	106.79(15)
C2 C3 C4	107.44(14)
N1 C4 C5	125.70(15)
N1 C4 C3	109.97(14)
C5 C4 C3	124.31(15)
C6 C5 C4	124.99(15)
C6 C5 C10	119.79(14)
C4 C5 C10	115.19(14)
N2 C6 C5	125.37(14)
N2 C6 C7	110.09(14)
C5 C6 C7	124.50(14)
C8 C7 C6	107.20(14)
C7 C8 C9	106.94(15)
N2 C9 C32	125.24(15)
N2 C9 C8	110.04(14)
C32 C9 C8	124.71(15)
C15 C10 C11	117.40(15)
C15 C10 C5	120.52(14)
C11 C10 C5	121.67(14)
O1 C11 C12	122.98(15)
O1 C11 C10	115.60(14)
C12 C11 C10	121.42(15)
C11 C12 C13	119.27(16)
C14 C13 C12	120.86(15)
C13 C14 C15	118.83(16)
C14 C15 O2	119.54(15)
C14 C15 C10	122.15(15)

O2 C15 C10	118.25(14)
C21 C16 C17	122.02(17)
C21 C16 O1	118.55(17)
C17 C16 O1	119.42(17)
C16 C17 C18	119.69(18)
C17 C18 C19	118.30(19)
C17 C18 C28	121.19(19)
C19 C18 C28	120.49(19)
C20 C19 C18	122.22(18)
C19 C20 C21	118.62(17)
C19 C20 C29	121.20(17)
C21 C20 C29	120.17(18)
C16 C21 C20	119.13(18)
C27 C22 C23	120.92(17)
C27 C22 O2	115.80(16)
C23 C22 O2	123.20(16)
C22 C23 C24	119.87(17)
C23 C24 C25	119.03(18)
C23 C24 C30	119.98(18)
C25 C24 C30	120.98(18)
C26 C25 C24	121.35(19)
C25 C26 C27	118.99(19)
C25 C26 C31	120.7(2)
C27 C26 C31	120.2(2)
C22 C27 C26	119.81(19)
C9 C32 C1	123.83(15)
C9 C32 C33	119.89(14)
C1 C32 C33	116.11(14)
C34 C33 C38	116.80(15)
C34 C33 C32	124.11(15)
C38 C33 C32	118.92(14)
O3 C34 C35	122.15(15)
O3 C34 C33	116.51(14)
C35 C34 C33	121.25(16)
C36 C35 C34	119.73(16)
C37 C36 C35	120.84(16)
C36 C37 C38	118.66(17)
O4 C38 C37	120.49(16)
O4 C38 C33	116.75(15)
C37 C38 C33	122.71(16)
C40 C39 C44	121.54(16)
C40 C39 O3	117.38(15)

C44 C39 O3	121.01(16)
C39 C40 C41	119.35(17)
C42 C41 C40	118.87(17)
C42 C41 C45	120.77(18)
C40 C41 C45	120.35(18)
C41 C42 C43	121.90(17)
C44 C43 C42	118.69(17)
C44 C43 C46	119.71(18)
C42 C43 C46	121.58(17)
C39 C44 C43	119.62(17)
O4 C47 C52	115.57(15)
O4 C47 C48	123.04(16)
C52 C47 C48	121.32(16)
C47 C48 C49	119.66(17)
C48 C49 C50	119.06(17)
C48 C49 C53	119.07(16)
C50 C49 C53	121.86(16)
C51 C50 C49	121.28(17)
C52 C51 C50	119.07(17)
C52 C51 C54	119.60(17)
C50 C51 C54	121.32(17)
C47 C52 C51	119.59(17)
C56 C55 C60	123.1(8)
C56 C55 N3	122.7(9)
C60 C55 N3	113.9(9)
C57 C56 C55	116.7(5)
C58 C57 C56	122.3(4)
C57 C58 C59	120.4(4)
C58 C59 C60	119.8(5)
C55 C60 C59	117.6(8)
O6A C61A C65A	112.0(8)
O6A C61A C62A	102.1(8)
C65A C61A C62A	113.4(10)
C61A C62A C63A	101.3(4)
C64A C63A C62A	101.0(4)
O6A C64A C63A	104.8(5)

Table S31. Torsion angles for [Fe(3,5-Me-BAFP)(2-MeTHF)(PhNO)].

Atom–Atom–Atom–Atom	Torsion Angle [°]
C4 N1 C1 C32	176.96(16)
Fe1 N1 C1 C32	-1.6(2)
C4 N1 C1 C2	-1.69(18)
Fe1 N1 C1 C2	179.70(11)
N1 C1 C2 C3	0.68(19)
C32 C1 C2 C3	-178.01(16)
C1 C2 C3 C4	0.61(19)
C1 N1 C4 C5	-176.20(16)
Fe1 N1 C4 C5	2.4(2)
C1 N1 C4 C3	2.06(18)
Fe1 N1 C4 C3	-179.30(11)
C2 C3 C4 N1	-1.71(19)
C2 C3 C4 C5	176.58(16)
N1 C4 C5 C6	-3.8(3)
C3 C4 C5 C6	178.15(16)
N1 C4 C5 C10	174.29(15)
C3 C4 C5 C10	-3.7(2)
C9 N2 C6 C5	-177.09(15)
Fe1 N2 C6 C5	0.3(2)
C9 N2 C6 C7	0.66(17)
Fe1 N2 C6 C7	178.03(11)
C4 C5 C6 N2	2.4(3)
C10 C5 C6 N2	-175.67(15)
C4 C5 C6 C7	-175.06(16)
C10 C5 C6 C7	6.9(2)
N2 C6 C7 C8	-1.13(19)
C5 C6 C7 C8	176.64(16)
C6 C7 C8 C9	1.09(19)
C6 N2 C9 C32	-178.83(15)
Fe1 N2 C9 C32	3.8(2)
C6 N2 C9 C8	0.03(17)
Fe1 N2 C9 C8	-177.30(11)
C7 C8 C9 N2	-0.73(19)
C7 C8 C9 C32	178.14(16)
C6 C5 C10 C15	83.5(2)
C4 C5 C10 C15	-94.69(18)
C6 C5 C10 C11	-103.96(19)
C4 C5 C10 C11	77.8(2)

C16 O1 C11 C12	10.2(2)
C16 O1 C11 C10	-169.62(15)
C15 C10 C11 O1	-177.72(14)
C5 C10 C11 O1	9.5(2)
C15 C10 C11 C12	2.4(2)
C5 C10 C11 C12	-170.31(15)
O1 C11 C12 C13	179.55(15)
C10 C11 C12 C13	-0.6(2)
C11 C12 C13 C14	-1.5(2)
C12 C13 C14 C15	1.8(3)
C13 C14 C15 O2	-177.05(15)
C13 C14 C15 C10	0.2(3)
C22 O2 C15 C14	-73.9(2)
C22 O2 C15 C10	108.79(17)
C11 C10 C15 C14	-2.2(2)
C5 C10 C15 C14	170.61(15)
C11 C10 C15 O2	175.03(14)
C5 C10 C15 O2	-12.1(2)
C11 O1 C16 C21	-106.55(19)
C11 O1 C16 C17	72.3(2)
C21 C16 C17 C18	1.3(3)
O1 C16 C17 C18 -	-177.57(17)
C16 C17 C18 C19	-0.7(3)
C16 C17 C18 C28	177.9(2)
C17 C18 C19 C20	-0.6(3)
C28 C18 C19 C20	-179.1(2)
C18 C19 C20 C21	1.2(3)
C18 C19 C20 C29	-179.82(19)
C17 C16 C21 C20	-0.6(3)
O1 C16 C21 C20	178.23(16)
C19 C20 C21 C16	-0.6(3)
C29 C20 C21 C16	-179.59(18)
C15 O2 C22 C27	162.60(16)
C15 O2 C22 C23	-20.6(2)
C27 C22 C23 C24	0.5(3)
O2 C22 C23 C24	-176.10(16)
C22 C23 C24 C25	-1.5(3)
C22 C23 C24 C30	177.15(18)
C23 C24 C25 C26	1.9(3)
C30 C24 C25 C26	-176.8(2)
C24 C25 C26 C27	-1.2(4)
C24 C25 C26 C31	176.7(3)

C23 C22 C27 C26	0.2(3)
O2 C22 C27 C26	177.0(2)
C25 C26 C27 C22	0.1(4)
C31 C26 C27 C22	-177.8(3)
N1 C1 C32 C9	3.8(3)
C2 C1 C32 C9	-177.76(16)
N1 C1 C32 C33	-171.52(15)
C2 C1 C32 C33	7.0(2)
C9 C32 C33 C34	85.3(2)
C1 C32 C33 C34	-99.24(19)
C9 C32 C33 C38	-99.53(19)
C1 C32 C33 C38	75.94(19)
C39 O3 C34 C35	29.5(2)
C39 O3 C34 C33	-153.80(15)
C38 C33 C34 O3	-177.64(14)
C32 C33 C34 O3	-2.4(2)
C38 C33 C34 C35	-0.9(2)
C32 C33 C34 C35	174.42(15)
O3 C34 C35 C36	176.96(15)
C33 C34 C35 C36	0.4(2)
C34 C35 C36 C37	0.3(3)
C35 C36 C37 C38	-0.4(3)
C47 O4 C38 C37	-53.3(2)
C47 O4 C38 C33	129.38(16)
C36 C37 C38 O4	-177.33(15)
C36 C37 C38 C33	-0.1(3)
C34 C33 C38 O4	178.05(14)
C32 C33 C38 O4	2.5(2)
C34 C33 C38 C37	0.7(2)
C32 C33 C38 C37	-174.79(15)
C34 O3 C39 C40	-136.18(16)
C34 O3 C39 C44	46.9(2)
C44 C39 C40 C41	0.4(3)
O3 C39 C40 C41	-176.51(15)
C39 C40 C41 C42	-1.3(3)
C39 C40 C41 C45	-179.91(17)
C40 C41 C42 C43	0.7(3)
C45 C41 C42 C43	179.30(18)
C41 C42 C43 C44	0.8(3)
C41 C42 C43 C46	-177.68(18)
C40 C39 C44 C43	1.1(3)
O3 C39 C44 C43	177.91(15)

C42 C43 C44 C39	-1.7(3)
C46 C43 C44 C39	176.84(17)
C38 O4 C47 C52	160.43(16)
C38 O4 C47 C48	-22.6(2)
O4 C47 C48 C49	-177.78(16)
C52 C47 C48 C49	-1.0(3)
C47 C48 C49 C50	1.2(3)
C47 C48 C49 C53	-178.04(16)
C48 C49 C50 C51	-0.3(3)
C53 C49 C50 C51	178.88(17)
C49 C50 C51 C52	-0.8(3)
C49 C50 C51 C54	178.18(18)
O4 C47 C52 C51	176.89(16)
C48 C47 C52 C51	-0.1(3)
C50 C51 C52 C47	1.0(3)
C54 C51 C52 C47	-177.97(18)
O5 N3 C55 C56	-90.9(11)
Fe1 N3 C55 C56	86.9(11)
O5 N3 C55 C60	83.4(12)
Fe1 N3 C55 C60	-98.9(11)
C60 C55 C56 C57	-0.1(12)
N3 C55 C56 C57	173.6(8)
C55 C56 C57 C58	0.8(7)
C56 C57 C58 C59	0.0(6)
C57 C58 C59 C60	-1.6(8)
C56 C55 C60 C59	-1.4(15)
N3 C55 C60 C59	-175.6(9)
C58 C59 C60 C55	2.2(13)
C64A O6A C61A C65A	103.0(11)
Fe1 O6A C61A C65A	-95.2(12)
C64A O6A C61A C62A	-18.6(11)
Fe1 O6A C61A C62A	143.1(8)
O6A C61A C62A C63A	37.4(9)
C65A C61A C62A C63A	-83.2(7)
C61A C62A C63A C64A	-43.0(7)
C61A O6A C64A C63A	-9.0(10)
Fe1 O6A C64A C63A	-172.5(5)
C62A C63A C64A O6A	32.0(6)

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