Supporting Information for

2-Phenoxypyridyl Dinucleating Ligands for Assembly of Diiron(II) Complexes; Efficient Reactivity with O_2 to Form μ-Oxodiiron(III) Units

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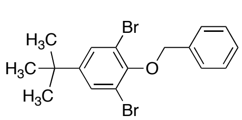
Experimental

Materials and Methods. Reagents purchased from Strem, Aldrich Chemical Co., and Alfa Aesar were used as received. All air-sensitive manipulations were performed using standard Schlenk techniques or under a nitrogen atmosphere inside an MBraun drybox. Solvents were saturated with argon and purified by passage over two columns of activated Al_2O_3.

General Physical Methods. NMR spectra were recorded on a 500 MHz Varian Mercury spectrometer. ^1H and ^{13}C chemical shifts referenced to residual solvent peaks. IR spectra were measured on a ThermoNicolet Avatar 360 spectrophotometer with the OMNIC software. Absorption spectra were recorded on a Cary 50 spectrophotometer using 6Q Spectrosil quartz cuvettes (Starna) with 1 cm path lengths. Cyclic and differential pulse voltammetric measurements were recorded using a VersaSTAT3 potentiostat from Princeton Applied Research using the V3 Studio software. Electrospray ionization mass spectra were acquired using an Agilent Technologies 1100 Series LC-MSD Trap. Gas-chromatographic mass spectra were obtained using an Agilent Technologies 6890 N GC system equipped with a 5973N MSD unit.

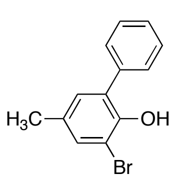
Synthesis

1-Benzyloxy-2,6-dibromo-4-*tert*-butylbenzene. Solid 2,6-dibromo-4-*t*-butylphenol (10.0 g, 32.5 mmol), K_2CO_3 (6.7 g,48.8 mmol), and benzyl bromide (4.7 mL, 39.0 mmol) were combined in 300 mL of CH_3CN and refluxed for 3 h. Water was added to the reaction mixture and the organic phase was extracted with CH_2Cl_2 (3 x 200 mL). The organic layer was separated, dried over Na_2SO_4, and evaporated to dryness. Purification of the crude material by silica gel column chromatography (5:95 EtOAc/hexanes) gave a yellow oil

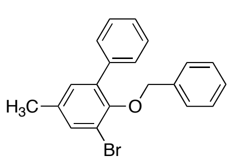


(5.54 g, 42 %). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.64 (d, *J* = 7.0 Hz, 2H), 7.55 (s, 2H), 7.44 (t, *J* = 7.0 Hz, 2H), 7.40 (d, *J* = 7.0 Hz, 1H), 5.03 (s, 2H), 1.32 (s, 9H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 150.55, 150.35, 136.63, 130.14, 128.68, 128.66, 128.54, 118.23, 74.78, 34.84, 31.37. GC-MS = 398 $[M]^+$.

3-Bromo-5-methylbiphenyl-2-ol (**5**). The protected 2-(5-methylbiphenyl-2-yloxy)tetrahydro-2*H*-pyran[1] (20.0 g, 74.6 mmmol) was dissolved in 100 mL of CH_3OH/CH_3CN (1:1). The mixture was treated with conc. HCl (10 mL), refluxed for 1h, and concentrated by evaporation. About 200 mL of H_2O was added and the product was extracted with CH_2Cl_2 (3x 100 mL). The organic layer was dried over Na_2SO_4, filtered, and evaporated to afford a white solid. The resulting 3-bromo-5-methylbiphenyl-2-ol was re-dissolved in CH_2Cl_2 (100 mL) and cooled to 0 ºC. Liquid bromine (3.8 mL, 74.6 mmol) was added in a dropwise manner to the reaction flask. The reaction mixture was stirred for 1 h, washed with sat. Na_2SO_2 (aq), dried over Na_2SO_4, and evaporated to yield a pale brown oil (18.8 g, 96%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.58 (d, *J* = 9 Hz, 2H), 7.50 (t, *J* = 8 Hz, 2H), 7.42 (t, *J* = 8 Hz, 1H), 7.35 (s, 1H), 7.11 (s, 1H), 5.59 (s, 1H), 2.36 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 147.10, 137.50, 131.73, 131.29, 130.96, 129.31, 129.26, 128.63, 127.81, 110.78, 20.42. GC-MS = 262 $[M]^+$.

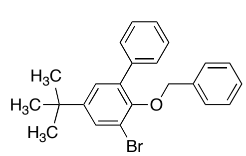


2-Benzyloxy-1-bromo-5-methyl-3-phenylbenzene (**6**). **Method A:** Solid 2-benzyloxy-1,3-dibromo-5-methylbenzene (**8**)[2] (12.0 g, 33.7 mmol), phenyl boronic acid (4.11 g, 33.7 mmol), and $[Pd(PPh_3)_4]$ (1.94 g, 1.68 mmol) were combined in solvent containing 100 mL THF and 100 mL of 1.0 M aqueous Na_2CO_3 in a



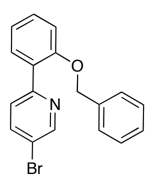
500 mL Schlenk flask. The mixture was degassed with nitrogen for 30 min and then refluxed for 20 h. The organic phase was then extracted with CH_2Cl_2 (3 x 150 mL), dried over Na_2SO_4, and evaporated to dryness. Purification of the crude material by silica gel column chromatography (5:95 EtOAc/hexanes) gave a colorless oil (10.12 g) that contained a mixture of 2-benzyloxy-1,3-dibromo-5-methylbenzene (929 mg, 7%), 1-benzyloxy-2,6-diphenyl-4-methylbenzene (1.83 g, 15%) and 2-benzyloxy-1-bromo-5-methyl-3-phenylbenzene (7.26 g, 62%). The three compounds could not be separated so the mixture was used in the next step. GC-MS = 356 [2-benzyloxy-1,3-dibromo-5-methylbenzene]$^+$, 350 [1-benzyloxy-2,6-diphenyl-4-methylbenzene]$^+$, and 352 [2-benzyloxy-1-bromo-5-methyl-3-phenylbenzene]$^+$. **Method B:** Solid 3-bromo-5-methylbiphenyl-2-ol (**5**) (18.8 g, 71.5 mmol) and benzyl bromide (9.3 mL, 78.6 mmol) were dissolved in CH_3CN (400 mL). The solution was refluxed for 4 h, evaporated to dryness, and the residue was re-dissolved in CH_2Cl_2 (300 mL). The organic phase was washed with H_2O (3 x 100 mL), dried over Na_2SO_4, filtered, and evaporated to give an oil. The crude material was purified by silica gel column chromatography (5 % EtOAc/ hexanes) and re-crystallized from hot hexanes to give a white solid (16.0 g, 72 %). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.62 (m, 2H), 7.48-7.43 (m, 4H), 7.32 (m 3H), 7.22 (m, 2H), 7.18 (s, 1H), 4.55(s, 2 H), 2.40 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 150.89, 137.99, 137.00, 136.61, 135.57, 132.98, 131.06, 129.46, 128.90, 128.42, 128.39, 128.24, 127.76, 118.29, 74.95, 20.78. GC-MS: m/z = 352 [M]$^+$. Mp = 64-65 °C.

2-Benzyloxy-1-bromo-3-phenyl-5-*tert*-butylbenzene. The same procedure was employed as



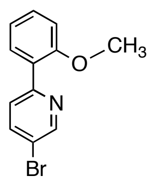
described for the synthesis of 2-benzyloxy-1-bromo-5-methyl-3-phenylbenzene (**6**) (Method A), except that 1-benzyloxy-2,6-dibromo-4-*tert*-butylbenzene was used in place of 2-benzyloxy-1,3-dibromo-5-methylbenzene. The reaction was performed with the following reagents: 1-benzyloxy-2,6-dibromo-4-*tert*-butylbenzene (1.0 g, 2.51 mmol), phenyl boronic acid (306 mg, 2.51 mmol), [Pd(PPh_3)$_4$] (146 mg, 0.126 mmol), and 1.0 M Na_2CO_3 (20 mL, H_2O/THF). Purification of the crude material by silica gel column chromatography (2:1 hexanes/CH_2Cl_2) gave a colorless oil (997 mg) that contained a mixture of 1-benzyloxy-2,6-dibromo-4-*tert*-butylbenzene (170 mg, 17%), 1-benzyloxy-2,6-diphenyl-4-*tert*-butylbenzene (257 mg, 26%), and 2-benzyloxy-1-bromo-3-phenyl 5-*tert*-butylbenzene (576 mg, 57%). The three compounds could not be separated so the mixture was used in the next step. GC-MS = 398 [1-benzyloxy-2,6-dibromo-4-*tert*-butylbenzene]$^+$, 392 [1-benzyloxy-2,6-diphenyl-4-*tert*-butylbenzene]$^+$, and 394 [2-benzyloxy-1-bromo-3-phenyl 5-*tert*-butylbenzene]$^+$.

2-(2-Benzyloxyphenyl)-5-bromopyridine. The compound 1-benzyloxy-2-iodobenzene (1.00 g,

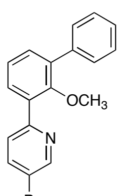


3.22 mmol) was dissolved in 15 mL dry THF in a 50 mL Schlenk flask and the mixture was cooled to -78 °C. A 1.6 M hexanes solution of *n*-butyllithium (2.0 mL, 3.22 mmol) was added slowly to the reaction flask. The mixture was stirred at -78 °C for 30 min. Solid anhydrous $ZnCl_2$ (351 mg, 3.22 mmol) was added and the mixture was stirred at RT for 30 min. The reaction flask was brought inside a drybox and charged with 2,5-dibromopyridine (694 mg, 2.93 mmol) and [Pd(PPh_3)$_4$] (169 mg, 0.146 mmol). The resulting solution was transferred to a sealed reaction vessel and stirred at 80 °C for 15h. Water was added to the reaction mixture and the organic phase was extracted with dichloromethane (3x15 mL). The organic layer was separated, dried over Na_2SO_4, and evaporated to dryness. The crude material was purified by silica gel column chromatography (5:95 EtOAc/hexanes) to afford a fluffy white solid (368 mg, 37%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.77 (d, *J* = 2.00 Hz,1H), 7.86 (m, 2H), 7.78 (dd, *J* = 11.0, 2.5 Hz, 1H), 7.40-7.33 (m, 6H), 7.12 (t, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 8.5 Hz, 1H), 5.15 (s, 2H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 156.19, 154.44, 150.48, 138.34, 136.87, 131.27, 130.55, 128.74, 128.35, 128.09, 127.29, 126.61, 121.72, 119.01, 113.25, 70.77. GC-MS: m/z = 339 $[M]^+$. Mp = 69-70 °C.

5-Bromo-2-(2-methoxyphenyl)pyridine. The same procedure was employed as for the synthesis of 2-(2-benzyloxyphenyl)-5-bromopyridine, except that 2-bromoanisole was used in place of 1-benzyloxy-2-iodobenzene. The reaction was performed with the following reagents: 2-bromoanisole (2.97 g, 15.9 mmol), 1.6 M *n*-butyllithium in hexanes (10 mL, 15.9 mmol), anhydrous $ZnCl_2$ (1.73 g, 15.9 mmol), $[Pd(PPh_3)_4]$ (873 mg, 0.755 mmol), and 2,5-dibromopyridine (3.58 g, 15.1 mmol). Purification of the crude material by silica gel column chromatography (5 :95 EtOAc/hexanes) gave a light yellow oil (2.29 g, 57%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.75 (d, J = 2.5 Hz, 1H), 7.81-7.75 (m, 3H), 7.38 (t, J = 1.0 Hz, 1H), 7.08 (t, J = 1.0 Hz, 1H), 7.99 (d, J = 10 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 156.94, 154.53, 150.40, 138.32, 131.03, 130.46, 127.86, 126.40, 121.19, 118.88, 111.47, 55.65. GC-MS = 263 $[M]^+$.

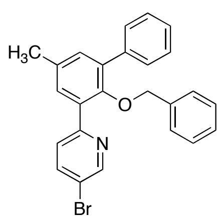


5-Bromo-2-(2-methoxybiphenyl-3-yl)pyridine. The same procedure was employed as for the synthesis of 2-(2-benzyloxyphenyl)-5-bromopyridine, except that 2-bromo-6-phenylanisole was used in place of 1-benzyloxy-2-iodobenzene. The reaction was performed with the following reagents: 2-bromo-6-phenylanisole (1.16 g, 4.43 mmol), 1.6 M *n*-butyllithium in hexanes (2.8 mL, 4.43 mmol), anhydrous $ZnCl_2$ (483 mg, 4.43 mmol), $[Pd(PPh_3)_4]$ (243 mg, 0.211 mmol), and 2,5-dibromopyridine (1.00 g, 4.22 mmol). Purification of the crude material by silica gel column chromatography (5 :95 EtOAc/hexanes) gave

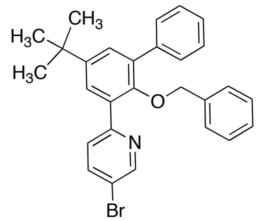


a white crystalline solid (868 mg, 57%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.80 (s, 1H), 7.87 (s, 2H), 7.74 (dd, *J* = 9.5, 2.0 Hz, 1H), 7.62 (d, *J* = 10 Hz, 2H), 7.47-7.42 (m, 3H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 155.49, 154.91, 150.66, 138.82, 138.44, 136.03, 133.20, 132.26, 130.43, 129.40, 128.44, 127.46, 126.25, 124.79, 119.41, 61.11. GC-MS = 339 $[M]^+$. Mp = 88-89 °C.

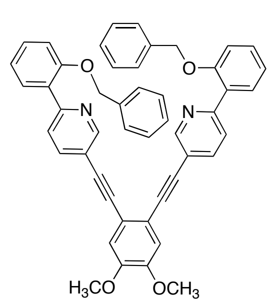
5-Bromo-2-(2-benzyloxy-5-methylbiphenyl-3-yl)pyridine (**7**). The same procedure was employed as for the synthesis of 2-(2-benzyloxyphenyl)-5-bromopyridine, except that 2-benzyloxy-1-bromo-5-methyl-3-phenylbenzene was used in place of 1-benzyloxy-2-iodobenzene. The reaction was performed with the following reagents: 2-benzyloxy-1-bromo-5-methyl-3-phenylbenzene (~60% purity, 6.00 g, ~10.2 mmol), 1.6 M *n*-butyllithium in hexanes (10 mL, 16.3 mmol), anhydrous $ZnCl_2$ (1.78 g, 16.3 mmol), $[Pd(PPh_3)_4]$ (751 mg, 0.65 mmol), and 2,5-dibromopyridine (3.06 g, 12.9 mmol). Purification of the crude material by silica gel column chromatography (10:90 EtOAc/hexanes) gave a white solid (2.47 g, ~ 60 %). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.77 (d, *J* = 2.0 Hz, 1H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.78 (dd, *J* = 12, 2.5 Hz, 1H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 1.5 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 2.0 Hz, 1H), 7.20 (d, *J* = 7.0 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 2H), 6.75 (d, *J* = 8.0 Hz, 2H). 4.24 (s, 2H). 2.44 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 155.05, 151.72, 138.62, 138.46, 136.48, 136.38, 134.57, 133.50, 132.84, 130.65, 129.76, 128.82, 128.41, 128.27, 128.12, 127.50, 126.86, 119.30, 75.91, 21.08. ESI-MS = 430.3 $[M+H]^+$. Mp = 93-95 °C.



5-Bromo-2-(2-benzyloxy-5-*tert*-butylbiphenyl-3-yl)pyridine. The same procedure was employed as for the synthesis of 2-(2-benzyloxyphenyl)-5-bromopyridine, except that 2-benzyloxy-1-bromo-3-phenyl-5-*tert*-butylbenzene was used in place of 1-benzyloxy-2-iodobenzene. The reaction was performed with the following reagents: 2-benzyloxy-1-bromo-3-phenyl-5-*tert*-butylbenzene (~60% purity, 3.26 g, ~8.25 mmol), 1.6 M *n*-butyllithium in hexanes (5.9 mL, 9.43 mmol), anhydrous $ZnCl_2$ (1.03 g, 9.43 mmol), $[Pd(PPh_3)_4]$ (454 mg, 0.393 mmol), and 2,5-dibromopyridine (1.86 g, 7.86 mmol). Purification of the crude material by silica gel column chromatography (5:95 EtOAc/hexanes) gave a white solid (909 mg, 39%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.83 (s, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.81 (s, 2H), 7.70 (d, J = 7.0 Hz, 2H), 7.52-7.44 (m, 4H), 7.24-7.20 (m, 3H), 6.80 (d, J = 7.0 Hz, 2H), 4.29 (s, 2H), 1.45 (s, 9H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 155.40, 151.76, 150.58, 147.69, 139.03, 138.39, 136.63, 135.96, 133.05, 129.84, 129.45, 128.70, 128.39, 128.26, 128.06, 127.44, 127.22, 126.87, 119.27, 75.87, 34.82, 31.66. ESI-MS = 472.2 $[M+H]^+$. Mp = 164-166 °C.

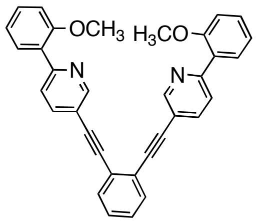


Benz$_2$LV^{H,H} (5,5'-(4,5-dimethoxy-1,2-phenylene)bis(ethyne-2,1-diyl)bis(2-(2-(benzyloxy) phenyl)-pyridine). Solid 2-(2-benzyloxyphenyl)-5-bromopyridine (600 mg, 1.76 mmol), 4,5-diethynylveratrole (149 mg, 0.802 mmol), $[Pd(PPh_3)_4]$ (93 mg, 80.2 μmol), and triethylamine (0.28 mL, 2.00 mmol) were combined with 20 mL dry THF in a sealed reaction vessel. The reaction was stirred at 80 °C for 3d. A 20 mL solution of dichloromethane was added and the mixture was washed with H_2O (2 x 50 mL). The organic layer was separated, dried over Na_2SO_4, and evaporated to dryness. The crude material was purified by silica gel col-



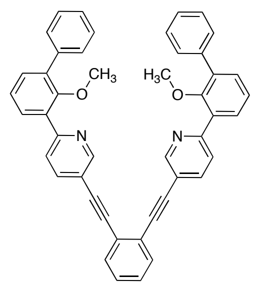
umn chromatography (20:80 EtOAc/hexanes) to afford a beige solid (381 mg, 67%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.91 (d, *J* = 1.5 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.91 (dd, *J* = 9.0, 1.5 Hz, 2H), 7.80 (dd, *J* = 10.5, 2.0 Hz, 2H), 7.38-7.31 (m, 8H), 7.25 (d, *J* = 7.5 Hz, 2H), 7.13-7.05 (m, 8H), 5.14 (s, 4H), 3.96 (s, 6H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 156.38, 154.94, 151.82, 149.55, 137.98, 136.96, 131.46, 130.50, 128.93, 128.70, 128.00, 127.21, 124.85, 121.70, 118.57, 118.34, 114.27, 113.32, 91.57, 89.76, 70.79, 56.28. ESI-MS = 705.6 $[M+H]^+$. Mp = 51-54 °C.

$Me_2LV^{H,H}$ (1,2-bis((6-(2-methoxyphenyl)pyridin-3-yl)ethynyl)benzene). The same procedure was employed as for the synthesis of **$Benz_2LV$**^{H,H} , except that 5-bromo-2-(2-methoxyphenyl)pyridine was used instead of 2-(2-benzyloxyphenyl)-5-bromopyridine, and 1,2-diethynylbenzene was used instead of 4,5-diethynylveratrole. The reaction was performed with the following reagents: 1,2-diethynylbenzene (331 mg, 2.63 mmol), 5-bromo-2-(2-methoxyphenyl)pyridine (2.00 g, 5.78 mmol), $[Pd(PPh_3)_4]$ (304 mg, 0.263 mmol), and triethylamine (0.92 mL, 6.58 mmol). Purification of the crude material by silica gel column chromatography (20:80 EtOAc/hexanes) gave a light yellow solid (341 mg, 26%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.91 (d, *J* = 3.0 Hz, 2H), 7.92-7.86 (m, 6H), 7.63 (m, 2H), 7.42-7.37 (m, 4H), 7.11 (t, 7.5 Hz, 2H), 7.02 (2, *J* = 8.0 Hz, 2H), 3.89 (s, 6H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 157.32, 155.33, 151.98, 138.42, 132.34, 131.41, 130.67, 128.72, 128.43, 125.57, 124.83, 121.36, 118.26, 111.63, 91.44, 91.08, 55.84. ESI-MS = 493.3 $[M+H]^+$. Mp = 150-151 °C.



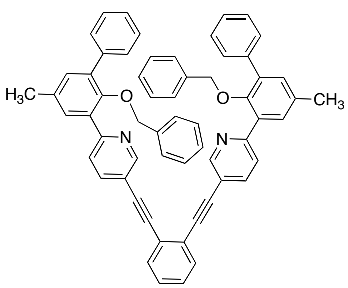
$Me_2L^{H,Ph}$ (1,2-bis((6-(2-methoxybiphenyl-3-yl)pyridin-3-yl)ethynyl)benzene). The same procedure was employed as for the synthesis of **$Benz_2LV$**^{H,H} , except that 5-bromo-2-(2-

methoxybiphenyl-3-yl)pyridine was used instead of 2-(2-benzyloxyphenyl)-5-bromopyridine, and 1,2-diethynylbenzene was used instead of 4,5-diethynylveratrole. The reaction was performed with the following reagents: 1,2-diethynylbenzene (529 mg, 4.20 mmol), 5-bromo-2-(2-



methoxybiphenyl-3-yl)pyridine (3.0 g, 8.82 mmol), $[Pd(PPh_3)_4]$ (486 mg, 0.420 mmol), and triethylamine (1.5 mL, 10.5 mmol). Purification of the crude material by silica gel column chromatography (CH_2Cl_2) gave a light yellow solid (1.84 g, 68%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.96 (d, *J* = 1.0 Hz, 2H), 8.00 (d, *J* = 8.5 Hz, 2H), 7.92 (dd, *J* = 10.5, 1.5 Hz, 2H), 7.81 (dd, *J* = 9.0, 1.5 Hz, 2H), 7.66-7.62 (m, 6H), 7.47-7.38 (m, 10H), 7.31 (t, *J* = 8.0 Hz, 2H), 3.26 (s, 6H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 155.70, 155.63, 152.08, 138.61, 138.54, 136.02, 133.63, 132.28, 130.65, 129.45, 128.73, 128.42, 127.42, 125.44, 124.76, 124.47, 118.53, 91.65, 90.84, 61.15. ESI-MS = 645.5 $[M+H]^+$. Mp = 128-130 °C.

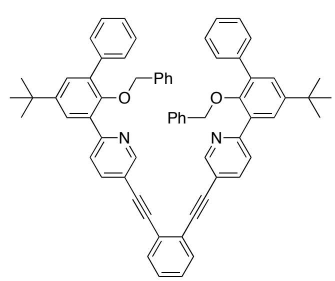
$Benz_2L^{Me,Ph}$ (1,2-bis((6-(2-(benzyloxy)-5-methylbiphenyl-3-yl)pyridin-3-yl)ethynyl)benzene).



Method A: The same procedure was employed as for the synthesis of **$Benz_2LV^{H,H}$** , except that 5-bromo-2-(2-benzyloxy-5-methylbiphenyl-3-yl)pyridine was used instead of 2-(2-benzyloxyphenyl)-5-bromopyridine, and 1,2-diethynylbenzene was used instead of 4,5-diethynylveratrole. The reaction was performed with the following reagents: 1,2-diethynylbenzene (345 mg, 2.74 mmol), 5-bromo-2-(2-benzyloxy-5-methylbiphenyl-3-yl)pyridine (2.47 g, 5.74 mmol), $[Pd(PPh_3)_4]$ (317 mg, 0.274 mmol), and triethylamine (1 mL, 6.85 mmol). Purification of the crude material by silica gel column chromatography (10:90 EtOAc/hexanes) gave a light yellow solid (1.26 g, 56%). **Method B:** Solid 1,2-

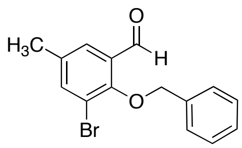
bis((trimethylsilyl)ethynyl)benzene (1.31 g, 4.85 mmol) was dissolved in THF (50 mL) and treated with a 1.0 M solution of NBu_4F (10.2 mL, 10.2 mmol). The mixture was stirred for 4.5 h and then charged with 5-bromo-2-(2-benzyloxy-5-methylbiphenyl-3-yl)pyridine (**7**) (5.21 g, 12.1 mmol), $[Pd(PPh_3)]_4$ (560 mg, 0.485 mmol), and NEt_3 (2.0 mL, 14.6 mmol). The reaction was stirred at 70ºC for 2 d. The workup and purification procedure was identical to method A. The product was obtained in 45% yield (1.80 g). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.96 (d, *J* = 1.5 Hz, 2H), 8.02 (d, *J* = 8.5 Hz, 2H), 7.86 (dd, *J* = 10.5, 2.0 Hz, 2H), 7.69-7.67 (m, 8H), 7.47 (t, *J* = 7.0 Hz, 4H), 7.42-7.41 (m, 4H), 7.29 (d, *J* = 2.0 Hz, 2H), 7.17-7.14 (m, 6H), 6.78 (dd, *J* = 9.0, 1.5 Hz, 4H), 4.27 (s, 4H), 2.46 (s, 6H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 155.82, 152.07, 151.99, 138.79, 138.40, 136.58, 136.48, 134.62, 133.93, 132.97, 132.41, 131.03, 129.90, 128.96, 128.87, 128.48, 128.36, 128.20, 127.55, 125.54, 125.20, 118.52, 91.71, 91.05, 76.02, 21.18. ESI-MS = 825.8 $[M+H]^+$. Mp = 111-114 °C.

$Benz_2L^{tBu,Ph}$ (1,2-bis((6-(2-(benzyloxy)-5-*tert*-butylbiphenyl-3-yl)pyridin-3-yl)ethynyl)benzene). The same procedure was employed as for the synthesis of **$Benz_2LV^{H,H}$**, except that 5-bromo-2-(2-benzyloxy-5-*tert*-butylbiphenyl-3-yl)pyridine was used instead of 2-(2-benzyloxyphenyl)-5-bromopyridine, and 1,2-diethynylbenzene was used instead of 4,5-diethynylveratrole. The reaction was performed with the following reagents: 1,2-diethynylbenzene (64 mg, 0.508 mmol), 5-bromo-2-(2-benzyloxy-5-*tert*-butylbiphenyl-3-yl)pyridine (576 mg, 1.22 mmol), $[Pd(PPh_3)_4]$ (59 mg, 0.051 mmol), and triethylamine (0.2 mL, 1.27 mmol). Purification of the crude material by silica gel column chromatography (5:95 to 10:90 EtOAc/hexanes) gave a yellow solid (260 mg, 56%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.97

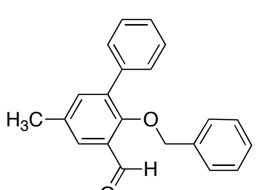


(d, J = 1.5 Hz, 2H), 7.99 (d, J = 8.0 Hz, 2H), 7.86-7.83 (m, 4H), 7.69-7.67 (m, 6H), 7.49-7.46 (m, 6H), 7.43-7.41 (m, 4H), 7.15-7.14 (m, 6H), 6.78-6.76 (m, 4H), 4.26 (s, 4H), 1.42 (s, 18H). ESI-MS = 909.9 $[M+H]^+$. Mp = 176-177 °C.

2-Benzyloxy-3-bromo-5-methylbenzaldehyde (**9**). Solid 2-benzyloxy-1,3-dibromo-5-methylbenzene (**8**) (27.7 g, 77.8 mmol) was dissolved in 500 mL of dry toluene and cooled to -78 °C. A 1.6 M nBuLi solution in hexanes (58 mL, 93.4 mmol) was slowly added to the reaction mixture and stirred for 1.5 h. The mixture was then treated with neat DMF (9.0 mL, 117 mmol) and continued to stir at –78 °C for 10 h. Once the reaction was complete, formation of a white precipitate was observed. The reaction mixture was washed with H_2O (3x200 mL), dried over Na_2SO_4, and evaporated to dryness. The resulting oil was dissolved in MeOH (200 mL) and cooled to -25 °C to induce crystallization. After 4 h, the material was isolated by filtration to give a white solid (15.5 g, 65 %). ^1H NMR ($CDCl_3$, 500 MHz): δ 10.09 (s, 1H), 7.67 (d, J = 2.5 Hz, 1H), 7.57 (d, J = 2.0 Hz, 1H), 7.47-7.39 (m, 5H), 5.09 (s, 2H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 189.18, 156.28, 140.06, 136.08, 135.44, 130.96, 128.8, 127.85, 118.08, 77.85, 20.57. GC-MS = 304 $[M]^+$. Mp = 53-55 °C.

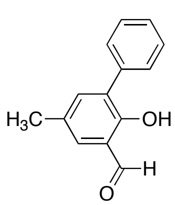


2-Benzyloxy-5-methyl-3-phenylbenzaldehyde (**10**). Solid 2-Benzyloxy-3-bromo-5-methylbenzaldehyde (**9**) (5.26 g, 17.2 mmol), phenyl boronic acid (3.16 g, 25.9 mmol), $Pd(PPh_3)_4$ (0.99 g, 0.86 mmol), and $NaCO_3$ (3.65 g, 34.4 mmol) were combined with 100 mL of H_2O/THF (1:1) and degassed with N_2 for 30 min. The reaction mixture was stirred rigorously and refluxed for 12 h. A solution of CH_2Cl_2 (200 mL) was added and the organic phase was separated from the aqueous layer. The organic



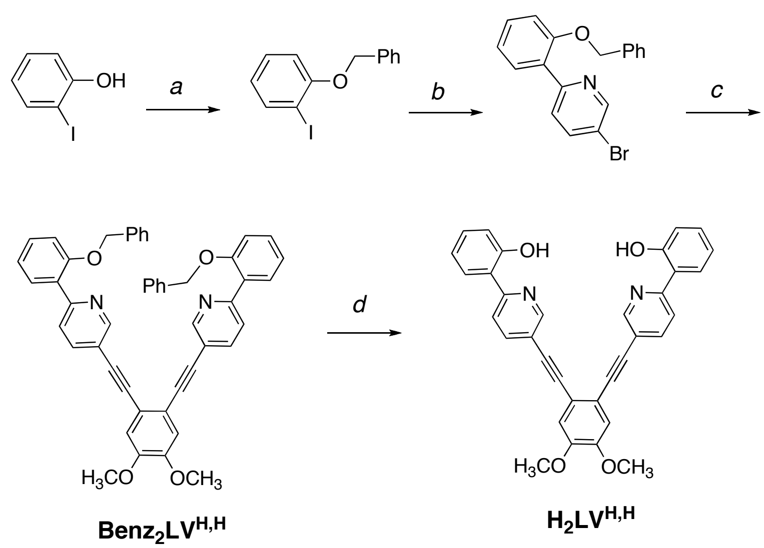
mixture was dried over Na_2SO_4 and evaporated to yield an oil. The crude material was purified by silica gel column chromatography (5% EtOAc/hexanes) and the desired product was further crystallized from hot hexanes to afford a white solid (3.92 g, 76 %). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 10.32 (s, 1H), 7.64 (m, 3H), 7.50-7.43 (m, 4H), 7.30-7.27 (m, 3H), 7.08-7.06 (m, 2H), 4.53 (s, 2H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 190.22, 157.07, 138.05, 137.30, 136.04, 135.66, 134.27, 129.78, 129.12, 128.73, 128.57, 128.44, 127.80, 127.34, 77.06, 20.71. GC-MS = 302 $[M]^+$. Mp = 98-99 °C.

2-Hydroxy-5-methyl-3-phenylbenzaldehyde (**11**). The 2-benzyloxy-5-methyl-3-phenyl-

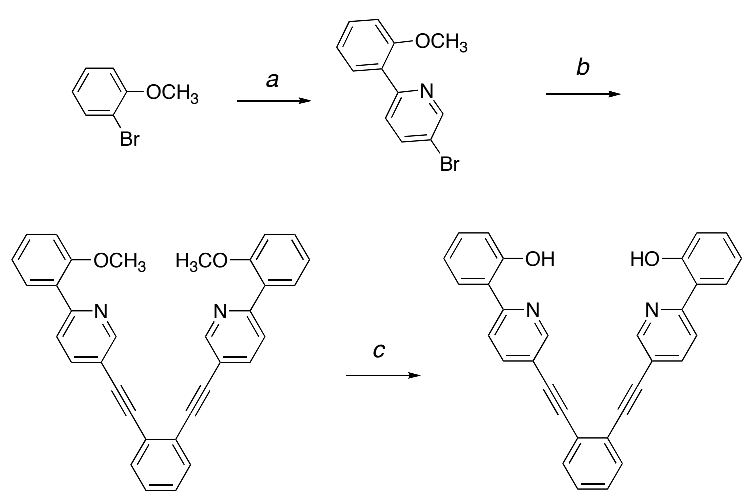


benzaldehyde compound (**10**) (3.92 g, 13 mmol) was dissolved in 50 mL of dry CH_2Cl_2 and cooled to 0 °C. A 1.0 M boron tribromide solution in CH_2Cl_2 (26 mL, 26 mmol) was added slowly to the reaction flask and the solution immediately became a dark red-orange color. The reaction was stirred for 2 h and then quenched with H_2O (50 mL). The organic layer was separated, dried over Na_2SO_4 and evaporated to dryness. The crude material was purified by silica gel column chromatography (5% EtOAc/hexanes) to give the desired product as a yellow oil (3.92 g, 76%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ 11.40 (s, 1H), 9.90 (s, 1H), 7.62 (d, J = 8 Hz, 2H), 7.49-7.45 (m, 3 H), 7.39 (m, 1H), 7.34 (s, 1H), 7.40 (s, 3H). ^{13}C NMR ($CDCl_3$, 500 MHz): δ 197.56, 157.52, 139.64, 137.17, 133.78, 130.90, 129.99, 129.88, 129.01, 126.33, 121.35, 21.06. GC-MS = 212 $[M]^+$..

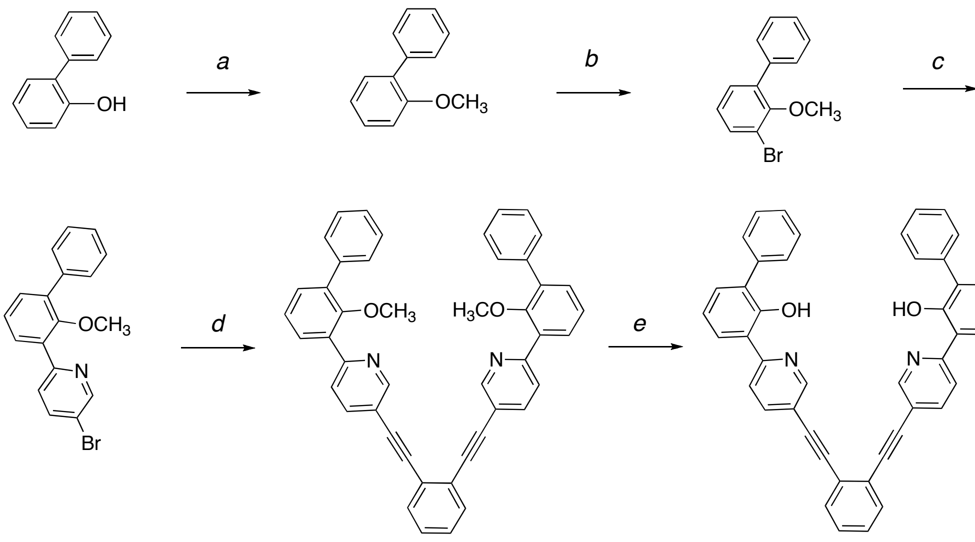
Synthetic Schemes



Scheme S1. a) Benzyl bromide, K_2CO_3, CH_3CN**;** b) *i.* *n*BuLi, THF, -78°C, *ii.* $ZnCl_2$, *iii.* 2,5-dibromopyridine, $[Pd(PPh_3)_4]$; c) 4,5-diethynylveratrole, $[Pd(PPh_3)_4]$, NEt_3, THF, reflux; d) TMSI, CH_2Cl_2.

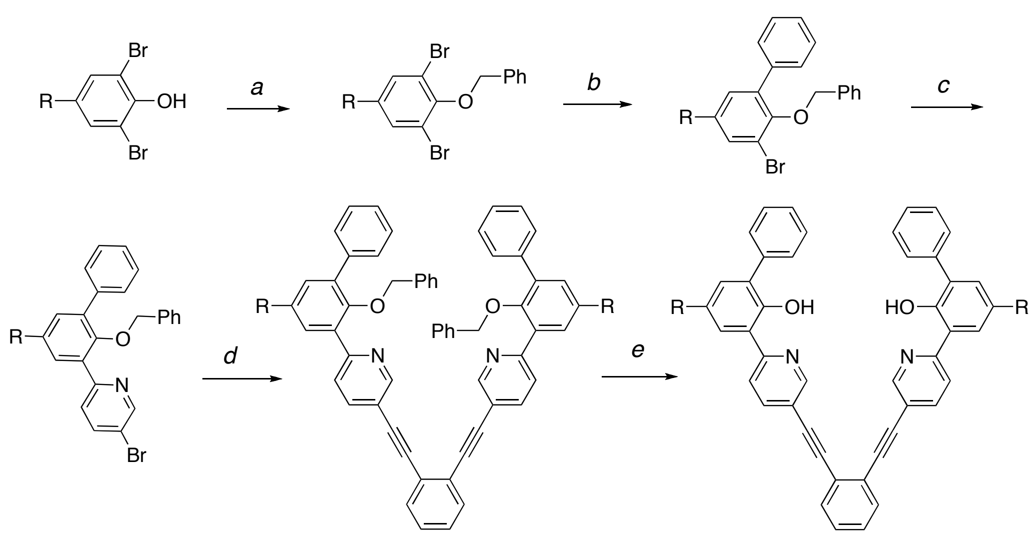


Scheme S2. a) *i.* *n*BuLi, THF, -78°C, *ii.* $ZnCl_2$, *iii.* 2,5-dibromopyridine, $[Pd(PPh_3)_4]$; b) 1,2-diethynylbenzene, $[Pd(PPh_3)_4]$, NEt_3, THF, reflux; c) *i.* BBr_3, CH_2Cl_2. *ii.* TFA.



Me$_2$L$^{H, Ph}$ **H$_2$L$^{H, Ph}$**

Scheme S3. a) *i.* NaH, THF, 0^{o}C; *ii.* CH_3I, reflux; b) *i.* TMEDA, Et_2O. *ii.* Br_2; c) *i.* *n*BuLi, THF, -78 ^{o}C. *ii.* $ZnCl_2$, *iii.* 2,5-dibromopyridine, [Pd(PPh_3)$_4$]; d) 1,2-diethynylbenzene, [Pd(PPh_3)$_4$], NEt_3, THF, reflux; e) BBr_3, CH_2Cl_2, 0^{o}C.



Benz$_2$L^{Me,Ph} (R = Me)
Benz$_2$L^{tBu,Ph} (R = *t*-Bu)

H$_2$L^{Me,Ph} (R = Me)
H$_2$L^{tBu,Ph} (R = *t*-Bu)

Scheme S4. a) Benzyl bromide, K_2CO_3, CH_3CN, reflux; b) phenylboronic acid, [Pd(PPh_3)$_4$], Na_2CO_3(aq), THF, reflux; c) *i.* *n*BuLi, THF, -78 ^{o}C, *ii.* $ZnCl_2$, *iii.* 2,5-dibromopyridine, [Pd(PPh_3)$_4$]; d) 1,2-diethynylbenzene, [Pd(PPh_3)$_4$], NEt_3, THF, reflux; e) TMSI, toluene, reflux.

Spectroscopic Data

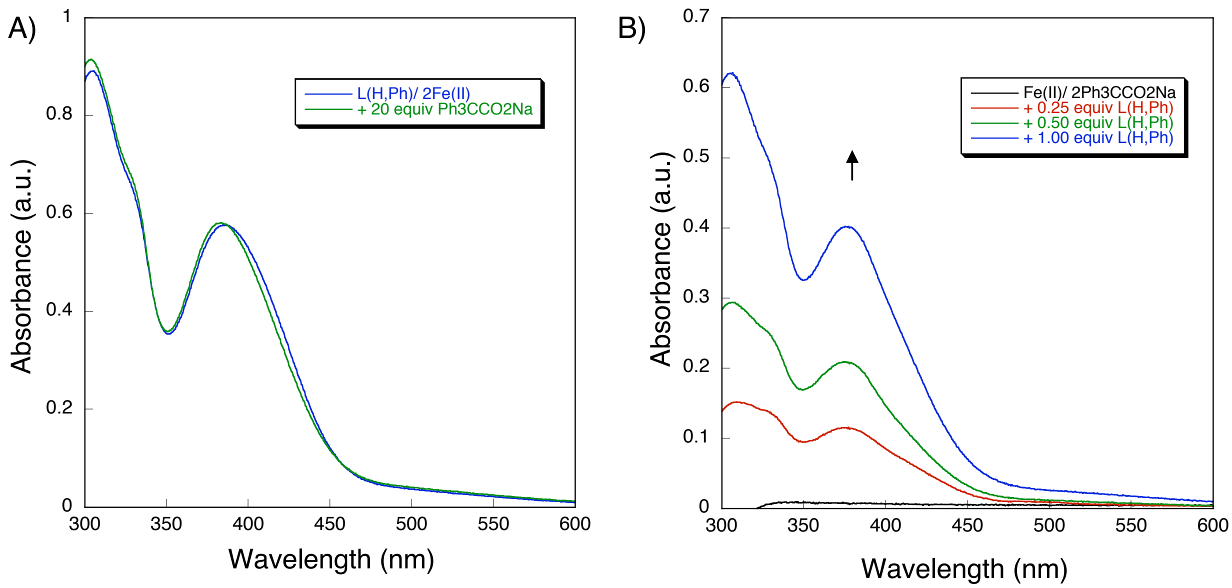


Figure S1. Electronic absorption spectra of **A**) addition of sodium triphenylacetate to a THF solution of Fe(II) and $\mathbf{L}^{\mathbf{H,Ph}}$ and **B**) addition of $\mathbf{L}^{\mathbf{H,Ph}}$ to a THF solution of Fe(II) and sodium triphenylacetate. For **A**, the equiv of triphenylacetate added is relative to the amount of $\mathbf{L}^{\mathbf{H,Ph}}$. For **B**, the equiv of $\mathbf{L}^{\mathbf{H,Ph}}$ added is relative to the amount of Fe(II).

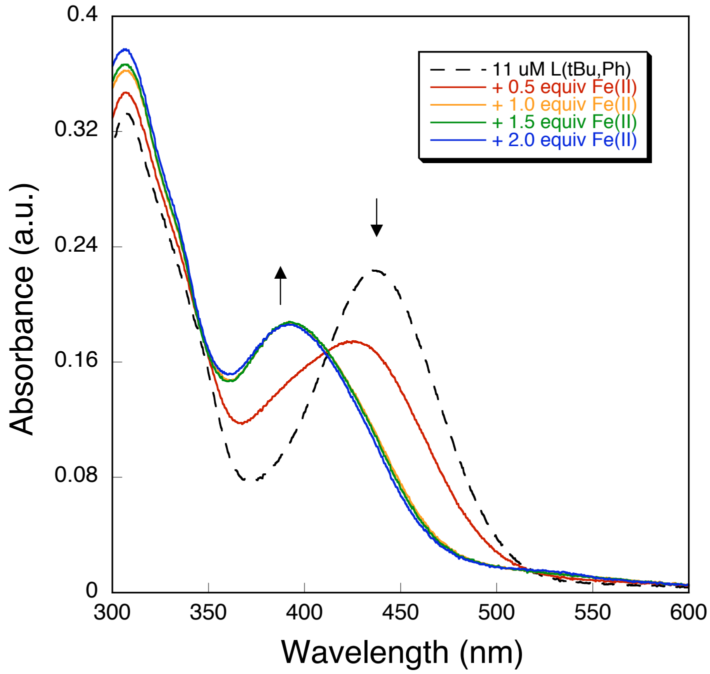


Figure S2. Electronic absorption spectra from the addition of $Fe^{II}(OSO_2CF_3)_2$ to a THF solution containing $\mathbf{L}^{tBu,Ph}$. The dashed line represents the spectrum of the deprotonated apo-ligand, whereas the solid lines are spectra acquired after addition of various equiv of Fe(II).

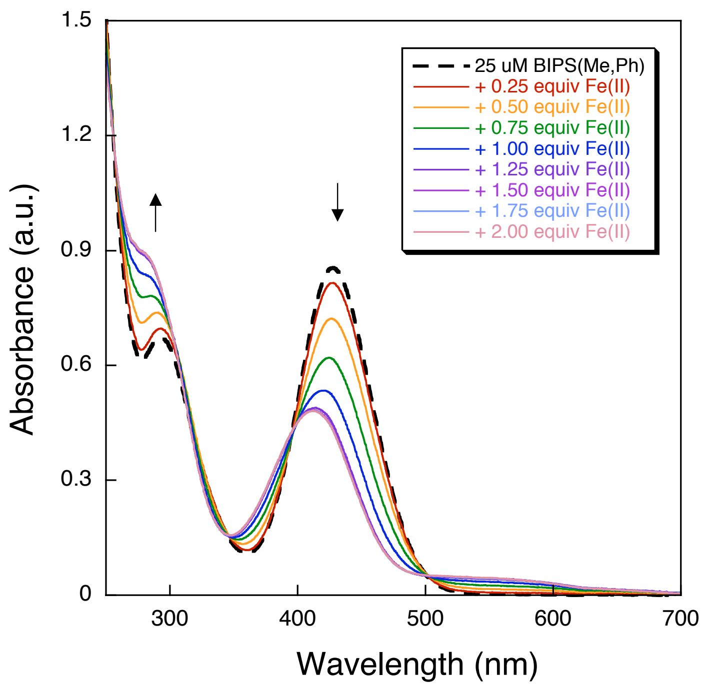


Figure S3. Electronic absorption spectra from the addition of $Fe^{II}(OSO_2CF_3)_2$ to a THF solution containing **BIPS^{Me,Ph}**. The dashed line represents the spectrum of the deprotonated apo-ligand, whereas the solid lines are spectra acquired after addition of various equiv of Fe(II).

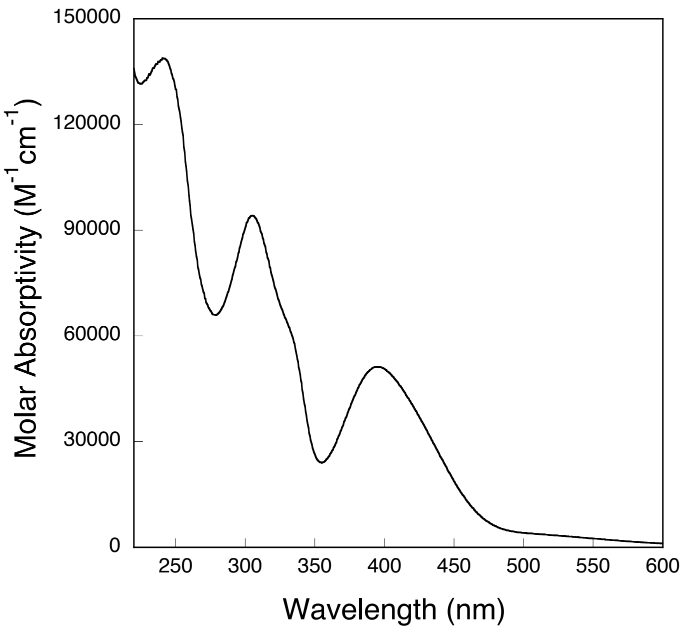


Figure S4. The electronic absorption spectrum of complex **1** in THF.

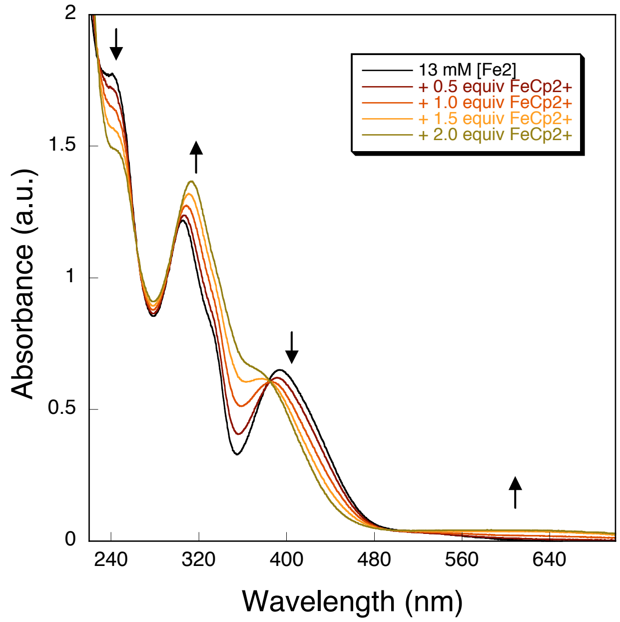


Figure S5. Electronic absorption spectra from the addition of $[FeCp_2](BF_4)$ to a THF solution containing $\mathbf{L}^{\mathbf{Me,Ph}}$.

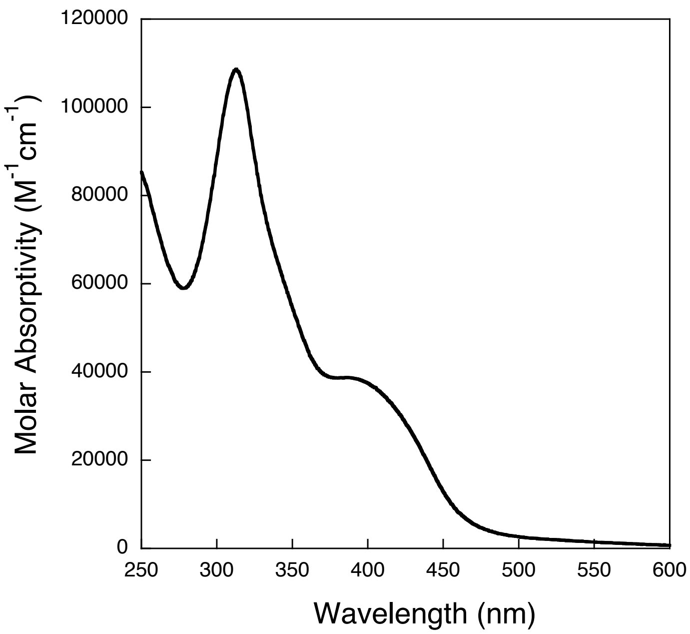


Figure S6. The electronic absorption spectrum of complex **2** in THF.

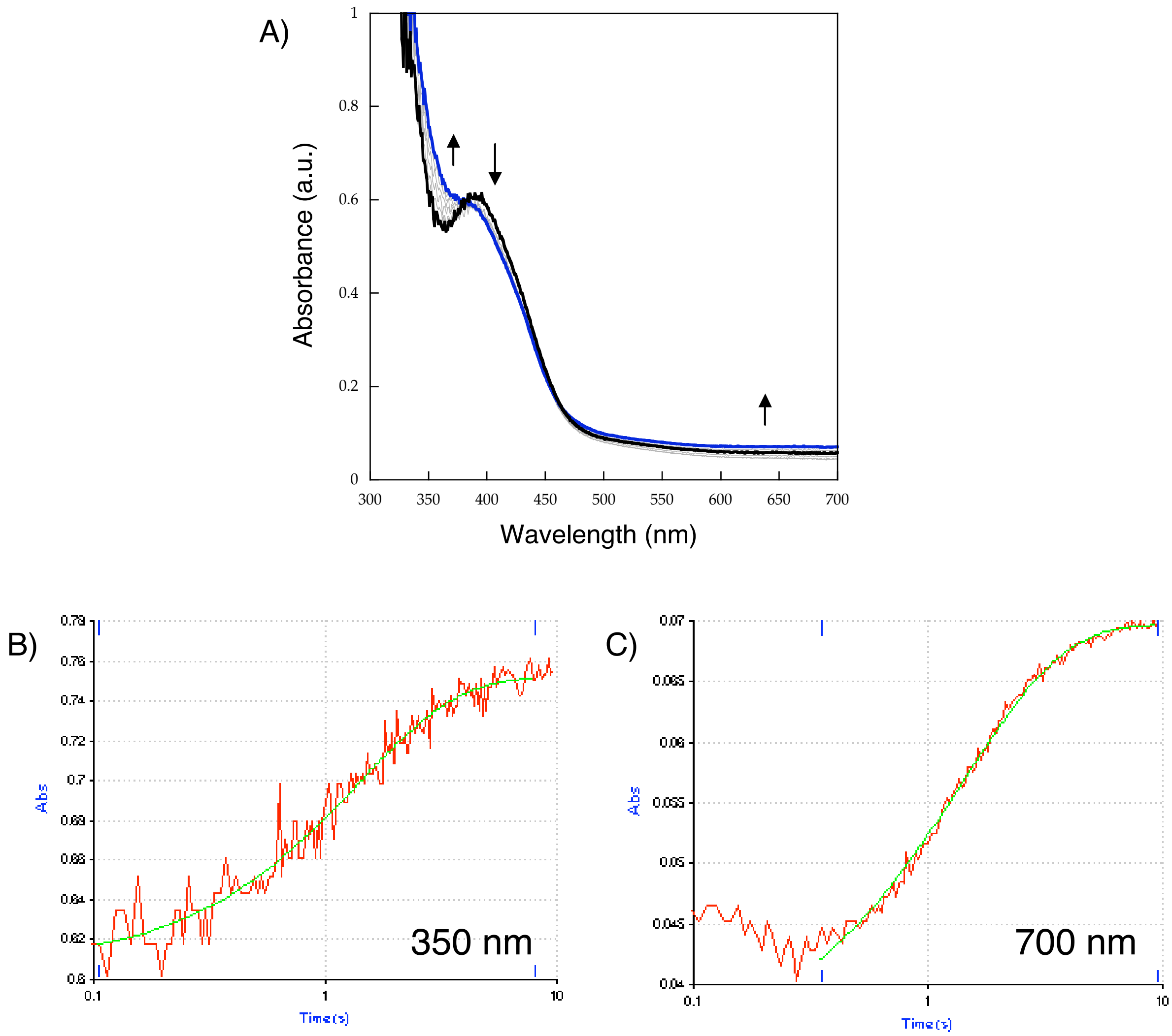


Figure S7. Single-mixing stopped-flowed spectral data from the reaction of **1** with O_2 in THF. The absorbance spectra from 300-600 nm (**A**, top) clearly show rapid conversion of **1** to **2**. The kinetic traces at 350 nm (**B**, bottom) and 700 nm (**C**, bottom) were fit to single exponential functions, giving pseudo-first order rate constants of ~ 0.7 s^{-1}.

Electrochemical Data

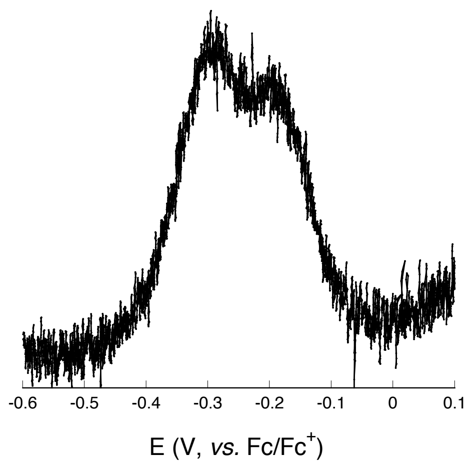


Figure S8. Differential pulse voltammogram of a 0.2 mM solution of complex **2** containing 0.1 M tetrabutylammonium hexafluorophosphate in THF. The measurement was carried out with a Pt working electrode at a scan rate of 50 mV/s and referenced to the Fc/Fc^+ redox couple.

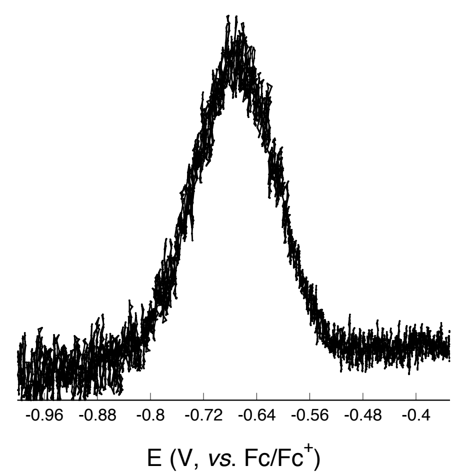


Figure S9. Differential pulse voltammogram of a 0.2 mM solution of complex **2** containing 0.1 M tetrabutylammonium hexafluorophosphate in DMF. The measurement was carried out with a Pt working electrode at a scan rate of 50 mV/s and referenced to the Fc/Fc^+ redox couple.

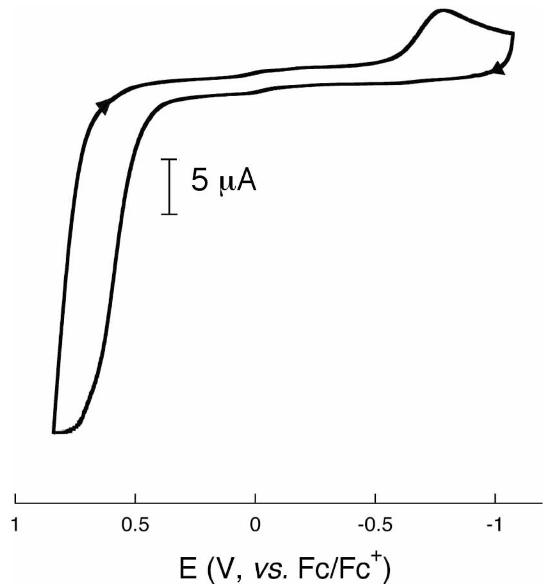


Figure S10. Cyclic voltammogram of a 0.2 mM solution of complex **2** containing 0.1 M tetrabutylammonium hexafluorophosphate in THF at a scan rate of 50 mV/s. The measurements were carried out with a Pt working electrode and referenced to the Fc/Fc^{+} redox couple.

Crystallographic Data

Additional Structural Details for 1·$(THF)_{3.5}$(pentane)$_{0.5}$. The parent $[Fe^{II}_2(\mathbf{L}^{Me,Ph})_2(THF)_3]$ complex shows positional disorder about two ligand phenyl rings. The C40-C45 ring was refined anisotropically as a two-part disorder and gave acceptable atomic displacement parameters. The C7-C12 ring, on the other hand, appears to have greater thermal motion and the atoms were best modeled in an isotropic manner. Due to the crystal packing of **1**, large spaces in the solid-state lattice were occupied by solvent molecules. In the asymmetric unit, 3.5 THF and 0.5 pentane molecules were identified. One of the THF molecules (O600, C601-C604) was disordered over two positions and another THF molecule (O700, C701-C704) sits on a special position with 50% occupancy. The remaining two THF molecules were refined with complete 100% occupancy. Lastly, a pentane molecule (C800-C804) was found to reside on an inversion center. The pentane was modeled with a total occupancy of 50% and had a great deal of dynamic disorder, as indicated by the large carbon atom atomic displacement parameters.

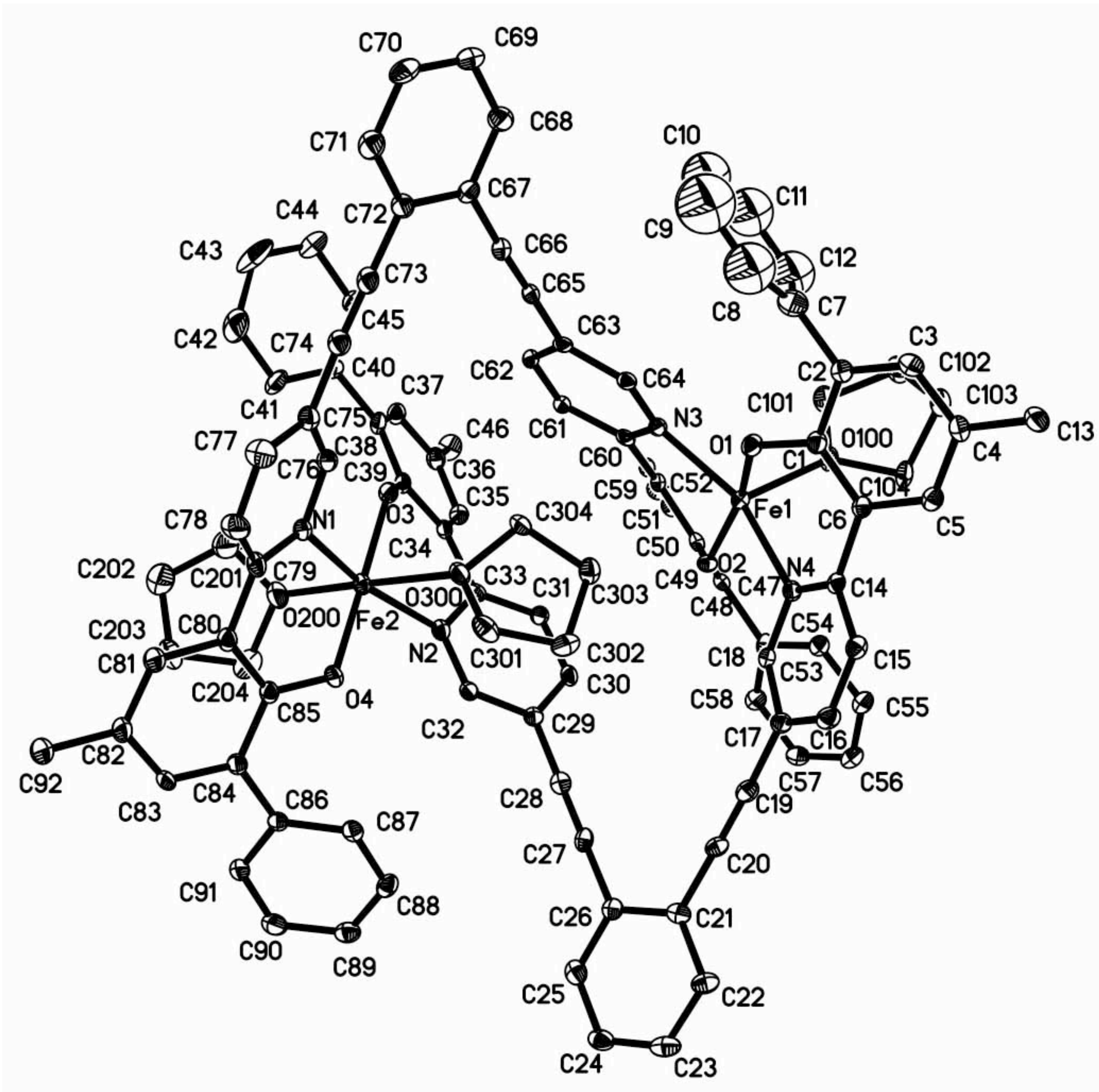


Figure S11. Fully labeled drawing of the X-ray structure of **1** showing 30% thermal ellipsoids. Hydrogen atoms and solvent molecules are omitted for clarity.

Table S1. Bond lengths [Å] and angles [º] for **1**·$(THF)_{3.5}(pentane)_{0.5}$.

Fe(1)-O(2)	1.936(3)
Fe(1)-O(1)	1.944(3)
Fe(1)-O(100)	2.122(3)
Fe(1)-N(3)	2.185(4)
Fe(1)-N(4)	2.193(4)
Fe(2)-O(3)	1.968(3)
Fe(2)-O(4)	1.977(3)
Fe(2)-N(1)	2.180(4)
Fe(2)-N(2)	2.191(4)
Fe(2)-O(200)	2.205(4)
Fe(2)-O(300)	2.320(3)
N(1)-C(76)	1.343(6)
N(1)-C(79)	1.359(5)
N(2)-C(32)	1.336(5)
N(2)-C(33)	1.366(5)
N(3)-C(64)	1.347(5)
N(3)-C(60)	1.369(5)
N(4)-C(18)	1.341(5)
N(4)-C(14)	1.361(5)
O(1)-C(1)	1.330(5)
O(2)-C(47)	1.319(5)
O(3)-C(39)	1.315(5)
O(4)-C(85)	1.318(5)
C(1)-C(6)	1.409(6)
C(1)-C(2)	1.417(6)
C(2)-C(3)	1.383(7)
C(2)-C(7)	1.489(6)
C(3)-C(4)	1.391(7)
C(3)-H(3)	0.9300
C(4)-C(5)	1.383(6)
C(4)-C(13)	1.508(6)
C(5)-C(6)	1.416(6)
C(5)-H(5)	0.9300
C(6)-C(14)	1.469(6)
C(7)-C(8)	1.3900
C(7)-C(12)	1.3900
C(8)-C(9)	1.3900
C(8)-H(8)	0.9300
C(9)-C(10)	1.3900
C(9)-H(9)	0.9300
C(10)-C(11)	1.3900
C(10)-H(10)	0.9300
C(11)-C(12)	1.3900
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.395(6)
C(15)-C(16)	1.376(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.405(6)
C(16)-H(16)	0.9300
C(17)-C(18)	1.387(6)
C(17)-C(19)	1.431(6)
C(18)-H(18)	0.9300
C(19)-C(20)	1.192(6)
C(20)-C(21)	1.440(6)
C(21)-C(22)	1.399(6)
C(21)-C(26)	1.412(6)
C(22)-C(23)	1.389(7)
C(22)-H(22)	0.9300
C(23)-C(24)	1.362(7)
C(23)-H(23)	0.9300
C(24)-C(25)	1.375(7)
C(24)-H(24)	0.9300
C(25)-C(26)	1.395(6)
C(25)-H(25)	0.9300
C(26)-C(27)	1.436(6)
C(27)-C(28)	1.200(6)
C(28)-C(29)	1.439(6)
C(29)-C(32)	1.394(6)
C(29)-C(30)	1.395(6)
C(30)-C(31)	1.379(6)
C(30)-H(30)	0.9300
C(31)-C(33)	1.400(6)
C(31)-H(31)	0.9300
C(32)-H(32)	0.9300
C(33)-C(34)	1.482(6)
C(34)-C(35)	1.390(6)
C(34)-C(39)	1.429(6)
C(35)-C(36)	1.377(6)
C(35)-H(35)	0.9300
C(36)-C(37)	1.392(6)
C(36)-C(46)	1.506(6)
C(37)-C(38)	1.394(6)
C(37)-H(37)	0.9300
C(38)-C(39)	1.428(6)
C(38)-C(40)	1.508(6)
C(40)-C(45A)	1.341(7)
C(40)-C(41)	1.3900
C(40)-C(45)	1.3900
C(40)-C(41A)	1.402(7)
C(41)-C(42)	1.3900
C(41)-H(41)	0.9300
C(42)-C(43)	1.3900
C(42)-H(42)	0.9300
C(43)-C(44A)	1.300(9)
C(43)-C(44)	1.3900
C(43)-C(42A)	1.462(10)
C(43)-H(43)	0.9300
C(44)-C(45)	1.3900
C(44)-H(44)	0.9300
C(45)-H(45)	0.9300

C(41A)-C(42A)	1.389(9)
C(41A)-H(41A)	0.9300
C(42A)-H(42A)	0.9300
C(44A)-C(45A)	1.395(9)
C(44A)-H(44A)	0.9300
C(45A)-H(45A)	0.9300
C(46)-H(46A)	0.9600
C(46)-H(46B)	0.9600
C(46)-H(46C)	0.9600
C(47)-C(52)	1.424(6)
C(47)-C(48)	1.428(6)
C(48)-C(49)	1.385(6)
C(48)-C(53)	1.504(6)
C(49)-C(50)	1.388(6)
C(49)-H(49)	0.9300
C(50)-C(51)	1.386(6)
C(50)-C(59)	1.508(6)
C(51)-C(52)	1.404(6)
C(51)-H(51)	0.9300
C(52)-C(60)	1.474(6)
C(53)-C(58)	1.380(6)
C(53)-C(54)	1.396(6)
C(54)-C(55)	1.377(6)
C(54)-H(54)	0.9300
C(55)-C(56)	1.380(7)
C(55)-H(55)	0.9300
C(56)-C(57)	1.384(7)
C(56)-H(56)	0.9300
C(57)-C(58)	1.384(7)
C(57)-H(57)	0.9300
C(58)-H(58)	0.9300
C(59)-H(59A)	0.9600
C(59)-H(59B)	0.9600
C(59)-H(59C)	0.9600
C(60)-C(61)	1.407(6)
C(61)-C(62)	1.364(6)
C(61)-H(61)	0.9300
C(62)-C(63)	1.396(6)
C(62)-H(62)	0.9300
C(63)-C(64)	1.388(6)
C(63)-C(65)	1.442(6)
C(64)-H(64)	0.9300
C(65)-C(66)	1.197(6)
C(66)-C(67)	1.437(6)
C(67)-C(68)	1.391(6)
C(67)-C(72)	1.410(6)
C(68)-C(69)	1.381(7)
C(68)-H(68)	0.9300
C(69)-C(70)	1.381(7)
C(69)-H(69)	0.9300
C(70)-C(71)	1.373(7)
C(70)-H(70)	0.9300
C(71)-C(72)	1.393(6)
C(71)-H(71)	0.9300
C(72)-C(73)	1.431(7)
C(73)-C(74)	1.200(6)
C(74)-C(75)	1.433(7)
C(75)-C(76)	1.386(6)
C(75)-C(77)	1.405(6)
C(76)-H(76)	0.9300
C(77)-C(78)	1.370(7)
C(77)-H(77)	0.9300
C(78)-C(79)	1.395(7)
C(78)-H(78)	0.9300
C(79)-C(80)	1.471(6)
C(80)-C(81)	1.407(6)
C(80)-C(85)	1.430(6)
C(81)-C(82)	1.378(7)
C(81)-H(81)	0.9300
C(82)-C(83)	1.383(7)
C(82)-C(92)	1.515(6)
C(83)-C(84)	1.385(6)
C(83)-H(83)	0.9300
C(84)-C(85)	1.434(6)
C(84)-C(86)	1.499(6)
C(86)-C(87)	1.387(6)
C(86)-C(91)	1.396(6)
C(87)-C(88)	1.395(6)
C(87)-H(87)	0.9300
C(88)-C(89)	1.381(7)
C(88)-H(88)	0.9300
C(89)-C(90)	1.382(7)
C(89)-H(89)	0.9300
C(90)-C(91)	1.386(7)
C(90)-H(90)	0.9300
C(91)-H(91)	0.9300
C(92)-H(92A)	0.9600
C(92)-H(92B)	0.9600
C(92)-H(92C)	0.9600
O(100)-C(104)	1.445(5)
O(100)-C(101)	1.449(5)
C(101)-C(102)	1.511(7)
C(101)-H(10A)	0.9700
C(101)-H(10B)	0.9700
C(102)-C(103)	1.528(7)
C(102)-H(10C)	0.9700
C(102)-H(10D)	0.9700
C(103)-C(104)	1.504(7)
C(103)-H(10E)	0.9700
C(103)-H(10F)	0.9700
C(104)-H(10G)	0.9700
C(104)-H(10H)	0.9700
O(200)-C(201)	1.379(7)
O(200)-C(204)	1.513(7)
C(201)-C(202)	1.497(9)
C(201)-H(20A)	0.9700
C(201)-H(20B)	0.9700
C(202)-C(203)	1.513(8)
C(202)-H(20C)	0.9700
C(202)-H(20D)	0.9700
C(203)-C(204)	1.506(7)
C(203)-H(20E)	0.9700

C(203)-H(20F)	0.9700
C(204)-H(20G)	0.9700
C(204)-H(20H)	0.9700
O(300)-C(301)	1.430(6)
O(300)-C(304)	1.439(5)
C(301)-C(302)	1.518(7)
C(301)-H(30A)	0.9700
C(301)-H(30B)	0.9700
C(302)-C(303)	1.542(6)
C(302)-H(30C)	0.9700
C(302)-H(30D)	0.9700
C(303)-C(304)	1.508(6)
C(303)-H(30E)	0.9700
C(303)-H(30F)	0.9700
C(304)-H(30G)	0.9700
C(304)-H(30H)	0.9700
O(400)-C(401)	1.326(15)
O(400)-C(404)	1.329(14)
C(401)-C(402)	1.468(18)
C(401)-H(40A)	0.9700
C(401)-H(40B)	0.9700
C(402)-C(403)	1.444(14)
C(402)-H(40C)	0.9700
C(402)-H(40D)	0.9700
C(403)-C(404)	1.484(16)
C(403)-H(40E)	0.9700
C(403)-H(40F)	0.9700
C(404)-H(40G)	0.9700
C(404)-H(40H)	0.9700
O(500)-C(501)	1.425(7)
O(500)-C(504)	1.431(7)
C(501)-C(502)	1.470(10)
C(501)-H(50A)	0.9700
C(501)-H(50B)	0.9700
C(502)-C(503)	1.391(11)
C(502)-H(50C)	0.9700
C(502)-H(50D)	0.9700
C(503)-C(504)	1.488(9)
C(503)-H(50E)	0.9700
C(503)-H(50F)	0.9700
C(504)-H(50G)	0.9700
C(504)-H(50H)	0.9700
O(600)-C(614)	1.27(4)
O(600)-C(604)	1.346(10)
O(600)-C(601)	1.486(11)
O(600)-C(613)	1.83(4)
C(601)-C(602)	1.463(13)
C(601)-C(612)	1.52(4)
C(601)-H(60A)	0.9700
C(601)-H(60B)	0.9700
C(601)-H(60A)	0.9700
C(601)-H(60B)	0.9699
C(602)-C(603)	1.475(12)
C(602)-H(60A)	0.7273
C(602)-H(60C)	0.9700
C(602)-H(60D)	0.9700
C(603)-C(604)	1.321(11)
C(603)-H(60E)	0.9700
C(603)-H(60F)	0.9700
C(604)-H(60G)	0.9700
C(604)-H(60H)	0.9700
C(612)-C(613)	1.26(4)
C(612)-H(61A)	0.9700
C(612)-H(61B)	0.9700
C(613)-C(614)	1.48(5)
C(613)-H(61C)	0.9700
C(613)-H(61D)	0.9700
C(614)-H(61E)	0.9700
C(614)-H(61F)	0.9700
O(700)-C(701)	1.50(3)
O(700)-C(704)	1.60(3)
C(701)-C(702)	1.48(3)
C(701)-H(70A)	0.9700
C(701)-H(70B)	0.9700
C(702)-C(703)	1.407(18)
C(702)-H(70C)	0.9700
C(702)-H(70D)	0.9700
C(703)-C(704)	1.39(2)
C(703)-H(70E)	0.9700
C(703)-H(70F)	0.9700
C(704)-H(70G)	0.9700
C(704)-H(70H)	0.9700
C(800)-C(801)	1.498(17)
C(800)-H(80A)	0.9600
C(800)-H(80B)	0.9600
C(800)-H(80C)	0.9600
C(801)-C(802)	1.622(14)
C(801)-H(80A)	0.9700
C(801)-H(80B)	0.9700
C(802)-C(803)#1	1.546(17)
C(802)-C(803)	1.546(17)
C(802)-C(801)#1	1.622(14)
C(802)-H(80D)	0.9700
C(802)-H(80E)	0.9700
C(803)-C(804)	1.549(19)
C(803)-H(80E)	0.9700
C(803)-H(80F)	0.9700
C(804)-H(80G)	0.9600
C(804)-H(80H)	0.9600
C(804)-H(80I)	0.9600
O(2)-Fe(1)-O(1)	163.22(13)
O(2)-Fe(1)-O(100)	96.87(13)
O(1)-Fe(1)-O(100)	99.87(13)
O(2)-Fe(1)-N(3)	85.91(13)
O(1)-Fe(1)-N(3)	92.30(13)
O(100)-Fe(1)-N(3)	99.70(12)
O(2)-Fe(1)-N(4)	91.46(13)
O(1)-Fe(1)-N(4)	84.30(13)
O(100)-Fe(1)-N(4)	101.09(13)
N(3)-Fe(1)-N(4)	159.21(13)
O(3)-Fe(2)-O(4)	177.24(13)

O(3)-Fe(2)-N(1)	92.25(13)
O(4)-Fe(2)-N(1)	85.21(13)
O(3)-Fe(2)-N(2)	85.66(13)
O(4)-Fe(2)-N(2)	96.53(13)
N(1)-Fe(2)-N(2)	165.83(14)
O(3)-Fe(2)-O(200)	89.31(13)
O(4)-Fe(2)-O(200)	92.25(13)
N(1)-Fe(2)-O(200)	101.12(14)
N(2)-Fe(2)-O(200)	92.88(14)
O(3)-Fe(2)-O(300)	90.12(12)
O(4)-Fe(2)-O(300)	88.44(12)
N(1)-Fe(2)-O(300)	81.73(13)
N(2)-Fe(2)-O(300)	84.25(13)
O(200)-Fe(2)-O(300)	177.11(13)
C(76)-N(1)-C(79)	118.7(4)
C(76)-N(1)-Fe(2)	114.2(3)
C(79)-N(1)-Fe(2)	125.1(3)
C(32)-N(2)-C(33)	118.5(4)
C(32)-N(2)-Fe(2)	113.8(3)
C(33)-N(2)-Fe(2)	124.2(3)
C(64)-N(3)-C(60)	118.1(4)
C(64)-N(3)-Fe(1)	117.3(3)
C(60)-N(3)-Fe(1)	122.6(3)
C(18)-N(4)-C(14)	118.6(4)
C(18)-N(4)-Fe(1)	116.3(3)
C(14)-N(4)-Fe(1)	123.7(3)
C(1)-O(1)-Fe(1)	123.2(3)
C(47)-O(2)-Fe(1)	122.7(3)
C(39)-O(3)-Fe(2)	126.8(3)
C(85)-O(4)-Fe(2)	126.6(3)
O(1)-C(1)-C(6)	122.9(4)
O(1)-C(1)-C(2)	118.7(4)
C(6)-C(1)-C(2)	118.4(4)
C(3)-C(2)-C(1)	120.1(4)
C(3)-C(2)-C(7)	121.3(4)
C(1)-C(2)-C(7)	118.6(4)
C(2)-C(3)-C(4)	123.1(5)
C(2)-C(3)-H(3)	118.5
C(4)-C(3)-H(3)	118.5
C(5)-C(4)-C(3)	116.3(4)
C(5)-C(4)-C(13)	122.7(4)
C(3)-C(4)-C(13)	120.9(4)
C(4)-C(5)-C(6)	123.5(4)
C(4)-C(5)-H(5)	118.3
C(6)-C(5)-H(5)	118.3
C(1)-C(6)-C(5)	118.6(4)
C(1)-C(6)-C(14)	122.4(4)
C(5)-C(6)-C(14)	118.7(4)
C(8)-C(7)-C(12)	120.0
C(8)-C(7)-C(2)	119.9(4)
C(12)-C(7)-C(2)	120.0(4)
C(7)-C(8)-C(9)	120.0
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	120.0
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	120.0
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(12)-C(11)-C(10)	120.0
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(7)	120.0
C(11)-C(12)-H(12)	120.0
C(7)-C(12)-H(12)	120.0
C(4)-C(13)-H(13A)	109.5
C(4)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(4)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(4)-C(14)-C(15)	119.4(4)
N(4)-C(14)-C(6)	119.6(4)
C(15)-C(14)-C(6)	120.9(4)
C(16)-C(15)-C(14)	121.6(4)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(15)-C(16)-C(17)	119.1(4)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-H(16)	120.5
C(18)-C(17)-C(16)	116.3(4)
C(18)-C(17)-C(19)	122.2(4)
C(16)-C(17)-C(19)	121.4(4)
N(4)-C(18)-C(17)	125.1(4)
N(4)-C(18)-H(18)	117.5
C(17)-C(18)-H(18)	117.5
C(20)-C(19)-C(17)	176.6(5)
C(19)-C(20)-C(21)	177.0(5)
C(22)-C(21)-C(26)	118.9(4)
C(22)-C(21)-C(20)	121.2(4)
C(26)-C(21)-C(20)	119.9(4)
C(23)-C(22)-C(21)	120.2(5)
C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9
C(24)-C(23)-C(22)	120.5(5)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	120.5(5)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	120.8(5)
C(24)-C(25)-H(25)	119.6
C(26)-C(25)-H(25)	119.6
C(25)-C(26)-C(21)	119.0(4)
C(25)-C(26)-C(27)	121.1(4)
C(21)-C(26)-C(27)	119.9(4)
C(28)-C(27)-C(26)	179.8(5)
C(27)-C(28)-C(29)	178.8(5)
C(32)-C(29)-C(30)	116.9(4)
C(32)-C(29)-C(28)	120.0(4)
C(30)-C(29)-C(28)	123.0(4)

C(31)-C(30)-C(29)	119.2(4)
C(31)-C(30)-H(30)	120.4
C(29)-C(30)-H(30)	120.4
C(30)-C(31)-C(33)	121.0(4)
C(30)-C(31)-H(31)	119.5
C(33)-C(31)-H(31)	119.5
N(2)-C(32)-C(29)	124.6(4)
N(2)-C(32)-H(32)	117.7
C(29)-C(32)-H(32)	117.7
N(2)-C(33)-C(31)	119.8(4)
N(2)-C(33)-C(34)	119.5(4)
C(31)-C(33)-C(34)	120.7(4)
C(35)-C(34)-C(39)	120.1(4)
C(35)-C(34)-C(33)	117.7(4)
C(39)-C(34)-C(33)	122.2(4)
C(36)-C(35)-C(34)	122.8(4)
C(36)-C(35)-H(35)	118.6
C(34)-C(35)-H(35)	118.6
C(35)-C(36)-C(37)	117.2(4)
C(35)-C(36)-C(46)	121.5(4)
C(37)-C(36)-C(46)	121.2(4)
C(36)-C(37)-C(38)	123.1(4)
C(36)-C(37)-H(37)	118.4
C(38)-C(37)-H(37)	118.4
C(37)-C(38)-C(39)	119.2(4)
C(37)-C(38)-C(40)	119.5(4)
C(39)-C(38)-C(40)	121.3(4)
O(3)-C(39)-C(38)	119.8(4)
O(3)-C(39)-C(34)	122.6(4)
C(38)-C(39)-C(34)	117.5(4)
C(45A)-C(40)-C(41)	71.2(7)
C(45A)-C(40)-C(45)	78.0(6)
C(41)-C(40)-C(45)	120.0
C(45A)-C(40)-C(41A)	120.0(5)
C(41)-C(40)-C(41A)	80.0(7)
C(45)-C(40)-C(41A)	72.9(7)
C(45A)-C(40)-C(38)	124.0(4)
C(41)-C(40)-C(38)	125.4(3)
C(45)-C(40)-C(38)	114.6(3)
C(41A)-C(40)-C(38)	115.7(4)
C(40)-C(41)-C(42)	120.0
C(40)-C(41)-H(41)	120.0
C(42)-C(41)-H(41)	120.0
C(43)-C(42)-C(41)	120.0
C(43)-C(42)-H(42)	120.0
C(41)-C(42)-H(42)	120.0
C(44A)-C(43)-C(42)	72.3(7)
C(44A)-C(43)-C(44)	77.7(7)
C(42)-C(43)-C(44)	120.0
C(44A)-C(43)-C(42A)	118.7(5)
C(42)-C(43)-C(42A)	78.6(7)
C(44)-C(43)-C(42A)	72.2(7)
C(44A)-C(43)-H(43)	121.1
C(42)-C(43)-H(43)	120.0
C(44)-C(43)-H(43)	120.0
C(42A)-C(43)-H(43)	120.2
C(45)-C(44)-C(43)	120.0
C(45)-C(44)-H(44)	120.0
C(43)-C(44)-H(44)	120.0
C(44)-C(45)-C(40)	120.0
C(44)-C(45)-H(45)	120.0
C(40)-C(45)-H(45)	120.0
C(42A)-C(41A)-C(40)	118.9(6)
C(42A)-C(41A)-H(41A)	120.5
C(40)-C(41A)-H(41A)	120.5
C(41A)-C(42A)-C(43)	119.2(6)
C(41A)-C(42A)-H(42A)	120.4
C(43)-C(42A)-H(42A)	120.4
C(43)-C(44A)-C(45A)	122.1(7)
C(43)-C(44A)-H(44A)	118.9
C(45A)-C(44A)-H(44A)	118.9
C(40)-C(45A)-C(44A)	121.1(6)
C(40)-C(45A)-H(45A)	119.4
C(44A)-C(45A)-H(45A)	119.4
C(36)-C(46)-H(46A)	109.5
C(36)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(36)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
O(2)-C(47)-C(52)	122.4(4)
O(2)-C(47)-C(48)	119.8(4)
C(52)-C(47)-C(48)	117.8(4)
C(49)-C(48)-C(47)	119.6(4)
C(49)-C(48)-C(53)	119.4(4)
C(47)-C(48)-C(53)	121.0(4)
C(48)-C(49)-C(50)	123.4(4)
C(48)-C(49)-H(49)	118.3
C(50)-C(49)-H(49)	118.3
C(51)-C(50)-C(49)	116.9(4)
C(51)-C(50)-C(59)	121.4(4)
C(49)-C(50)-C(59)	121.8(4)
C(50)-C(51)-C(52)	122.9(4)
C(50)-C(51)-H(51)	118.6
C(52)-C(51)-H(51)	118.6
C(51)-C(52)-C(47)	119.4(4)
C(51)-C(52)-C(60)	118.5(4)
C(47)-C(52)-C(60)	122.0(4)
C(58)-C(53)-C(54)	118.3(4)
C(58)-C(53)-C(48)	120.5(4)
C(54)-C(53)-C(48)	121.0(4)
C(55)-C(54)-C(53)	120.4(5)
C(55)-C(54)-H(54)	119.8
C(53)-C(54)-H(54)	119.8
C(54)-C(55)-C(56)	120.7(5)
C(54)-C(55)-H(55)	119.7
C(56)-C(55)-H(55)	119.7
C(55)-C(56)-C(57)	119.4(5)
C(55)-C(56)-H(56)	120.3
C(57)-C(56)-H(56)	120.3
C(58)-C(57)-C(56)	119.7(5)
C(58)-C(57)-H(57)	120.1

C(56)-C(57)-H(57)	120.1
C(53)-C(58)-C(57)	121.4(5)
C(53)-C(58)-H(58)	119.3
C(57)-C(58)-H(58)	119.3
C(50)-C(59)-H(59A)	109.5
C(50)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(50)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
N(3)-C(60)-C(61)	119.7(4)
N(3)-C(60)-C(52)	119.7(4)
C(61)-C(60)-C(52)	120.5(4)
C(62)-C(61)-C(60)	121.2(4)
C(62)-C(61)-H(61)	119.4
C(60)-C(61)-H(61)	119.4
C(61)-C(62)-C(63)	119.3(4)
C(61)-C(62)-H(62)	120.4
C(63)-C(62)-H(62)	120.4
C(64)-C(63)-C(62)	117.3(4)
C(64)-C(63)-C(65)	121.1(4)
C(62)-C(63)-C(65)	121.6(4)
N(3)-C(64)-C(63)	124.4(4)
N(3)-C(64)-H(64)	117.8
C(63)-C(64)-H(64)	117.8
C(66)-C(65)-C(63)	177.0(5)
C(65)-C(66)-C(67)	177.2(5)
C(68)-C(67)-C(72)	119.2(4)
C(68)-C(67)-C(66)	119.3(4)
C(72)-C(67)-C(66)	121.5(4)
C(69)-C(68)-C(67)	121.1(5)
C(69)-C(68)-H(68)	119.5
C(67)-C(68)-H(68)	119.5
C(68)-C(69)-C(70)	119.7(5)
C(68)-C(69)-H(69)	120.1
C(70)-C(69)-H(69)	120.1
C(71)-C(70)-C(69)	120.1(5)
C(71)-C(70)-H(70)	120.0
C(69)-C(70)-H(70)	120.0
C(70)-C(71)-C(72)	121.4(5)
C(70)-C(71)-H(71)	119.3
C(72)-C(71)-H(71)	119.3
C(71)-C(72)-C(67)	118.5(4)
C(71)-C(72)-C(73)	120.8(4)
C(67)-C(72)-C(73)	120.7(4)
C(74)-C(73)-C(72)	178.8(5)
C(73)-C(74)-C(75)	177.3(5)
C(76)-C(75)-C(77)	117.0(4)
C(76)-C(75)-C(74)	120.1(4)
C(77)-C(75)-C(74)	122.8(4)
N(1)-C(76)-C(75)	124.4(4)
N(1)-C(76)-H(76)	117.8
C(75)-C(76)-H(76)	117.8
C(78)-C(77)-C(75)	118.5(5)
C(78)-C(77)-H(77)	120.8
C(75)-C(77)-H(77)	120.8
C(77)-C(78)-C(79)	122.0(5)
C(77)-C(78)-H(78)	119.0
C(79)-C(78)-H(78)	119.0
N(1)-C(79)-C(78)	119.4(4)
N(1)-C(79)-C(80)	119.7(4)
C(78)-C(79)-C(80)	120.8(4)
C(81)-C(80)-C(85)	119.4(4)
C(81)-C(80)-C(79)	117.6(4)
C(85)-C(80)-C(79)	123.0(4)
C(82)-C(81)-C(80)	122.8(5)
C(82)-C(81)-H(81)	118.6
C(80)-C(81)-H(81)	118.6
C(81)-C(82)-C(83)	117.2(4)
C(81)-C(82)-C(92)	121.1(5)
C(83)-C(82)-C(92)	121.6(5)
C(82)-C(83)-C(84)	123.7(4)
C(82)-C(83)-H(83)	118.2
C(84)-C(83)-H(83)	118.2
C(83)-C(84)-C(85)	119.4(4)
C(83)-C(84)-C(86)	119.4(4)
C(85)-C(84)-C(86)	121.2(4)
O(4)-C(85)-C(80)	122.3(4)
O(4)-C(85)-C(84)	120.2(4)
C(80)-C(85)-C(84)	117.4(4)
C(87)-C(86)-C(91)	117.7(4)
C(87)-C(86)-C(84)	121.9(4)
C(91)-C(86)-C(84)	120.1(4)
C(86)-C(87)-C(88)	121.1(4)
C(86)-C(87)-H(87)	119.4
C(88)-C(87)-H(87)	119.4
C(89)-C(88)-C(87)	120.1(4)
C(89)-C(88)-H(88)	119.9
C(87)-C(88)-H(88)	119.9
C(88)-C(89)-C(90)	119.4(5)
C(88)-C(89)-H(89)	120.3
C(90)-C(89)-H(89)	120.3
C(89)-C(90)-C(91)	120.2(5)
C(89)-C(90)-H(90)	119.9
C(91)-C(90)-H(90)	119.9
C(90)-C(91)-C(86)	121.3(4)
C(90)-C(91)-H(91)	119.4
C(86)-C(91)-H(91)	119.4
C(82)-C(92)-H(92A)	109.5
C(82)-C(92)-H(92B)	109.5
H(92A)-C(92)-H(92B)	109.5
C(82)-C(92)-H(92C)	109.5
H(92A)-C(92)-H(92C)	109.5
H(92B)-C(92)-H(92C)	109.5
C(104)-O(100)-C(101)	108.0(3)
C(104)-O(100)-Fe(1)	126.2(3)
C(101)-O(100)-Fe(1)	124.1(3)
O(100)-C(101)-C(102)	107.0(4)
O(100)-C(101)-H(10A)	110.3
C(102)-C(101)-H(10A)	110.3
O(100)-C(101)-H(10B)	110.3
C(102)-C(101)-H(10B)	110.3

H(10A)-C(101)-H(10B)	108.6
C(101)-C(102)-C(103)	103.6(4)
C(101)-C(102)-H(10C)	111.0
C(103)-C(102)-H(10C)	111.0
C(101)-C(102)-H(10D)	111.0
C(103)-C(102)-H(10D)	111.0
H(10C)-C(102)-H(10D)	109.0
C(104)-C(103)-C(102)	101.6(4)
C(104)-C(103)-H(10E)	111.4
C(102)-C(103)-H(10E)	111.4
C(104)-C(103)-H(10F)	111.4
C(102)-C(103)-H(10F)	111.4
H(10E)-C(103)-H(10F)	109.3
O(100)-C(104)-C(103)	104.1(4)
O(100)-C(104)-H(10G)	110.9
C(103)-C(104)-H(10G)	110.9
O(100)-C(104)-H(10H)	110.9
C(103)-C(104)-H(10H)	110.9
H(10G)-C(104)-H(10H)	109.0
C(201)-O(200)-C(204)	107.7(4)
C(201)-O(200)-Fe(2)	123.2(4)
C(204)-O(200)-Fe(2)	124.5(3)
O(200)-C(201)-C(202)	108.2(5)
O(200)-C(201)-H(20A)	110.1
C(202)-C(201)-H(20A)	110.1
O(200)-C(201)-H(20B)	110.1
C(202)-C(201)-H(20B)	110.1
H(20A)-C(201)-H(20B)	108.4
C(201)-C(202)-C(203)	103.5(5)
C(201)-C(202)-H(20C)	111.1
C(203)-C(202)-H(20C)	111.1
C(201)-C(202)-H(20D)	111.1
C(203)-C(202)-H(20D)	111.1
H(20C)-C(202)-H(20D)	109.0
C(204)-C(203)-C(202)	100.7(5)
C(204)-C(203)-H(20E)	111.6
C(202)-C(203)-H(20E)	111.6
C(204)-C(203)-H(20F)	111.6
C(202)-C(203)-H(20F)	111.6
H(20E)-C(203)-H(20F)	109.4
C(203)-C(204)-O(200)	100.4(4)
C(203)-C(204)-H(20G)	111.7
O(200)-C(204)-H(20G)	111.7
C(203)-C(204)-H(20H)	111.7
O(200)-C(204)-H(20H)	111.7
H(20G)-C(204)-H(20H)	109.5
C(301)-O(300)-C(304)	105.4(3)
C(301)-O(300)-Fe(2)	127.1(3)
C(304)-O(300)-Fe(2)	124.4(3)
O(300)-C(301)-C(302)	105.6(4)
O(300)-C(301)-H(30A)	110.6
C(302)-C(301)-H(30A)	110.6
O(300)-C(301)-H(30B)	110.6
C(302)-C(301)-H(30B)	110.6
H(30A)-C(301)-H(30B)	108.8
C(301)-C(302)-C(303)	102.9(4)
C(301)-C(302)-H(30C)	111.2
C(303)-C(302)-H(30C)	111.2
C(301)-C(302)-H(30D)	111.2
C(303)-C(302)-H(30D)	111.2
H(30C)-C(302)-H(30D)	109.1
C(304)-C(303)-C(302)	104.9(4)
C(304)-C(303)-H(30E)	110.8
C(302)-C(303)-H(30E)	110.8
C(304)-C(303)-H(30F)	110.8
C(302)-C(303)-H(30F)	110.8
H(30E)-C(303)-H(30F)	108.8
O(300)-C(304)-C(303)	106.7(4)
O(300)-C(304)-H(30G)	110.4
C(303)-C(304)-H(30G)	110.4
O(300)-C(304)-H(30H)	110.4
C(303)-C(304)-H(30H)	110.4
H(30G)-C(304)-H(30H)	108.6
C(401)-O(400)-C(404)	110.6(14)
O(400)-C(401)-C(402)	102.5(13)
O(400)-C(401)-H(40A)	111.3
C(402)-C(401)-H(40A)	111.3
O(400)-C(401)-H(40B)	111.3
C(402)-C(401)-H(40B)	111.3
H(40A)-C(401)-H(40B)	109.2
C(403)-C(402)-C(401)	107.0(11)
C(403)-C(402)-H(40C)	110.3
C(401)-C(402)-H(40C)	110.3
C(403)-C(402)-H(40D)	110.3
C(401)-C(402)-H(40D)	110.3
H(40C)-C(402)-H(40D)	108.6
C(402)-C(403)-C(404)	101.7(12)
C(402)-C(403)-H(40E)	111.4
C(404)-C(403)-H(40E)	111.4
C(402)-C(403)-H(40F)	111.4
C(404)-C(403)-H(40F)	111.4
H(40E)-C(403)-H(40F)	109.3
O(400)-C(404)-C(403)	106.6(12)
O(400)-C(404)-H(40G)	110.4
C(403)-C(404)-H(40G)	110.4
O(400)-C(404)-H(40H)	110.4
C(403)-C(404)-H(40H)	110.4
H(40G)-C(404)-H(40H)	108.6
C(501)-O(500)-C(504)	108.2(5)
O(500)-C(501)-C(502)	106.7(6)
O(500)-C(501)-H(50A)	110.4
C(502)-C(501)-H(50A)	110.4
O(500)-C(501)-H(50B)	110.4
C(502)-C(501)-H(50B)	110.4
H(50A)-C(501)-H(50B)	108.6
C(503)-C(502)-C(501)	106.6(7)
C(503)-C(502)-H(50C)	110.4
C(501)-C(502)-H(50C)	110.4
C(503)-C(502)-H(50D)	110.4
C(501)-C(502)-H(50D)	110.4
H(50C)-C(502)-H(50D)	108.6
C(502)-C(503)-C(504)	106.1(7)

C(502)-C(503)-H(50E)	110.5
C(504)-C(503)-H(50E)	110.5
C(502)-C(503)-H(50F)	110.5
C(504)-C(503)-H(50F)	110.5
H(50E)-C(503)-H(50F)	108.7
O(500)-C(504)-C(503)	106.1(6)
O(500)-C(504)-H(50G)	110.5
C(503)-C(504)-H(50G)	110.5
O(500)-C(504)-H(50H)	110.5
C(503)-C(504)-H(50H)	110.5
H(50G)-C(504)-H(50H)	108.7
C(614)-O(600)-C(604)	122.3(18)
C(614)-O(600)-C(601)	120.1(19)
C(604)-O(600)-C(601)	109.8(8)
C(614)-O(600)-C(613)	53.2(19)
C(604)-O(600)-C(613)	112.5(13)
C(601)-O(600)-C(613)	81.9(12)
C(602)-C(601)-O(600)	103.6(8)
C(602)-C(601)-C(612)	91.6(17)
O(600)-C(601)-C(612)	81.0(13)
C(602)-C(601)-H(60A)	111.0
O(600)-C(601)-H(60A)	111.0
C(602)-C(601)-H(60B)	111.0
O(600)-C(601)-H(60B)	111.0
C(612)-C(601)-H(60B)	149.8
H(60A)-C(601)-H(60B)	109.0
O(600)-C(601)-H(60A)	115.3
C(612)-C(601)-H(60A)	115.6
H(60A)-C(601)-H(60A)	121.9
H(60B)-C(601)-H(60A)	85.1
C(602)-C(601)-H(60B)	134.7
O(600)-C(601)-H(60B)	115.6
C(612)-C(601)-H(60B)	115.3
H(60A)-C(601)-H(60B)	75.9
H(60A)-C(601)-H(60B)	111.2
C(601)-C(602)-C(603)	101.4(8)
C(603)-C(602)-H(60A)	109.2
C(601)-C(602)-H(60C)	111.5
C(603)-C(602)-H(60C)	111.5
H(60A)-C(602)-H(60C)	76.5
C(601)-C(602)-H(60D)	111.5
C(603)-C(602)-H(60D)	111.5
H(60A)-C(602)-H(60D)	132.5
H(60C)-C(602)-H(60D)	109.3
C(604)-C(603)-C(602)	110.1(8)
C(604)-C(603)-H(60E)	109.6
C(602)-C(603)-H(60E)	109.6
C(604)-C(603)-H(60F)	109.6
C(602)-C(603)-H(60F)	109.6
H(60E)-C(603)-H(60F)	108.2
C(603)-C(604)-O(600)	106.1(7)
C(603)-C(604)-H(60G)	110.5
O(600)-C(604)-H(60G)	110.5
C(603)-C(604)-H(60H)	110.5
O(600)-C(604)-H(60H)	110.5
H(60G)-C(604)-H(60H)	108.7
C(613)-C(612)-C(601)	103(4)
C(613)-C(612)-H(61A)	111.1
C(601)-C(612)-H(61A)	111.1
C(613)-C(612)-H(61B)	111.1
C(601)-C(612)-H(61B)	111.1
H(61A)-C(612)-H(61B)	109.0
C(612)-C(613)-C(614)	118(4)
C(612)-C(613)-O(600)	76(3)
C(614)-C(613)-O(600)	43(2)
C(612)-C(613)-H(61C)	107.7
C(614)-C(613)-H(61C)	107.7
O(600)-C(613)-H(61C)	116.7
C(612)-C(613)-H(61D)	107.7
C(614)-C(613)-H(61D)	107.7
O(600)-C(613)-H(61D)	132.7
H(61C)-C(613)-H(61D)	107.1
O(600)-C(614)-C(613)	83(3)
O(600)-C(614)-H(61E)	114.7
C(613)-C(614)-H(61E)	114.7
O(600)-C(614)-H(61F)	114.7
C(613)-C(614)-H(61F)	114.7
H(61E)-C(614)-H(61F)	111.8
C(701)-O(700)-C(704)	100.8(13)
C(702)-C(701)-O(700)	109.3(18)
C(702)-C(701)-H(70A)	109.8
O(700)-C(701)-H(70A)	109.8
C(702)-C(701)-H(70B)	109.8
O(700)-C(701)-H(70B)	109.8
H(70A)-C(701)-H(70B)	108.3
C(703)-C(702)-C(701)	105.9(16)
C(703)-C(702)-H(70C)	110.6
C(701)-C(702)-H(70C)	110.6
C(703)-C(702)-H(70D)	110.6
C(701)-C(702)-H(70D)	110.6
H(70C)-C(702)-H(70D)	108.7
C(704)-C(703)-C(702)	111.0(16)
C(704)-C(703)-H(70E)	109.4
C(702)-C(703)-H(70E)	109.4
C(704)-C(703)-H(70F)	109.4
C(702)-C(703)-H(70F)	109.4
H(70E)-C(703)-H(70F)	108.0
C(703)-C(704)-O(700)	105(2)
C(703)-C(704)-H(70G)	110.8
O(700)-C(704)-H(70G)	110.8
C(703)-C(704)-H(70H)	110.8
O(700)-C(704)-H(70H)	110.8
H(70G)-C(704)-H(70H)	108.8
C(801)-C(800)-H(80A)	109.5
C(801)-C(800)-H(80B)	109.5
H(80A)-C(800)-H(80B)	109.5
C(801)-C(800)-H(80C)	109.5
H(80A)-C(800)-H(80C)	109.5
H(80B)-C(800)-H(80C)	109.5
C(800)-C(801)-C(802)	107.4(15)
C(800)-C(801)-H(80A)	110.2
C(802)-C(801)-H(80A)	110.2

C(800)-C(801)-H(80B)	110.2
C(802)-C(801)-H(80B)	110.2
H(80A)-C(801)-H(80B)	108.5
C(803)#1-C(802)-C(803)	179.998(4)
C(803)#1-C(802)-C(801)	80.1(12)
C(803)-C(802)-C(801)	99.9(12)
C(803)#1-C(802)-C(801)#1	99.9(12)
C(803)-C(802)-C(801)#1	80.1(12)
C(801)-C(802)-C(801)#1	179.999(2)
C(803)#1-C(802)-H(80D)	68.2
C(803)-C(802)-H(80D)	111.8
C(801)-C(802)-H(80D)	111.8
C(801)#1-C(802)-H(80D)	68.2
C(803)#1-C(802)-H(80E)	68.2
C(803)-C(802)-H(80E)	111.8
C(801)-C(802)-H(80E)	111.8
C(801)#1-C(802)-H(80E)	68.2
H(80D)-C(802)-H(80E)	109.5
C(802)-C(803)-C(804)	105.6(19)
C(802)-C(803)-H(80E)	110.6
C(804)-C(803)-H(80E)	110.6
C(802)-C(803)-H(80F)	110.6
C(804)-C(803)-H(80F)	110.6
H(80E)-C(803)-H(80F)	108.7
C(803)-C(804)-H(80G)	109.5
C(803)-C(804)-H(80H)	109.5
H(80G)-C(804)-H(80H)	109.5
C(803)-C(804)-H(80I)	109.5
H(80G)-C(804)-H(80I)	109.5
H(80H)-C(804)-H(80I)	109.5

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