Supporting Information

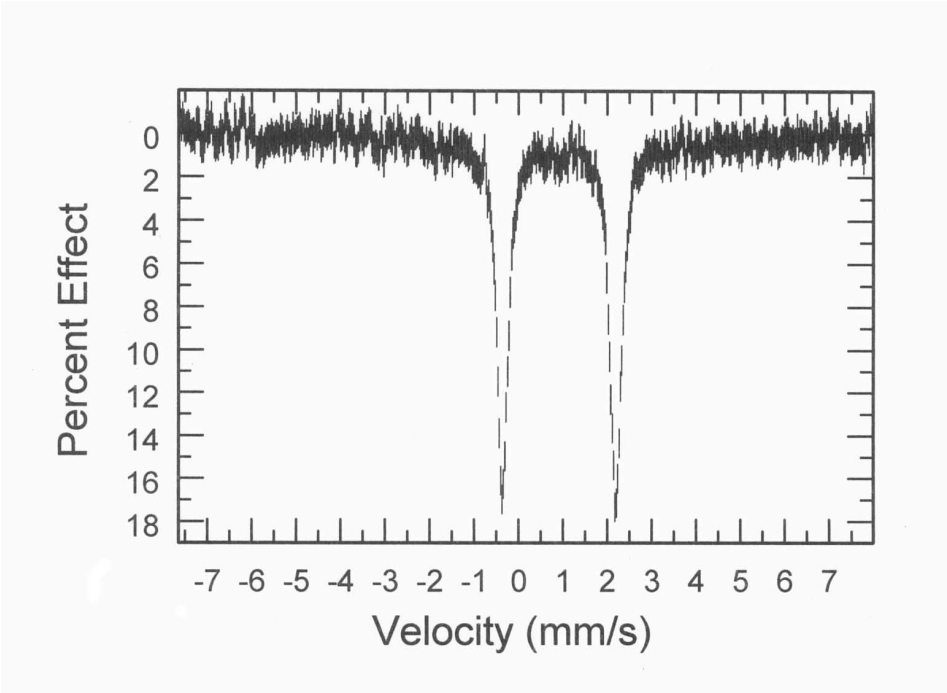

Figure S1. Zero-field Mössbauer spectrum of [Fe(TPP)(Hdmpz)] taken at 4.2 K. The fit parameters are: Quadrupole Splitting = 2.54 mm/s, isomer shift = 0.91 mm/s, Gamma = 0.31. Area = 16.2 %.mm/s.

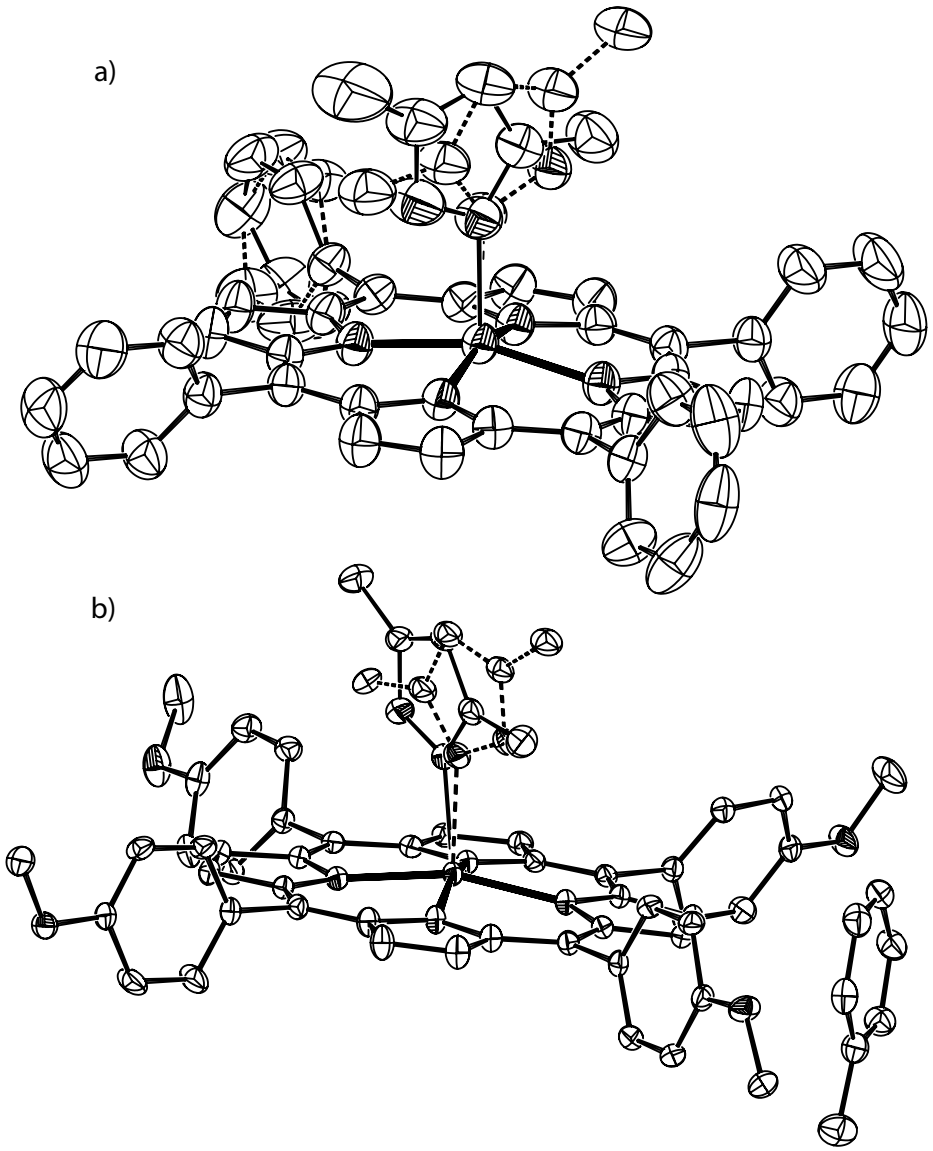

Figure S2. ORTEP diagram showing all nonhydrogen atoms in the independent unit including all the disordered atoms. The major pyrazole ligand orientation is drawn with heavy bonds, while the minor orientation is depicted with open bonds. Diagrams are for a) [Fe(TPP)(Hdmpz)] and b) [Fe(T*p*-OCH_3PP)(Hdmpz)].

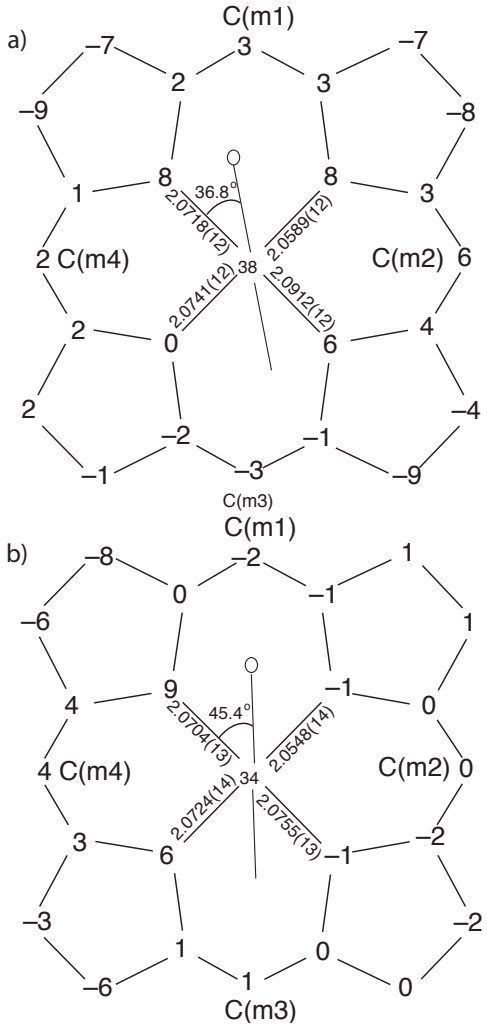

Figure S3. Formal diagrams of the porphyrinato cores. a) [Fe(TPP)(Hdmpz)]. b) [Fe(T*p*-OCH_3PP)(Hdmpz)]. Illustrated are the displacements of each atom from the mean plane of the 24-atom core in units of 0.01 Å. Positive values of displacement are toward the pyrazole ligand. The diagrams also show the orientation of the pyrazole ligand with respect to the atoms of the porphyrin core. The location of the methyl group at the α-position of the coordinated nitrogen is represented by the circle.

Table S1. Complete Crystallographic Details for [Fe(TPP)(Hdmpz)]

formula	$C_{49}H_{36}FeN_6$
FW, amu	764.69
a, Å	11.3032(2)
b, Å	30.8656(6)
c, Å	11.7462(2)
β, deg	105.3580(10)
V, Å^3	3951.67(12)
space group	$P2_1/c$
Z	4
D_c, g/cm^3	1.285
F(000)	1592
μ, mm^{-1}	0.424
crystal dimensions, mm	0.44 × 0.44 × 0.22
radiation	MoKα, $\bar{\lambda} = 0.71073$ Å
temperature, K	299(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.32–30.50
index range	$-16 \leq h \leq 16$
	$-44 \leq k \leq 43$
	$-16 \leq l \leq 15$
total data collected	84805
absorption correction	Semi-empirical from equivalent
relative transmission coefficients (I)	0.9124 and 0.8352
unique data	11989 ($R_{int} = 0.024$)
unique observed data [I > 2σ(I)]	8806
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	11989/84/582
goodness-of-fit (pased on F^2)	1.025
final R indices [I > 2σ(I)]	$R_1 = 0.0421$, $wR_2 = 0.1121$
final R indices (all data)	$R_1 = 0.0645$, $wR_2 = 0.1272$

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(Hdmpz)][a]

atom	x	y	z	U(eq)
Fe(1)	0.37554(2)	0.13193(1)	0.80577(2)	0.0377(1)
N(1)	0.34128(12)	0.19179(4)	0.87026(11)	0.0401(3)
N(2)	0.26137(11)	0.10397(4)	0.89542(11)	0.0408(3)
N(3)	0.44794(11)	0.07058(4)	0.78972(11)	0.0398(3)
N(4)	0.53049(12)	0.15819(4)	0.76945(11)	0.0410(3)
C(a1)	0.39624(15)	0.23049(5)	0.85671(13)	0.0416(3)
C(a2)	0.25196(14)	0.20092(5)	0.92674(13)	0.0411(3)
C(a3)	0.18342(14)	0.12552(5)	0.94834(13)	0.0426(3)
C(a4)	0.23978(14)	0.06045(5)	0.90426(13)	0.0423(3)
C(a5)	0.39836(14)	0.03178(5)	0.81108(13)	0.0421(3)
C(a6)	0.54445(14)	0.06096(5)	0.74392(14)	0.0417(3)
C(a7)	0.61351(14)	0.13666(5)	0.72284(14)	0.0413(3)
C(a8)	0.55364(14)	0.20167(5)	0.76345(13)	0.0416(3)
C(b1)	0.33859(17)	0.26500(5)	0.90556(15)	0.0510(4)
C(b2)	0.25036(16)	0.24705(5)	0.94795(15)	0.0502(4)
C(b3)	0.11171(16)	0.09419(6)	0.99230(16)	0.0520(4)
C(b4)	0.14653(17)	0.05446(6)	0.96570(16)	0.0532(4)
C(b5)	0.46630(16)	−0.00326(5)	0.77686(16)	0.0524(4)
C(b6)	0.55624(17)	0.01468(5)	0.73651(17)	0.0532(4)
C(b7)	0.69069(16)	0.16798(5)	0.68641(16)	0.0515(4)
C(b8)	0.65357(16)	0.20762(5)	0.71122(16)	0.0521(4)
C(m1)	0.17640(14)	0.17046(5)	0.96081(13)	0.0419(3)
C(m2)	0.29977(14)	0.02675(5)	0.86153(13)	0.0414(3)
C(m3)	0.62114(13)	0.09175(5)	0.71045(13)	0.0411(3)
C(m4)	0.49243(15)	0.23556(5)	0.80410(13)	0.0416(3)
C(11)	0.08060(14)	0.18753(5)	1.01613(14)	0.0451(3)
C(12)	−0.03830(18)	0.19285(8)	0.95014(19)	0.0696(5)
C(13)	−0.1267(2)	0.20888(9)	1.0008(2)	0.0864(7)
C(14)	−0.0969(2)	0.21976(7)	1.1170(2)	0.0745(6)
C(15)	0.0195(2)	0.21462(7)	1.18401(19)	0.0702(5)
C(16)	0.10903(18)	0.19863(7)	1.13417(16)	0.0587(4)
C(21)	0.25262(15)	−0.01810(5)	0.86940(14)	0.0446(3)
C(22)	0.3145(2)	−0.04770(6)	0.95325(17)	0.0617(5)
C(23)	0.2661(3)	−0.08849(6)	0.9587(2)	0.0784(7)

Table S2. Continued

atom	x	y	z	U(eq)
C(24)	0.1581(3)	−0.10045(7)	0.8815(3)	0.0835(8)
C(25)	0.0970(2)	−0.07162(8)	0.7986(3)	0.0854(7)
C(26)	0.14318(18)	−0.03063(6)	0.79252(19)	0.0631(5)
C(31)	0.71980(15)	0.07494(5)	0.65826(14)	0.0457(3)
C(32)	0.84223(17)	0.07982(6)	0.71733(18)	0.0593(4)
C(33)	0.93326(19)	0.06638(7)	0.6656(2)	0.0726(6)
C(34)	0.9033(2)	0.04777(8)	0.5566(2)	0.0780(6)
C(35)	0.7820(2)	0.04155(8)	0.4980(2)	0.0775(6)
C(36)	0.69003(19)	0.05493(7)	0.54834(17)	0.0608(4)
C(41)	0.53593(15)	0.28079(5)	0.79119(14)	0.0447(3)
C(44)	0.6175(3)	0.36439(6)	0.7663(2)	0.0731(6)
C(42a)	0.5985(12)	0.3029(4)	0.8859(10)	0.061(2)
C(43a)	0.6364(13)	0.3439(4)	0.8718(11)	0.074(3)
C(45a)	0.5516(13)	0.3412(4)	0.6692(11)	0.071(2)
C(46a)	0.5069(12)	0.2990(3)	0.6789(9)	0.0570(19)
C(42b)	0.6393(15)	0.2988(4)	0.8738(13)	0.070(3)
C(43b)	0.6819(15)	0.3413(5)	0.8637(14)	0.077(3)
C(45b)	0.5188(15)	0.3488(5)	0.6865(15)	0.079(3)
C(46b)	0.4828(14)	0.3081(5)	0.6994(13)	0.067(3)
N(5a)	0.26399(18)	0.13177(7)	0.62618(16)	0.0529(4)
N(6a)	0.31368(19)	0.11241(7)	0.54559(16)	0.0751(6)
C(1a)	0.2423(2)	0.11517(9)	0.43556(19)	0.0738(7)
C(2a)	0.1404(3)	0.13674(9)	0.4444(2)	0.0652(5)
C(3a)	0.15735(18)	0.14662(6)	0.56350(18)	0.0517(4)
C(4a)	0.2815(4)	0.09584(15)	0.3335(3)	0.1307(16)
C(5a)	0.0752(2)	0.17118(8)	0.6204(2)	0.0734(6)
N(5b)	0.2573(13)	0.1366(7)	0.6287(11)	0.0529(4)
N(6b)	0.1462(13)	0.1555(6)	0.6216(10)	0.050(2)
C(1b)	0.0718(11)	0.1552(4)	0.5125(10)	0.057(2)
C(2b)	0.1366(14)	0.1360(7)	0.4437(10)	0.0652(5)
C(3b)	0.2518(12)	0.1247(5)	0.5199(12)	0.059(2)
C(4b)	−0.0568(13)	0.1743(7)	0.4867(16)	0.069(5)
C(5b)	0.3570(15)	0.1015(7)	0.4913(18)	0.071(5)

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S3. Bond Lengths for [Fe(TPP)(Hdmpz)][a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(2)	2.0589(12)	C(25)–H(25)	0.9300
Fe(1)–N(1)	2.0718(12)	C(26)–H(26)	0.9300
Fe(1)–N(4)	2.0741(12)	C(31)–C(32)	1.382(3)
Fe(1)–N(3)	2.0912(12)	C(31)–C(36)	1.390(2)
Fe(1)–N(5a)	2.1519(18)	C(32)–C(33)	1.389(3)
Fe(1)–N(5b)	2.159(11)	C(32)–H(32)	0.9300
N(1)–C(a1)	1.3750(19)	C(33)–C(34)	1.363(3)
N(1)–C(a2)	1.3761(19)	C(33)–H(33)	0.9300
N(2)–C(a4)	1.3739(19)	C(34)–C(35)	1.375(3)
N(2)–C(a3)	1.3767(19)	C(34)–H(34)	0.9300
N(3)–C(a6)	1.3706(19)	C(35)–C(36)	1.388(3)
N(3)–C(a5)	1.3733(19)	C(35)–H(35)	0.9300
N(4)–C(a8)	1.3728(19)	C(36)–H(36)	0.9300
N(4)–C(a7)	1.3762(19)	C(41)–C(42a)	1.336(11)
C(a1)–C(m4)	1.394(2)	C(41)–C(46b)	1.374(14)
C(a1)–C(b1)	1.444(2)	C(41)–C(46a)	1.390(11)
C(a2)–C(m1)	1.398(2)	C(41)–C(42b)	1.419(15)
C(a2)–C(b2)	1.446(2)	C(44)–C(45b)	1.342(17)
C(a3)–C(m1)	1.399(2)	C(44)–C(43a)	1.356(13)
C(a3)–C(b3)	1.442(2)	C(44)–C(43b)	1.381(16)
C(a4)–C(m2)	1.405(2)	C(44)–C(45a)	1.385(14)
C(a4)–C(b4)	1.438(2)	C(44)–H(44)	0.9300
C(a5)–C(m2)	1.402(2)	C(42a)–C(43a)	1.361(16)
C(a5)–C(b5)	1.444(2)	C(42a)–H(42a)	0.9300
C(a6)–C(m3)	1.411(2)	C(43a)–H(43a)	0.9300
C(a6)–C(b6)	1.440(2)	C(45a)–C(46a)	1.413(16)
C(a7)–C(m3)	1.399(2)	C(45a)–H(45a)	0.9300
C(a7)–C(b7)	1.441(2)	C(46a)–H(46a)	0.9300
C(a8)–C(m4)	1.406(2)	C(42b)–C(43b)	1.413(18)
C(a8)–C(b8)	1.433(2)	C(42b)–H(42b)	0.9300
C(b1)–C(b2)	1.346(2)	C(43b)–H(43b)	0.9300
C(b1)–H(b1)	0.9300	C(45b)–C(46b)	1.34(2)
C(b2)–H(b2)	0.9300	C(45b)–H(45b)	0.9300
C(b3)–C(b4)	1.349(2)	C(46b)–H(46b)	0.9300

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(b3)–H(b3)	0.9300	N(5a)–C(3a)	1.317(3)
C(b4)–H(b4)	0.9300	N(5a)–N(6a)	1.360(3)
C(b5)–C(b6)	1.349(2)	N(6a)–C(1a)	1.333(3)
C(b5)–H(b5)	0.9300	N(6a)–H(6aa)	0.8600
C(b6)–H(b6)	0.9300	C(1a)–C(2a)	1.357(4)
C(b7)–C(b8)	1.350(2)	C(1a)–C(4a)	1.507(4)
C(b7)–H(b7)	0.9300	C(2a)–C(3a)	1.395(3)
C(b8)–H(b8)	0.9300	C(2a)–H(2aa)	0.9300
C(m1)–C(11)	1.498(2)	C(3a)–C(5a)	1.488(3)
C(m2)–C(21)	1.495(2)	C(4a)–H(4aa)	0.9600
C(m3)–C(31)	1.500(2)	C(4a)–H(4ab)	0.9600
C(m4)–C(41)	1.501(2)	C(4a)–H(4ac)	0.9600
C(11)–C(12)	1.372(3)	C(5a)–H(5aa)	0.9600
C(11)–C(16)	1.381(2)	C(5a)–H(5ab)	0.9600
C(12)–C(13)	1.383(3)	C(5a)–H(5ac)	0.9600
C(12)–H(12)	0.9300	N(5b)–C(3b)	1.3145
C(13)–C(14)	1.358(3)	N(5b)–N(6b)	1.3676
C(13)–H(13)	0.9300	N(6b)–C(1b)	1.3338
C(14)–C(15)	1.352(3)	N(6b)–H(6ba)	0.8600
C(14)–H(14)	0.9300	C(1b)–C(2b)	1.3622
C(15)–C(16)	1.387(3)	C(1b)–C(4b)	1.5225
C(15)–H(15)	0.9300	C(2b)–C(3b)	1.4143
C(16)–H(16)	0.9300	C(2b)–H(2ba)	0.9300
C(21)–C(26)	1.380(2)	C(3b)–C(5b)	1.5008
C(21)–C(22)	1.389(2)	C(4b)–H(4ba)	0.9600
C(22)–C(23)	1.381(3)	C(4b)–H(4bb)	0.9600
C(22)–H(22)	0.9300	C(4b)–H(4bc)	0.9600
C(23)–C(24)	1.365(4)	C(5b)–H(5ba)	0.9600
C(23)–H(23)	0.9300	C(5b)–H(5bb)	0.9600
C(24)–C(25)	1.364(4)	C(5b)–H(5bc)	0.9600
C(24)–H(24)	0.9300		
C(25)–C(26)	1.378(3)		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S4. Bond Angles for [Fe(TPP)(Hdmpz)][a]

angle	degree	angle	degree
N(2)–Fe(1)–N(1)	89.07(5)	C(24)–C(23)–H(23)	119.6
N(2)–Fe(1)–N(4)	161.22(5)	C(22)–C(23)–H(23)	119.6
N(1)–Fe(1)–N(4)	88.66(5)	C(25)–C(24)–C(23)	119.51(19)
N(2)–Fe(1)–N(3)	88.84(5)	C(25)–C(24)–H(24)	120.2
N(1)–Fe(1)–N(3)	162.93(5)	C(23)–C(24)–H(24)	120.2
N(4)–Fe(1)–N(3)	87.90(5)	C(24)–C(25)–C(26)	120.6(2)
N(2)–Fe(1)–N(5a)	102.50(7)	C(24)–C(25)–H(25)	119.7
N(1)–Fe(1)–N(5a)	104.05(6)	C(26)–C(25)–H(25)	119.7
N(4)–Fe(1)–N(5a)	96.13(7)	C(25)–C(26)–C(21)	120.7(2)
N(3)–Fe(1)–N(5a)	92.94(6)	C(25)–C(26)–H(26)	119.7
N(2)–Fe(1)–N(5b)	102.0(5)	C(21)–C(26)–H(26)	119.7
N(1)–Fe(1)–N(5b)	99.5(5)	C(32)–C(31)–C(36)	118.59(16)
N(4)–Fe(1)–N(5b)	96.7(5)	C(32)–C(31)–C(m3)	120.73(15)
N(3)–Fe(1)–N(5b)	97.5(5)	C(36)–C(31)–C(m3)	120.66(15)
N(5a)–Fe(1)–N(5b)	4.6(5)	C(31)–C(32)–C(33)	120.47(19)
C(a1)–N(1)–C(a2)	106.83(12)	C(31)–C(32)–H(32)	119.8
C(a1)–N(1)–Fe(1)	126.76(10)	C(33)–C(32)–H(32)	119.8
C(a2)–N(1)–Fe(1)	126.23(10)	C(34)–C(33)–C(32)	120.5(2)
C(a4)–N(2)–C(a3)	106.89(12)	C(34)–C(33)–H(33)	119.7
C(a4)–N(2)–Fe(1)	126.61(10)	C(32)–C(33)–H(33)	119.7
C(a3)–N(2)–Fe(1)	126.24(10)	C(33)–C(34)–C(35)	119.77(19)
C(a6)–N(3)–C(a5)	106.77(12)	C(33)–C(34)–H(34)	120.1
C(a6)–N(3)–Fe(1)	127.06(10)	C(35)–C(34)–H(34)	120.1
C(a5)–N(3)–Fe(1)	125.80(10)	C(34)–C(35)–C(36)	120.3(2)
C(a8)–N(4)–C(a7)	107.00(12)	C(34)–C(35)–H(35)	119.8
C(a8)–N(4)–Fe(1)	125.12(10)	C(36)–C(35)–H(35)	119.8
C(a7)–N(4)–Fe(1)	126.52(10)	C(35)–C(36)–C(31)	120.25(19)
N(1)–C(a1)–C(m4)	125.31(13)	C(35)–C(36)–H(36)	119.9
N(1)–C(a1)–C(b1)	109.24(13)	C(31)–C(36)–H(36)	119.9
C(m4)–C(a1)–C(b1)	125.45(14)	C(42a)–C(41)–C(46b)	111.5(7)
N(1)–C(a2)–C(m1)	125.59(13)	C(42a)–C(41)–C(46a)	121.6(7)
N(1)–C(a2)–C(b2)	109.21(13)	C(46b)–C(41)–C(42b)	114.0(8)
C(m1)–C(a2)–C(b2)	125.19(14)	C(46a)–C(41)–C(42b)	115.8(8)
N(2)–C(a3)–C(m1)	125.95(14)	C(42a)–C(41)–C(m4)	120.4(5)

Table S4. Continued

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	108.97(13)	C(46b)–C(41)–C(m4)	124.2(6)
C(m1)–C(a3)–C(b3)	125.06(14)	C(46a)–C(41)–C(m4)	118.0(5)
N(2)–C(a4)–C(m2)	125.78(13)	C(42b)–C(41)–C(m4)	121.8(5)
N(2)–C(a4)–C(b4)	109.39(13)	C(45b)–C(44)–C(43a)	111.8(7)
C(m2)–C(a4)–C(b4)	124.83(14)	C(45b)–C(44)–C(43b)	123.4(8)
N(3)–C(a5)–C(m2)	125.59(13)	C(43a)–C(44)–C(45a)	115.6(7)
N(3)–C(a5)–C(b5)	109.24(13)	C(43b)–C(44)–C(45a)	117.7(8)
C(m2)–C(a5)–C(b5)	125.14(14)	C(45b)–C(44)–H(44)	121.4
N(3)–C(a6)–C(m3)	125.11(13)	C(43a)–C(44)–H(44)	122.2
N(3)–C(a6)–C(b6)	109.56(13)	C(43b)–C(44)–H(44)	115.1
C(m3)–C(a6)–C(b6)	125.33(14)	C(45a)–C(44)–H(44)	122.2
N(4)–C(a7)–C(m3)	125.96(13)	C(41)–C(42a)–C(43a)	119.2(10)
N(4)–C(a7)–C(b7)	108.93(13)	C(41)–C(42a)–H(42a)	120.4
C(m3)–C(a7)–C(b7)	125.10(14)	C(43a)–C(42a)–H(42a)	120.4
N(4)–C(a8)–C(m4)	126.33(13)	C(44)–C(43a)–C(42a)	124.5(9)
N(4)–C(a8)–C(b8)	109.26(13)	C(44)–C(43a)–H(43a)	117.7
C(m4)–C(a8)–C(b8)	124.39(14)	C(42a)–C(43a)–H(43a)	117.7
C(b2)–C(b1)–C(a1)	107.43(14)	C(44)–C(45a)–C(46a)	122.4(10)
C(b2)–C(b1)–H(b1)	126.3	C(44)–C(45a)–H(45a)	118.8
C(a1)–C(b1)–H(b1)	126.3	C(46a)–C(45a)–H(45a)	118.8
C(b1)–C(b2)–C(a2)	107.29(14)	C(41)–C(46a)–C(45a)	116.7(9)
C(b1)–C(b2)–H(b2)	126.4	C(41)–C(46a)–H(46a)	121.6
C(a2)–C(b2)–H(b2)	126.4	C(45a)–C(46a)–H(46a)	121.6
C(b4)–C(b3)–C(a3)	107.48(14)	C(43b)–C(42b)–C(41)	122.9(11)
C(b4)–C(b3)–H(b3)	126.3	C(43b)–C(42b)–H(42b)	118.6
C(a3)–C(b3)–H(b3)	126.3	C(41)–C(42b)–H(42b)	118.6
C(b3)–C(b4)–C(a4)	107.27(14)	C(44)–C(43b)–C(42b)	115.6(11)
C(b3)–C(b4)–H(b4)	126.4	C(44)–C(43b)–H(43b)	122.2
C(a4)–C(b4)–H(b4)	126.4	C(42b)–C(43b)–H(43b)	122.2
C(b6)–C(b5)–C(a5)	107.23(14)	C(46b)–C(45b)–C(44)	118.6(12)
C(b6)–C(b5)–H(b5)	126.4	C(46b)–C(45b)–H(45b)	120.7
C(a5)–C(b5)–H(b5)	126.4	C(44)–C(45b)–H(45b)	120.7
C(b5)–C(b6)–C(a6)	107.19(14)	C(45b)–C(46b)–C(41)	125.4(13)
C(b5)–C(b6)–H(b6)	126.4	C(45b)–C(46b)–H(46b)	117.3

Table S4. Continued

angle	degree	angle	degree
C(a6)–C(b6)–H(b6)	126.4	C(41)–C(46b)–H(46b)	117.3
C(b8)–C(b7)–C(a7)	107.26(14)	C(3a)–N(5a)–N(6a)	104.43(18)
C(b8)–C(b7)–H(b7)	126.4	C(3a)–N(5a)–Fe(1)	139.38(16)
C(a7)–C(b7)–H(b7)	126.4	N(6a)–N(5a)–Fe(1)	116.14(14)
C(b7)–C(b8)–C(a8)	107.55(14)	C(1a)–N(6a)–N(5a)	113.0(2)
C(b7)–C(b8)–H(b8)	126.2	C(1a)–N(6a)–H(6aa)	123.5
C(a8)–C(b8)–H(b8)	126.2	N(5a)–N(6a)–H(6aa)	123.5
C(a2)–C(m1)–C(a3)	125.51(13)	N(6a)–C(1a)–C(2a)	105.4(2)
C(a2)–C(m1)–C(11)	117.00(13)	N(6a)–C(1a)–C(4a)	121.1(2)
C(a3)–C(m1)–C(11)	117.48(13)	C(2a)–C(1a)–C(4a)	133.5(2)
C(a5)–C(m2)–C(a4)	125.57(14)	C(1a)–C(2a)–C(3a)	106.9(2)
C(a5)–C(m2)–C(21)	117.69(13)	C(1a)–C(2a)–H(2aa)	126.6
C(a4)–C(m2)–C(21)	116.73(13)	C(3a)–C(2a)–H(2aa)	126.6
C(a7)–C(m3)–C(a6)	125.40(13)	N(5a)–C(3a)–C(2a)	110.3(2)
C(a7)–C(m3)–C(31)	117.27(13)	N(5a)–C(3a)–C(5a)	120.9(2)
C(a6)–C(m3)–C(31)	117.32(13)	C(2a)–C(3a)–C(5a)	128.7(2)
C(a1)–C(m4)–C(a8)	125.36(13)	C(3b)–N(5b)–N(6b)	104.7
C(a1)–C(m4)–C(41)	117.64(13)	C(3b)–N(5b)–Fe(1)	140.9(6)
C(a8)–C(m4)–C(41)	116.99(13)	N(6b)–N(5b)–Fe(1)	114.3(6)
C(12)–C(11)–C(16)	118.05(16)	C(1b)–N(6b)–N(5b)	113.0
C(12)–C(11)–C(m1)	120.62(15)	C(1b)–N(6b)–H(6ba)	123.5
C(16)–C(11)–C(m1)	121.32(15)	N(5b)–N(6b)–H(6ba)	123.5
C(11)–C(12)–C(13)	120.7(2)	N(6b)–C(1b)–C(2b)	105.8
C(11)–C(12)–H(12)	119.6	N(6b)–C(1b)–C(4b)	120.9
C(13)–C(12)–H(12)	119.6	C(2b)–C(1b)–C(4b)	133.3
C(14)–C(13)–C(12)	120.4(2)	C(1b)–C(2b)–C(3b)	106.3
C(14)–C(13)–H(13)	119.8	C(1b)–C(2b)–H(2ba)	126.8
C(12)–C(13)–H(13)	119.8	C(3b)–C(2b)–H(2ba)	126.8
C(15)–C(14)–C(13)	120.00(18)	N(5b)–C(3b)–C(2b)	110.2
C(15)–C(14)–H(14)	120.0	N(5b)–C(3b)–C(5b)	120.9
C(13)–C(14)–H(14)	120.0	C(2b)–C(3b)–C(5b)	128.8
C(14)–C(15)–C(16)	120.15(19)	C(1b)–C(4b)–H(4ba)	109.5
C(14)–C(15)–H(15)	119.9	C(1b)–C(4b)–H(4bb)	109.5
C(16)–C(15)–H(15)	119.9	H(4ba)–C(4b)–H(4bb)	109.5

Table S4. Continued

angle	degree	angle	degree
C(11)–C(16)–C(15)	120.67(18)	C(1b)–C(4b)–H(4bc)	109.5
C(11)–C(16)–H(16)	119.7	H(4ba)–C(4b)–H(4bc)	109.5
C(15)–C(16)–H(16)	119.7	H(4bb)–C(4b)–H(4bc)	109.5
C(26)–C(21)–C(22)	118.39(16)	C(3b)–C(5b)–H(5ba)	109.5
C(26)–C(21)–C(m2)	119.44(15)	C(3b)–C(5b)–H(5bb)	109.5
C(22)–C(21)–C(m2)	122.16(15)	H(5ba)–C(5b)–H(5bb)	109.5
C(23)–C(22)–C(21)	120.1(2)	C(3b)–C(5b)–H(5bc)	109.5
C(23)–C(22)–H(22)	119.9	H(5ba)–C(5b)–H(5bc)	109.5
C(21)–C(22)–H(22)	119.9	H(5bb)–C(5b)–H(5bc)	109.5
C(24)–C(23)–C(22)	120.8(2)		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S5. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(Hdmpz)][a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0404(1)	0.0341(1)	0.0413(1)	−0.0013(1)	0.0156(1)	−0.0001(1)
N(1)	0.0434(7)	0.0365(6)	0.0431(6)	−0.0022(5)	0.0160(5)	0.0008(5)
N(2)	0.0425(7)	0.0375(6)	0.0459(6)	−0.0030(5)	0.0180(5)	−0.0005(5)
N(3)	0.0420(6)	0.0356(6)	0.0447(6)	0.0005(5)	0.0169(5)	0.0006(5)
N(4)	0.0444(7)	0.0358(6)	0.0471(6)	−0.0009(5)	0.0196(5)	0.0005(5)
C(a1)	0.0491(8)	0.0349(7)	0.0418(7)	0.0006(5)	0.0141(6)	0.0026(6)
C(a2)	0.0420(8)	0.0401(7)	0.0422(7)	−0.0025(6)	0.0128(6)	0.0064(6)
C(a3)	0.0413(8)	0.0458(8)	0.0440(7)	−0.0041(6)	0.0168(6)	−0.0013(6)
C(a4)	0.0438(8)	0.0406(7)	0.0454(7)	−0.0028(6)	0.0171(6)	−0.0049(6)
C(a5)	0.0443(8)	0.0356(7)	0.0475(8)	−0.0032(6)	0.0143(6)	−0.0020(6)
C(a6)	0.0435(8)	0.0370(7)	0.0478(8)	−0.0025(6)	0.0176(6)	0.0024(6)
C(a7)	0.0418(8)	0.0414(7)	0.0442(7)	−0.0007(6)	0.0177(6)	−0.0005(6)
C(a8)	0.0465(8)	0.0372(7)	0.0441(7)	0.0009(6)	0.0172(6)	−0.0030(6)
C(b1)	0.0647(10)	0.0353(7)	0.0577(9)	0.0018(6)	0.0242(8)	0.0072(7)
C(b2)	0.0581(10)	0.0408(8)	0.0568(9)	0.0005(7)	0.0245(8)	0.0113(7)
C(b3)	0.0531(9)	0.0521(9)	0.0602(10)	−0.0077(7)	0.0316(8)	−0.0073(7)
C(b4)	0.0588(10)	0.0470(8)	0.0625(10)	−0.0043(7)	0.0312(8)	−0.0101(7)
C(b5)	0.0586(10)	0.0344(7)	0.0699(10)	−0.0072(7)	0.0270(8)	−0.0020(7)
C(b6)	0.0575(10)	0.0389(8)	0.0711(11)	−0.0068(7)	0.0309(8)	0.0024(7)
C(b7)	0.0537(9)	0.0476(8)	0.0630(10)	−0.0017(7)	0.0324(8)	−0.0044(7)
C(b8)	0.0567(10)	0.0434(8)	0.0645(10)	−0.0011(7)	0.0307(8)	−0.0079(7)
C(m1)	0.0389(7)	0.0463(8)	0.0423(7)	−0.0039(6)	0.0137(6)	0.0034(6)
C(m2)	0.0433(8)	0.0367(7)	0.0447(7)	−0.0021(6)	0.0124(6)	−0.0045(6)
C(m3)	0.0417(8)	0.0422(7)	0.0427(7)	−0.0036(6)	0.0169(6)	0.0022(6)
C(m4)	0.0499(8)	0.0348(7)	0.0409(7)	0.0016(5)	0.0134(6)	−0.0012(6)
C(11)	0.0437(8)	0.0449(8)	0.0510(8)	−0.0032(6)	0.0199(7)	0.0037(6)
C(12)	0.0513(11)	0.0958(15)	0.0611(11)	−0.0077(10)	0.0137(9)	0.0167(10)
C(13)	0.0495(11)	0.113(2)	0.0978(17)	−0.0073(15)	0.0212(11)	0.0263(12)
C(14)	0.0686(13)	0.0710(13)	0.0991(16)	−0.0098(11)	0.0489(13)	0.0126(10)
C(15)	0.0813(15)	0.0728(13)	0.0689(12)	−0.0173(10)	0.0413(11)	0.0004(11)
C(16)	0.0538(10)	0.0723(12)	0.0524(9)	−0.0111(8)	0.0184(8)	0.0052(8)
C(21)	0.0530(9)	0.0367(7)	0.0493(8)	−0.0049(6)	0.0228(7)	−0.0062(6)
C(22)	0.0834(13)	0.0467(9)	0.0544(10)	0.0033(7)	0.0172(9)	−0.0043(9)
C(23)	0.129(2)	0.0434(9)	0.0796(14)	0.0084(9)	0.0565(15)	−0.0008(11)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.1064(18)	0.0446(10)	0.127(2)	−0.0200(12)	0.0790(17)	−0.0244(12)
C(25)	0.0660(13)	0.0664(13)	0.130(2)	−0.0321(14)	0.0373(14)	−0.0286(11)
C(26)	0.0542(10)	0.0540(10)	0.0796(13)	−0.0088(9)	0.0149(9)	−0.0090(8)
C(31)	0.0480(9)	0.0428(7)	0.0519(8)	0.0000(6)	0.0232(7)	0.0038(6)
C(32)	0.0506(10)	0.0639(11)	0.0655(11)	−0.0056(8)	0.0189(8)	0.0072(8)
C(33)	0.0521(11)	0.0748(13)	0.0952(16)	0.0018(12)	0.0270(11)	0.0145(10)
C(34)	0.0754(15)	0.0821(14)	0.0918(16)	0.0006(12)	0.0488(13)	0.0241(11)
C(35)	0.0853(16)	0.0905(16)	0.0667(12)	−0.0144(11)	0.0377(12)	0.0179(12)
C(36)	0.0603(11)	0.0692(11)	0.0566(10)	−0.0104(8)	0.0218(8)	0.0070(9)
C(41)	0.0550(9)	0.0356(7)	0.0462(8)	0.0017(6)	0.0184(7)	−0.0013(6)
C(44)	0.1027(18)	0.0411(9)	0.0822(14)	0.0058(9)	0.0363(14)	−0.0115(10)
C(42a)	0.096(6)	0.042(3)	0.042(2)	−0.0070(18)	0.015(4)	−0.013(4)
C(43a)	0.100(7)	0.052(3)	0.066(3)	−0.016(2)	0.017(5)	−0.031(5)
C(45a)	0.085(7)	0.063(4)	0.063(3)	0.020(3)	0.018(4)	−0.014(4)
C(46a)	0.077(5)	0.044(4)	0.046(2)	0.005(2)	0.009(2)	−0.012(3)
C(42b)	0.095(8)	0.040(3)	0.063(5)	0.007(3)	−0.003(4)	−0.004(4)
C(43b)	0.087(7)	0.051(3)	0.083(5)	0.000(3)	0.005(5)	−0.028(5)
C(45b)	0.080(6)	0.063(5)	0.091(7)	0.045(5)	0.016(4)	0.006(4)
C(46b)	0.069(5)	0.056(5)	0.065(6)	0.013(4)	−0.004(4)	−0.007(4)
N(5a)	0.0537(8)	0.0576(9)	0.0456(7)	−0.0046(6)	0.0100(6)	0.0089(7)
N(6a)	0.0743(13)	0.0957(15)	0.0506(10)	−0.0149(9)	0.0080(9)	0.0306(11)
C(1a)	0.0843(17)	0.0803(15)	0.0492(11)	−0.0143(10)	0.0046(11)	0.0132(13)
C(2a)	0.0665(12)	0.0627(11)	0.0547(10)	−0.0046(8)	−0.0045(9)	0.0050(9)
C(3a)	0.0529(11)	0.0430(9)	0.0563(11)	−0.0006(8)	0.0093(9)	−0.0020(8)
C(4a)	0.146(3)	0.177(4)	0.0609(16)	−0.0392(19)	0.0121(18)	0.057(3)
C(5a)	0.0629(14)	0.0789(15)	0.0777(15)	−0.0012(12)	0.0175(11)	0.0150(12)
N(b)	0.0537(8)	0.0576(9)	0.0456(7)	−0.0046(6)	0.0100(6)	0.0089(7)
N(6b)	0.049(4)	0.055(4)	0.047(4)	−0.005(4)	0.014(4)	0.009(4)
C(1b)	0.056(4)	0.059(4)	0.053(4)	−0.002(4)	0.006(4)	0.006(4)
C(2b)	0.0665(12)	0.0627(11)	0.0547(10)	−0.0046(8)	−0.0045(9)	0.0050(9)
C(3b)	0.060(3)	0.061(3)	0.050(3)	−0.004(3)	0.004(3)	0.007(3)
C(4b)	0.063(8)	0.075(8)	0.057(8)	0.000(7)	−0.003(7)	0.008(8)
C(5b)	0.076(9)	0.078(8)	0.054(8)	−0.002(8)	0.007(7)	0.010(8)

[a]The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2\,\pi\,[h^2\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12}]$.

Table S6. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(Hdmpz)][a]

atom	x	y	z	U(eq)
H(b1)	0.3587	0.2943	0.9074	0.061
H(b2)	0.1981	0.2616	0.9841	0.060
H(b3)	0.0523	0.1003	1.0318	0.062
H(b4)	0.1159	0.0281	0.9837	0.064
H(b5)	0.4509	−0.0327	0.7817	0.063
H(b6)	0.6149	−0.0001	0.7090	0.064
H(b7)	0.7543	0.1620	0.6522	0.062
H(b8)	0.6868	0.2340	0.6970	0.062
H(12)	−0.0597	0.1856	0.8704	0.084
H(13)	−0.2070	0.2122	0.9551	0.104
H(14)	−0.1566	0.2308	1.1504	0.089
H(15)	0.0396	0.2218	1.2637	0.084
H(16)	0.1890	0.1953	1.1807	0.070
H(22)	0.3886	−0.0400	1.0058	0.074
H(23)	0.3076	−0.1080	1.0156	0.094
H(24)	0.1264	−0.1280	0.8855	0.100
H(25)	0.0235	−0.0797	0.7457	0.102
H(26)	0.1002	−0.0112	0.7360	0.076
H(32)	0.8638	0.0922	0.7922	0.071
H(33)	1.0153	0.0701	0.7058	0.087
H(34)	0.9646	0.0393	0.5219	0.094
H(35)	0.7615	0.0283	0.4242	0.093
H(36)	0.6082	0.0505	0.5084	0.073
H(44)	0.6467	0.3922	0.7597	0.088
H(42a)	0.6160	0.2903	0.9605	0.073
H(43a)	0.6781	0.3589	0.9391	0.088
H(45a)	0.5363	0.3538	0.5948	0.085
H(46a)	0.4603	0.2841	0.6134	0.068
H(42b)	0.6808	0.2819	0.9374	0.085
H(43b)	0.7490	0.3529	0.9189	0.092
H(45b)	0.4764	0.3658	0.6236	0.095
H(46b)	0.4163	0.2974	0.6415	0.081
H(6aa)	0.3839	0.0997	0.5637	0.090
H(2aa)	0.0724	0.1436	0.3828	0.078

Table S6. Continued

atom	x	y	z	U(eq)
H(4aa)	0.3693	0.0966	0.3502	0.196
H(4ab)	0.2463	0.1122	0.2632	0.196
H(4ac)	0.2538	0.0664	0.3220	0.196
H(5aa)	0.0584	0.1540	0.6825	0.110
H(5ab)	−0.0004	0.1777	0.5627	0.110
H(5ac)	0.1145	0.1977	0.6527	0.110
H(6ba)	0.1264	0.1665	0.6813	0.060
H(2ba)	0.1103	0.1312	0.3628	0.078
H(4ba)	−0.0620	0.1933	0.5500	0.103
H(4bb)	−0.1156	0.1513	0.4797	0.103
H(4bc)	−0.0738	0.1904	0.4142	0.103
H(5ba)	0.4231	0.0986	0.5617	0.107
H(5bb)	0.3846	0.1177	0.4336	0.107
H(5bc)	0.3307	0.0733	0.4605	0.107

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor the estimated standard deviations of the least significant digits are given in parentheses.

Table S7. Complete Crystallographic Details for [Fe(T*p*-OCH_3PP)(Hdmpz)]

formula	$C_{60}H_{52}FeN_6O_4$
FW, amu	976.93
a, Å	11.9585(3)
b, Å	35.4853(9)
c, Å	11.9857(3)
β, deg	106.9490(10)
V, Å^3	4865.2(2)
space group	$P2_1/c$
Z	4
D_c, g/cm^3	1.334
F(000)	2048
μ, mm^{-1}	0.367
crystal dimensions, mm	0.52 × 0.46 × 0.20
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.78–28.46
index range	$-15 \leq h \leq 15$
	$-47 \leq k \leq 47$
	$-15 \leq l \leq 16$
total data collected	86053
absorption correction	Semi-empirical from equivalents
relative transmission coefficients (I)	0.9303 and 0.8322
unique data	12075 (R_{int} = 0.048)
unique observed data [I > 2σ(I)]	10028
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	12075/58/692
goodness-of-fit (pased on F^2)	1.028
final R indices [I > 2σ(I)]	R_1 = 0.0428, wR_2 = 0.1047
final R indices (all data)	R_1 = 0.0554, wR_2 = 0.1132

Table S8. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(T*p*-OCH$_3$PP)(Hdmpz)][a]

atom	x	y	z	U(eq)
Fe(1)	0.63725(2)	0.14483(1)	0.21371(2)	0.0162(1)
N(1)	0.56250(12)	0.09290(4)	0.22528(11)	0.0177(3)
N(2)	0.49539(13)	0.17051(4)	0.24516(12)	0.0194(3)
N(3)	0.67946(12)	0.19597(4)	0.15224(11)	0.0174(3)
N(4)	0.74507(12)	0.11836(4)	0.13033(12)	0.0179(3)
C(a1)	0.60159(14)	0.05820(4)	0.20197(13)	0.0176(3)
C(a2)	0.46702(14)	0.08643(4)	0.26378(13)	0.0177(3)
C(a3)	0.41316(15)	0.15318(4)	0.28708(14)	0.0197(3)
C(a4)	0.47883(15)	0.20867(5)	0.25315(15)	0.0214(3)
C(a5)	0.63708(14)	0.23053(4)	0.17130(13)	0.0171(3)
C(a6)	0.77103(14)	0.20272(4)	0.10753(13)	0.0175(3)
C(a7)	0.82477(14)	0.13568(4)	0.08411(13)	0.0177(3)
C(a8)	0.75982(14)	0.08020(4)	0.12091(13)	0.0175(3)
C(b1)	0.52851(15)	0.02901(4)	0.22837(14)	0.0201(3)
C(b2)	0.44595(14)	0.04633(4)	0.26670(14)	0.0187(3)
C(b3)	0.34360(16)	0.18121(5)	0.32291(16)	0.0247(4)
C(b4)	0.38405(17)	0.21529(5)	0.30159(16)	0.0260(4)
C(b5)	0.70399(15)	0.25993(4)	0.13709(14)	0.0203(3)
C(b6)	0.78682(15)	0.24286(5)	0.09850(14)	0.0205(3)
C(b7)	0.89118(14)	0.10741(5)	0.04469(14)	0.0197(3)
C(b8)	0.85205(14)	0.07333(5)	0.06896(14)	0.0192(3)
C(m1)	0.39836(14)	0.11412(4)	0.29476(13)	0.0180(3)
C(m2)	0.54476(14)	0.23671(4)	0.21928(14)	0.0181(3)
C(m3)	0.83945(14)	0.17495(4)	0.07544(13)	0.0176(3)
C(m4)	0.69433(14)	0.05179(4)	0.15579(13)	0.0175(3)
C(11)	0.30321(14)	0.10178(4)	0.34448(14)	0.0176(3)
C(12)	0.32907(15)	0.09513(5)	0.46370(14)	0.0210(3)
C(13)	0.24267(15)	0.08639(5)	0.51449(14)	0.0221(3)
C(14)	0.12704(14)	0.08408(5)	0.44600(15)	0.0203(3)
C(15)	0.09919(15)	0.09013(5)	0.32693(15)	0.0219(3)
C(16)	0.18778(15)	0.09879(5)	0.27701(14)	0.0217(3)
O(1)	0.04737(11)	0.07545(4)	0.50391(11)	0.0284(3)
C(17)	−0.07048(16)	0.06947(6)	0.43572(17)	0.0297(4)
C(21)	0.51495(14)	0.27691(4)	0.23661(14)	0.0184(3)

Table S8. Continued

atom	x	y	z	U(eq)
C(22)	0.4270(2)	0.29596(5)	0.15451(16)	0.0362(5)
C(23)	0.4011(2)	0.33303(5)	0.17214(17)	0.0379(5)
C(24)	0.46318(15)	0.35206(4)	0.27226(15)	0.0209(3)
C(25)	0.55114(15)	0.33375(5)	0.35435(15)	0.0225(3)
C(26)	0.57496(14)	0.29619(5)	0.33530(15)	0.0222(3)
O(2)	0.42924(11)	0.38856(3)	0.28160(11)	0.0274(3)
C(27)	0.48252(17)	0.40759(5)	0.38848(16)	0.0289(4)
C(31)	0.93539(14)	0.18751(4)	0.02760(14)	0.0190(3)
C(32)	0.91281(15)	0.20575(5)	−0.07982(15)	0.0222(3)
C(33)	1.00294(16)	0.21528(5)	−0.12547(16)	0.0254(4)
C(34)	1.11795(16)	0.20623(5)	−0.06375(17)	0.0260(4)
C(35)	1.14221(16)	0.18927(5)	0.04409(17)	0.0272(4)
C(36)	1.05097(15)	0.18027(5)	0.08896(15)	0.0237(3)
O(3)	0.84811(13)	−0.09546(3)	0.09432(11)	0.0319(3)
C(37)	1.3141(2)	0.19776(6)	−0.0665(3)	0.0477(6)
C(41)	0.72765(14)	0.01185(4)	0.14094(14)	0.0183(3)
C(42)	0.70925(16)	−0.00432(5)	0.03082(14)	0.0226(3)
C(43)	0.74786(16)	−0.04031(5)	0.01796(15)	0.0250(4)
C(44)	0.80714(15)	−0.06100(4)	0.11570(15)	0.0219(3)
C(45)	0.82289(15)	−0.04612(4)	0.22578(14)	0.0204(3)
C(46)	0.78186(14)	−0.01004(4)	0.23727(14)	0.0192(3)
O(4)	1.20110(13)	0.21439(4)	−0.11802(13)	0.0354(3)
C(47)	0.9154(2)	−0.11575(6)	0.19374(19)	0.0446(6)
N(5a)	0.76474(17)	0.15476(6)	0.37827(16)	0.0224(4)
N(6a)	0.87217(15)	0.16826(5)	0.37985(15)	0.0272(4)
C(1a)	0.94266(18)	0.17329(5)	0.48863(18)	0.0285(5)
C(2a)	0.8782(2)	0.16295(7)	0.56165(19)	0.0278(4)
C(3a)	0.76900(18)	0.15166(5)	0.49007(16)	0.0233(4)
C(4a)	1.0654(2)	0.18733(7)	0.5119(2)	0.0424(6)
C(5a)	0.6662(2)	0.13797(6)	0.52419(19)	0.0337(5)
N(5b)	0.7570(12)	0.1497(5)	0.3898(8)	0.023(4)
N(6b)	0.7104(10)	0.1377(4)	0.4766(10)	0.021(3)
C(1b)	0.7824(10)	0.1448(3)	0.5839(9)	0.023(3)
C(2b)	0.8807(11)	0.1616(5)	0.5688(10)	0.0278(4)

Table S8. Continued

atom	x	y	z	U(eq)
C(3b)	0.8611(11)	0.1642(3)	0.4465(10)	0.024(3)
C(4b)	0.7491(15)	0.1345(5)	0.6921(10)	0.032(4)
C(5b)	0.9396(15)	0.1797(5)	0.3828(15)	0.033(4)
C(1S)	0.18843(16)	−0.02218(5)	0.26071(16)	0.0276(4)
C(2S)	0.20865(18)	−0.00695(5)	0.37103(17)	0.0295(4)
C(3S)	0.31100(19)	−0.01413(5)	0.45758(17)	0.0315(4)
C(4S)	0.39619(18)	−0.03659(5)	0.43576(16)	0.0308(4)
C(5S)	0.37736(18)	−0.05249(5)	0.32677(17)	0.0302(4)
C(6S)	0.27389(17)	−0.04561(5)	0.24029(16)	0.0291(4)
C(7S)	0.07959(18)	−0.01277(7)	0.16492(19)	0.0385(5)

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S9. Bond Lengths for [Fe(T*p*-OCH_3PP)(Hdmpz)][a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(2)	2.0548(14)	C(31)–C(36)	1.387(2)
Fe(1)–N(1)	2.0704(13)	C(31)–C(32)	1.395(2)
Fe(1)–N(4)	2.0724(14)	C(32)–C(33)	1.386(2)
Fe(1)–N(3)	2.0755(13)	C(32)–H(32a)	0.9500
Fe(1)–N(5a)	2.1414(18)	C(33)–C(34)	1.396(3)
Fe(1)–N(5b)	2.185(10)	C(33)–H(33a)	0.9500
N(1)–C(a2)	1.370(2)	C(34)–O(4)	1.368(2)
N(1)–C(a1)	1.374(2)	C(34)–C(35)	1.378(3)
N(2)–C(a3)	1.373(2)	C(35)–C(36)	1.387(2)
N(2)–C(a4)	1.376(2)	C(35)–H(35a)	0.9500
N(3)–C(a5)	1.371(2)	C(36)–H(36a)	0.9500
N(3)–C(a6)	1.373(2)	O(3)–C(44)	1.3693(19)
N(4)–C(a8)	1.374(2)	O(3)–C(47)	1.424(2)
N(4)–C(a7)	1.379(2)	C(37)–O(4)	1.439(3)
C(a1)–C(m4)	1.395(2)	C(37)–H(37a)	0.9800
C(a1)–C(b1)	1.449(2)	C(37)–H(37b)	0.9800
C(a2)–C(m1)	1.398(2)	C(37)–H(37c)	0.9800
C(a2)–C(b2)	1.447(2)	C(41)–C(46)	1.386(2)
C(a3)–C(m1)	1.404(2)	C(41)–C(42)	1.397(2)
C(a3)–C(b3)	1.440(2)	C(42)–C(43)	1.382(2)
C(a4)–C(m2)	1.401(2)	C(42)–H(42a)	0.9500
C(a4)–C(b4)	1.435(2)	C(43)–C(44)	1.389(2)
C(a5)–C(m2)	1.403(2)	C(43)–H(43a)	0.9500
C(a5)–C(b5)	1.445(2)	C(44)–C(45)	1.382(2)
C(a6)–C(m3)	1.404(2)	C(45)–C(46)	1.392(2)
C(a6)–C(b6)	1.445(2)	C(45)–H(45a)	0.9500
C(a7)–C(m3)	1.412(2)	C(46)–H(46a)	0.9500
C(a7)–C(b7)	1.442(2)	C(47)–H(47a)	0.9800
C(a8)–C(m4)	1.413(2)	C(47)–H(47b)	0.9800
C(a8)–C(b8)	1.437(2)	C(47)–H(47c)	0.9800
C(b1)–C(b2)	1.352(2)	N(5a)–C(3a)	1.331(3)
C(b1)–H(b1)	0.9500	N(5a)–N(6a)	1.366(3)
C(b2)–H(b2)	0.9500	N(6a)–C(1a)	1.342(3)
C(b3)–C(b4)	1.354(2)	N(6a)–H(6a)	0.8800

Table S9. Continued

bond	length (Å)	bond	length (Å)
C(b3)–H(b3)	0.9500	C(1a)–C(2a)	1.374(3)
C(b4)–H(b4)	0.9500	C(1a)–C(4a)	1.497(3)
C(b5)–C(b6)	1.352(2)	C(2a)–C(3a)	1.396(3)
C(b5)–H(b5)	0.9500	C(2a)–H(2a)	0.9500
C(b6)–H(b6)	0.9500	C(3a)–C(5a)	1.486(3)
C(b7)–C(b8)	1.358(2)	C(4a)–H(4a1)	0.9800
C(b7)–H(b7)	0.9500	C(4a)–H(4a2)	0.9800
C(b8)–H(b8)	0.9500	C(4a)–H(4a3)	0.9800
C(m1)–C(11)	1.496(2)	C(5a)–H(5a1)	0.9800
C(m2)–C(21)	1.499(2)	C(5a)–H(5a2)	0.9800
C(m3)–C(31)	1.492(2)	C(5a)–H(5a3)	0.9800
C(m4)–C(41)	1.497(2)	N(5b)–C(3b)	1.3337
C(11)–C(16)	1.386(2)	N(5b)–N(6b)	1.3830
C(11)–C(12)	1.391(2)	N(6b)–C(1b)	1.3473
C(12)–C(13)	1.379(2)	N(6b)–H(6ba)	0.8800
C(12)–H(12a)	0.9500	C(1b)–C(2b)	1.3765
C(13)–C(14)	1.390(2)	C(1b)–C(4b)	1.5089
C(13)–H(13a)	0.9500	C(2b)–C(3b)	1.4181
C(14)–O(1)	1.367(2)	C(2b)–H(2ba)	0.9500
C(14)–C(15)	1.384(2)	C(3b)–C(5b)	1.4788
C(15)–C(16)	1.394(2)	C(4b)–H(4b1)	0.9800
C(15)–H(15a)	0.9500	C(4b)–H(4b2)	0.9800
C(16)–H(16a)	0.9500	C(4b)–H(4b3)	0.9800
O(1)–C(17)	1.424(2)	C(5b)–H(5b1)	0.9800
C(17)–H(17a)	0.9800	C(5b)–H(5b2)	0.9800
C(17)–H(17b)	0.9800	C(5b)–H(5b3)	0.9800
C(17)–H(17c)	0.9800	C(1S)–C(2S)	1.383(3)
C(21)–C(26)	1.374(2)	C(1S)–C(6S)	1.393(3)
C(21)–C(22)	1.389(2)	C(1S)–C(7S)	1.501(3)
C(22)–C(23)	1.381(3)	C(2S)–C(3S)	1.378(3)
C(22)–H(22a)	0.9500	C(2S)–H(2Sa)	0.9500
C(23)–C(24)	1.389(2)	C(3S)–C(4S)	1.377(3)
C(23)–H(23a)	0.9500	C(3S)–H(3Sa)	0.9500
C(24)–O(2)	1.3715(19)	C(4S)–C(5S)	1.380(3)

Table S9. Continued

bond	length (Å)	bond	length (Å)
C(24)–C(25)	1.376(2)	C(4S)–H(4Sa)	0.9500
C(25)–C(26)	1.396(2)	C(5S)–C(6S)	1.385(3)
C(25)–H(25a)	0.9500	C(5S)–H(5Sa)	0.9500
C(26)–H(26a)	0.9500	C(6S)–H(6Sa)	0.9500
O(2)–C(27)	1.424(2)	C(7S)–H(7S1)	0.9800
C(27)–H(27a)	0.9800	C(7S)–H(7S2)	0.9800
C(27)–H(27b)	0.9800	C(7S)–H(7S3)	0.9800
C(27)–H(27c)	0.9800		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S10. Bond Angles for [Fe(T*p*-OCH_3PP)(Hdmpz)][a]

angle	degree	angle	degree
N(2)–Fe(1)–N(1)	89.24(5)	O(2)–C(24)–C(25)	124.77(15)
N(2)–Fe(1)–N(4)	162.24(5)	O(2)–C(24)–C(23)	115.69(15)
N(1)–Fe(1)–N(4)	88.30(5)	C(25)–C(24)–C(23)	119.54(15)
N(2)–Fe(1)–N(3)	88.67(5)	C(24)–C(25)–C(26)	118.94(15)
N(1)–Fe(1)–N(3)	163.03(5)	C(24)–C(25)–H(25a)	120.5
N(4)–Fe(1)–N(3)	88.58(5)	C(26)–C(25)–H(25a)	120.5
N(2)–Fe(1)–N(5a)	99.34(7)	C(21)–C(26)–C(25)	122.42(15)
N(1)–Fe(1)–N(5a)	106.87(6)	C(21)–C(26)–H(26a)	118.8
N(4)–Fe(1)–N(5a)	98.21(7)	C(25)–C(26)–H(26a)	118.8
N(3)–Fe(1)–N(5a)	90.09(6)	C(24)–O(2)–C(27)	117.12(13)
N(2)–Fe(1)–N(5b)	97.5(4)	O(2)–C(27)–H(27a)	109.5
N(1)–Fe(1)–N(5b)	100.4(4)	O(2)–C(27)–H(27b)	109.5
N(4)–Fe(1)–N(5b)	100.2(4)	H(27a)–C(27)–H(27b)	109.5
N(3)–Fe(1)–N(5b)	96.6(4)	O(2)–C(27)–H(27c)	109.5
N(5a)–Fe(1)–N(5b)	6.8(4)	H(27a)–C(27)–H(27c)	109.5
C(a2)–N(1)–C(a1)	106.53(13)	H(27b)–C(27)–H(27c)	109.5
C(a2)–N(1)–Fe(1)	126.18(10)	C(36)–C(31)–C(32)	118.03(15)
C(a1)–N(1)–Fe(1)	127.22(11)	C(36)–C(31)–C(m3)	119.98(15)
C(a3)–N(2)–C(a4)	106.39(13)	C(32)–C(31)–C(m3)	121.96(15)
C(a3)–N(2)–Fe(1)	125.89(11)	C(33)–C(32)–C(31)	120.94(16)
C(a4)–N(2)–Fe(1)	126.32(11)	C(33)–C(32)–H(32a)	119.5
C(a5)–N(3)–C(a6)	106.54(13)	C(31)–C(32)–H(32a)	119.5
C(a5)–N(3)–Fe(1)	125.65(11)	C(32)–C(33)–C(34)	119.62(16)
C(a6)–N(3)–Fe(1)	126.52(10)	C(32)–C(33)–H(33a)	120.2
C(a8)–N(4)–C(a7)	106.61(13)	C(34)–C(33)–H(33a)	120.2
C(a8)–N(4)–Fe(1)	126.80(11)	O(4)–C(34)–C(35)	123.69(17)
C(a7)–N(4)–Fe(1)	126.29(10)	O(4)–C(34)–C(33)	116.08(17)
N(1)–C(a1)–C(m4)	125.70(14)	C(35)–C(34)–C(33)	120.21(16)
N(1)–C(a1)–C(b1)	109.49(14)	C(34)–C(35)–C(36)	119.34(17)
C(m4)–C(a1)–C(b1)	124.76(14)	C(34)–C(35)–H(35a)	120.3
N(1)–C(a2)–C(m1)	125.67(14)	C(36)–C(35)–H(35a)	120.3
N(1)–C(a2)–C(b2)	109.95(14)	C(35)–C(36)–C(31)	121.77(16)
C(m1)–C(a2)–C(b2)	124.38(15)	C(35)–C(36)–H(36a)	119.1
N(2)–C(a3)–C(m1)	125.70(15)	C(31)–C(36)–H(36a)	119.1

Table S10. Continued

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	109.72(14)	C(44)–O(3)–C(47)	116.16(14)
C(m1)–C(a3)–C(b3)	124.58(15)	O(4)–C(37)–H(37a)	109.5
N(2)–C(a4)–C(m2)	125.04(15)	O(4)–C(37)–H(37b)	109.5
N(2)–C(a4)–C(b4)	109.63(14)	H(37a)–C(37)–H(37b)	109.5
C(m2)–C(a4)–C(b4)	125.33(15)	O(4)–C(37)–H(37c)	109.5
N(3)–C(a5)–C(m2)	125.55(14)	H(37a)–C(37)–H(37c)	109.5
N(3)–C(a5)–C(b5)	109.65(14)	H(37b)–C(37)–H(37c)	109.5
C(m2)–C(a5)–C(b5)	124.78(14)	C(46)–C(41)–C(42)	117.62(14)
N(3)–C(a6)–C(m3)	125.40(14)	C(46)–C(41)–C(m4)	120.52(14)
N(3)–C(a6)–C(b6)	109.72(14)	C(42)–C(41)–C(m4)	121.82(14)
C(m3)–C(a6)–C(b6)	124.88(15)	C(43)–C(42)–C(41)	121.29(15)
N(4)–C(a7)–C(m3)	125.79(14)	C(43)–C(42)–H(42a)	119.4
N(4)–C(a7)–C(b7)	109.43(14)	C(41)–C(42)–H(42a)	119.4
C(m3)–C(a7)–C(b7)	124.78(15)	C(42)–C(43)–C(44)	119.96(16)
N(4)–C(a8)–C(m4)	125.68(15)	C(42)–C(43)–H(43a)	120.0
N(4)–C(a8)–C(b8)	109.63(14)	C(44)–C(43)–H(43a)	120.0
C(m4)–C(a8)–C(b8)	124.68(14)	O(3)–C(44)–C(45)	124.28(15)
C(b2)–C(b1)–C(a1)	107.22(14)	O(3)–C(44)–C(43)	115.89(15)
C(b2)–C(b1)–H(b1)	126.4	C(45)–C(44)–C(43)	119.82(15)
C(a1)–C(b1)–H(b1)	126.4	C(44)–C(45)–C(46)	119.46(15)
C(b1)–C(b2)–C(a2)	106.81(14)	C(44)–C(45)–H(45a)	120.3
C(b1)–C(b2)–H(b2)	126.6	C(46)–C(45)–H(45a)	120.3
C(a2)–C(b2)–H(b2)	126.6	C(41)–C(46)–C(45)	121.73(15)
C(b4)–C(b3)–C(a3)	106.94(15)	C(41)–C(46)–H(46a)	119.1
C(b4)–C(b3)–H(b3)	126.5	C(45)–C(46)–H(46a)	119.1
C(a3)–C(b3)–H(b3)	126.5	C(34)–O(4)–C(37)	115.55(15)
C(b3)–C(b4)–C(a4)	107.32(15)	O(3)–C(47)–H(47a)	109.5
C(b3)–C(b4)–H(b4)	126.3	O(3)–C(47)–H(47b)	109.5
C(a4)–C(b4)–H(b4)	126.3	H(47a)–C(47)–H(47b)	109.5
C(b6)–C(b5)–C(a5)	107.16(14)	O(3)–C(47)–H(47c)	109.5
C(b6)–C(b5)–H(b5)	126.4	H(47a)–C(47)–H(47c)	109.5
C(a5)–C(b5)–H(b5)	126.4	H(47b)–C(47)–H(47c)	109.5
C(b5)–C(b6)–C(a6)	106.93(14)	C(3a)–N(5a)–N(6a)	104.79(17)
C(b5)–C(b6)–H(b6)	126.5	C(3a)–N(5a)–Fe(1)	136.21(16)

Table S10. Continued

angle	degree	angle	degree
C(a6)–C(b6)–H(b6)	126.5	N(6a)–N(5a)–Fe(1)	118.99(13)
C(b8)–C(b7)–C(a7)	106.99(14)	C(1a)–N(6a)–N(5a)	112.45(18)
C(b8)–C(b7)–H(b7)	126.5	C(1a)–N(6a)–H(6a)	123.8
C(a7)–C(b7)–H(b7)	126.5	N(5a)–N(6a)–H(6a)	123.8
C(b7)–C(b8)–C(a8)	107.32(14)	N(6a)–C(1a)–C(2a)	105.86(18)
C(b7)–C(b8)–H(b8)	126.3	N(6a)–C(1a)–C(4a)	122.0(2)
C(a8)–C(b8)–H(b8)	126.3	C(2a)–C(1a)–C(4a)	132.2(2)
C(a2)–C(m1)–C(a3)	125.55(15)	C(1a)–C(2a)–C(3a)	106.45(19)
C(a2)–C(m1)–C(11)	118.28(14)	C(1a)–C(2a)–H(2a)	126.8
C(a3)–C(m1)–C(11)	116.13(14)	C(3a)–C(2a)–H(2a)	126.8
C(a4)–C(m2)–C(a5)	125.76(14)	N(5a)–C(3a)–C(2a)	110.5(2)
C(a4)–C(m2)–C(21)	117.32(14)	N(5a)–C(3a)–C(5a)	120.82(19)
C(a5)–C(m2)–C(21)	116.92(14)	C(2a)–C(3a)–C(5a)	128.73(19)
C(a6)–C(m3)–C(a7)	125.27(15)	C(3b)–N(5b)–N(6b)	104.9
C(a6)–C(m3)–C(31)	118.06(14)	C(3b)–N(5b)–Fe(1)	140.7(6)
C(a7)–C(m3)–C(31)	116.67(14)	N(6b)–N(5b)–Fe(1)	114.0(6)
C(a1)–C(m4)–C(a8)	125.06(14)	C(1b)–N(6b)–N(5b)	111.9
C(a1)–C(m4)–C(41)	118.13(14)	C(1b)–N(6b)–H(6ba)	124.0
C(a8)–C(m4)–C(41)	116.80(14)	N(5b)–N(6b)–H(6ba)	124.0
C(16)–C(11)–C(12)	118.15(15)	N(6b)–C(1b)–C(2b)	106.8
C(16)–C(11)–C(m1)	122.28(14)	N(6b)–C(1b)–C(4b)	121.3
C(12)–C(11)–C(m1)	119.46(15)	C(2b)–C(1b)–C(4b)	131.9
C(13)–C(12)–C(11)	121.39(15)	C(1b)–C(2b)–C(3b)	105.8
C(13)–C(12)–H(12a)	119.3	C(1b)–C(2b)–H(2ba)	127.1
C(11)–C(12)–H(12a)	119.3	C(3b)–C(2b)–H(2ba)	127.1
C(12)–C(13)–C(14)	119.81(15)	N(5b)–C(3b)–C(2b)	110.5
C(12)–C(13)–H(13a)	120.1	N(5b)–C(3b)–C(5b)	121.3
C(14)–C(13)–H(13a)	120.1	C(2b)–C(3b)–C(5b)	128.2
O(1)–C(14)–C(15)	124.36(15)	C(2S)–C(1S)–C(6S)	117.93(18)
O(1)–C(14)–C(13)	115.72(15)	C(2S)–C(1S)–C(7S)	121.02(18)
C(15)–C(14)–C(13)	119.92(15)	C(6S)–C(1S)–C(7S)	121.02(17)
C(14)–C(15)–C(16)	119.47(15)	C(3S)–C(2S)–C(1S)	121.12(18)
C(14)–C(15)–H(15a)	120.3	C(3S)–C(2S)–H(2Sa)	119.4
C(16)–C(15)–H(15a)	120.3	C(1S)–C(2S)–H(2Sa)	119.4

Table S10. Continued

angle	degree	angle	degree
C(11)–C(16)–C(15)	121.25(15)	C(4S)–C(3S)–C(2S)	120.53(18)
C(11)–C(16)–H(16a)	119.4	C(4S)–C(3S)–H(3Sa)	119.7
C(15)–C(16)–H(16a)	119.4	C(2S)–C(3S)–H(3Sa)	119.7
C(14)–O(1)–C(17)	117.49(14)	C(3S)–C(4S)–C(5S)	119.39(18)
O(1)–C(17)–H(17a)	109.5	C(3S)–C(4S)–H(4Sa)	120.3
O(1)–C(17)–H(17b)	109.5	C(5S)–C(4S)–H(4Sa)	120.3
H(17a)–C(17)–H(17b)	109.5	C(4S)–C(5S)–C(6S)	120.00(18)
O(1)–C(17)–H(17c)	109.5	C(4S)–C(5S)–H(5Sa)	120.0
H(17a)–C(17)–H(17c)	109.5	C(6S)–C(5S)–H(5Sa)	120.0
H(17b)–C(17)–H(17c)	109.5	C(5S)–C(6S)–C(1S)	120.99(18)
C(26)–C(21)–C(22)	117.73(15)	C(5S)–C(6S)–H(6Sa)	119.5
C(26)–C(21)–C(m2)	120.49(15)	C(1S)–C(6S)–H(6Sa)	119.5
C(22)–C(21)–C(m2)	121.78(15)	C(1S)–C(7S)–H(7S1)	109.5
C(23)–C(22)–C(21)	120.81(17)	C(1S)–C(7S)–H(7S2)	109.5
C(23)–C(22)–H(22a)	119.6	H(7S1)–C(7S)–H(7S2)	109.5
C(21)–C(22)–H(22a)	119.6	C(1S)–C(7S)–H(7S3)	109.5
C(22)–C(23)–C(24)	120.55(17)	H(7S1)–C(7S)–H(7S3)	109.5
C(22)–C(23)–H(23a)	119.7	H(7S2)–C(7S)–H(7S3)	109.5
C(24)–C(23)–H(23a)	119.7		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S11. Anisotropic Displacement Parameters (Å^2) for [Fe(T*p*-OCH_3PP)(Hdmpz)][a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0184(1)	0.0120(1)	0.0182(1)	0.0005(1)	0.0054(1)	0.0001(1)
N(1)	0.0200(7)	0.0138(6)	0.0197(6)	0.0005(5)	0.0064(5)	−0.0002(5)
N(2)	0.0238(7)	0.0131(6)	0.0232(7)	0.0011(5)	0.0097(5)	0.0000(5)
N(3)	0.0176(7)	0.0160(6)	0.0182(6)	0.0006(5)	0.0049(5)	0.0001(5)
N(4)	0.0183(7)	0.0151(6)	0.0197(6)	0.0012(5)	0.0046(5)	−0.0002(5)
C(a1)	0.0199(8)	0.0134(7)	0.0181(7)	0.0001(5)	0.0035(6)	−0.0008(6)
C(a2)	0.0193(8)	0.0162(7)	0.0166(7)	0.0016(5)	0.0034(6)	−0.0012(6)
C(a3)	0.0220(8)	0.0165(7)	0.0225(8)	0.0008(6)	0.0095(6)	−0.0001(6)
C(a4)	0.0261(9)	0.0163(7)	0.0242(8)	−0.0008(6)	0.0109(7)	0.0004(6)
C(a5)	0.0189(8)	0.0138(7)	0.0173(7)	0.0002(5)	0.0036(6)	−0.0011(6)
C(a6)	0.0174(8)	0.0158(7)	0.0179(7)	0.0015(6)	0.0029(6)	−0.0018(6)
C(a7)	0.0173(8)	0.0186(7)	0.0163(7)	0.0009(6)	0.0034(6)	0.0001(6)
C(a8)	0.0182(8)	0.0156(7)	0.0170(7)	0.0005(5)	0.0026(6)	0.0020(6)
C(b1)	0.0219(8)	0.0142(7)	0.0224(8)	0.0008(6)	0.0036(6)	−0.0017(6)
C(b2)	0.0201(8)	0.0160(7)	0.0186(7)	0.0011(6)	0.0033(6)	−0.0025(6)
C(b3)	0.0291(10)	0.0189(8)	0.0313(9)	0.0005(7)	0.0173(7)	0.0010(7)
C(b4)	0.0328(10)	0.0171(8)	0.0336(9)	0.0001(7)	0.0184(8)	0.0015(7)
C(b5)	0.0222(8)	0.0146(7)	0.0240(8)	0.0002(6)	0.0066(6)	−0.0030(6)
C(b6)	0.0205(8)	0.0175(7)	0.0225(8)	0.0001(6)	0.0049(6)	−0.0033(6)
C(b7)	0.0191(8)	0.0201(7)	0.0191(7)	−0.0001(6)	0.0047(6)	0.0020(6)
C(b8)	0.0189(8)	0.0189(7)	0.0192(7)	−0.0008(6)	0.0046(6)	0.0027(6)
C(m1)	0.0199(8)	0.0159(7)	0.0181(7)	0.0017(6)	0.0057(6)	−0.0009(6)
C(m2)	0.0218(8)	0.0136(7)	0.0189(7)	−0.0009(6)	0.0059(6)	0.0004(6)
C(m3)	0.0160(8)	0.0188(7)	0.0170(7)	0.0019(6)	0.0030(6)	−0.0010(6)
C(m4)	0.0201(8)	0.0141(7)	0.0164(7)	0.0002(5)	0.0023(6)	0.0015(6)
C(11)	0.0195(8)	0.0121(7)	0.0224(8)	0.0004(6)	0.0078(6)	−0.0002(6)
C(12)	0.0166(8)	0.0226(8)	0.0219(8)	0.0013(6)	0.0028(6)	−0.0023(6)
C(13)	0.0214(9)	0.0255(8)	0.0178(7)	0.0014(6)	0.0033(6)	−0.0041(7)
C(14)	0.0182(8)	0.0180(7)	0.0252(8)	0.0015(6)	0.0071(6)	−0.0027(6)
C(15)	0.0168(8)	0.0227(8)	0.0237(8)	0.0018(6)	0.0019(6)	−0.0025(6)
C(16)	0.0240(9)	0.0205(8)	0.0189(7)	0.0023(6)	0.0038(6)	−0.0002(6)
O(1)	0.0182(6)	0.0418(8)	0.0252(6)	0.0044(5)	0.0065(5)	−0.0078(5)
C(17)	0.0166(9)	0.0332(10)	0.0372(10)	0.0032(8)	0.0047(7)	−0.0058(7)
C(21)	0.0216(8)	0.0134(7)	0.0220(8)	0.0000(6)	0.0093(6)	−0.0002(6)

Table S11. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(22)	0.0577(14)	0.0170(8)	0.0218(9)	−0.0016(7)	−0.0074(8)	0.0048(8)
C(23)	0.0528(13)	0.0179(8)	0.0280(10)	0.0002(7)	−0.0117(9)	0.0089(8)
C(24)	0.0240(9)	0.0132(7)	0.0248(8)	−0.0001(6)	0.0061(6)	0.0004(6)
C(25)	0.0185(8)	0.0200(8)	0.0263(8)	−0.0074(6)	0.0021(6)	−0.0001(6)
C(26)	0.0160(8)	0.0192(8)	0.0280(9)	−0.0031(6)	0.0009(6)	0.0033(6)
O(2)	0.0314(7)	0.0141(5)	0.0304(7)	−0.0030(5)	−0.0010(5)	0.0043(5)
C(27)	0.0337(10)	0.0190(8)	0.0306(9)	−0.0065(7)	0.0039(7)	0.0022(7)
C(31)	0.0188(8)	0.0163(7)	0.0224(8)	−0.0005(6)	0.0066(6)	−0.0005(6)
C(32)	0.0218(9)	0.0201(8)	0.0245(8)	0.0028(6)	0.0065(6)	0.0018(6)
C(33)	0.0326(10)	0.0198(8)	0.0276(9)	0.0050(7)	0.0148(7)	0.0024(7)
C(34)	0.0287(10)	0.0174(8)	0.0381(10)	−0.0032(7)	0.0194(8)	−0.0025(7)
C(35)	0.0188(9)	0.0290(9)	0.0342(10)	0.0001(7)	0.0082(7)	0.0002(7)
C(36)	0.0200(9)	0.0264(8)	0.0238(8)	0.0027(7)	0.0051(6)	−0.0008(7)
O(3)	0.0440(8)	0.0172(6)	0.0296(7)	−0.0020(5)	0.0030(6)	0.0108(5)
C(37)	0.0395(13)	0.0344(11)	0.0856(18)	0.0172(11)	0.0440(13)	0.0099(9)
C(41)	0.0183(8)	0.0149(7)	0.0221(8)	0.0000(6)	0.0064(6)	−0.0003(6)
C(42)	0.0273(9)	0.0172(7)	0.0198(8)	0.0018(6)	0.0016(6)	0.0025(6)
C(43)	0.0316(10)	0.0198(8)	0.0210(8)	−0.0034(6)	0.0034(7)	0.0027(7)
C(44)	0.0234(9)	0.0133(7)	0.0274(8)	−0.0007(6)	0.0050(7)	0.0016(6)
C(45)	0.0218(8)	0.0167(7)	0.0217(8)	0.0040(6)	0.0046(6)	0.0011(6)
C(46)	0.0207(8)	0.0180(7)	0.0194(7)	0.0001(6)	0.0065(6)	0.0001(6)
O(4)	0.0356(8)	0.0289(7)	0.0530(9)	0.0085(6)	0.0306(7)	0.0034(6)
C(47)	0.0648(16)	0.0220(9)	0.0386(11)	0.0004(8)	0.0020(10)	0.0203(10)
N(5a)	0.0219(9)	0.0198(9)	0.0240(8)	0.0020(7)	0.0045(7)	−0.0008(7)
N(6a)	0.0217(9)	0.0296(9)	0.0280(9)	0.0033(7)	0.0037(7)	−0.0040(7)
C(1a)	0.0244(11)	0.0204(9)	0.0335(11)	−0.0001(8)	−0.0030(8)	0.0025(7)
C(2a)	0.0319(10)	0.0201(8)	0.0249(9)	−0.0013(7)	−0.0019(7)	0.0039(7)
C(3a)	0.0296(11)	0.0168(8)	0.0211(9)	−0.0002(7)	0.0039(7)	0.0037(7)
C(4a)	0.0260(12)	0.0391(13)	0.0516(15)	0.0022(11)	−0.0051(10)	−0.0052(9)
C(5a)	0.0400(13)	0.0366(11)	0.0254(10)	−0.0003(8)	0.0108(9)	−0.0077(9)
N(5b)	0.020(5)	0.024(6)	0.024(4)	0.000(4)	0.006(3)	0.003(4)
N(6b)	0.020(4)	0.019(5)	0.024(4)	0.003(4)	0.007(3)	0.005(4)
C(1b)	0.026(5)	0.021(5)	0.022(4)	−0.004(4)	0.005(3)	0.009(4)
C(2b)	0.0319(10)	0.0201(8)	0.0249(9)	−0.0013(7)	−0.0019(7)	0.0039(7)

Table S11. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(3b)	0.024(5)	0.020(5)	0.025(4)	0.000(4)	0.003(4)	0.002(4)
C(4b)	0.036(6)	0.033(6)	0.026(4)	−0.002(4)	0.006(4)	0.003(4)
C(5b)	0.031(6)	0.032(6)	0.034(5)	−0.001(4)	0.007(4)	−0.007(4)
C(1S)	0.0265(10)	0.0285(9)	0.0292(9)	0.0035(7)	0.0104(7)	−0.0039(7)
C(2S)	0.0358(11)	0.0229(8)	0.0348(10)	0.0006(7)	0.0180(8)	−0.0014(7)
C(3S)	0.0452(12)	0.0253(9)	0.0252(9)	−0.0007(7)	0.0121(8)	−0.0025(8)
C(4S)	0.0363(11)	0.0257(9)	0.0265(9)	0.0038(7)	0.0031(8)	−0.0013(8)
C(5S)	0.0337(11)	0.0272(9)	0.0289(9)	0.0034(7)	0.0078(8)	0.0054(8)
C(6S)	0.0319(10)	0.0310(9)	0.0242(9)	−0.0009(7)	0.0077(7)	0.0006(8)
C(7S)	0.0261(10)	0.0511(13)	0.0389(11)	0.0024(9)	0.0103(8)	0.0031(9)

[a]The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2\ \pi\ [h^2\ U_{11}\ +...+\ 2\ h\ k\ a^*\ b^*\ U_{12}]$.

Table S12. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(T*p*-OCH_3PP)(Hdmpz)][a]

atom	x	y	z	U(eq)
H(b1)	0.5370	0.0026	0.2203	0.024
H(b2)	0.3857	0.0345	0.2909	0.022
H(b3)	0.2812	0.1767	0.3553	0.030
H(b4)	0.3551	0.2392	0.3160	0.031
H(b5)	0.6920	0.2863	0.1410	0.024
H(b6)	0.8444	0.2550	0.0707	0.025
H(b7)	0.9510	0.1118	0.0086	0.024
H(b8)	0.8804	0.0494	0.0543	0.023
H(12a)	0.4079	0.0967	0.5111	0.025
H(13a)	0.2621	0.0820	0.5961	0.027
H(15a)	0.0204	0.0884	0.2796	0.026
H(16a)	0.1686	0.1027	0.1952	0.026
H(17a)	−0.1025	0.0929	0.3959	0.044
H(17b)	−0.1172	0.0616	0.4866	0.044
H(17c)	−0.0729	0.0498	0.3777	0.044
H(22a)	0.3840	0.2834	0.0854	0.043
H(23a)	0.3404	0.3456	0.1153	0.045
H(25a)	0.5950	0.3465	0.4229	0.027
H(26a)	0.6349	0.2835	0.3927	0.027
H(27a)	0.4677	0.3935	0.4531	0.043
H(27b)	0.4496	0.4330	0.3855	0.043
H(27c)	0.5670	0.4093	0.4004	0.043
H(32a)	0.8345	0.2117	−0.1223	0.027
H(33a)	0.9866	0.2279	−0.1984	0.030
H(35a)	1.2206	0.1838	0.0873	0.033
H(36a)	1.0681	0.1688	0.1637	0.028
H(37a)	1.3516	0.2100	0.0085	0.072
H(37b)	1.3629	0.2012	−0.1188	0.072
H(37c)	1.3050	0.1708	−0.0540	0.072
H(42a)	0.6694	0.0097	−0.0366	0.027
H(43a)	0.7339	−0.0509	−0.0577	0.030
H(45a)	0.8614	−0.0604	0.2931	0.025
H(46a)	0.7913	−0.0002	0.3131	0.023
H(47a)	0.9814	−0.1002	0.2375	0.067

Table S12. Continued

atom	x	y	z	U(eq)
H(47b)	0.9450	−0.1390	0.1684	0.067
H(47c)	0.8663	−0.1220	0.2438	0.067
H(6a)	0.8928	0.1731	0.3166	0.033
H(2a)	0.9031	0.1634	0.6445	0.033
H(4a1)	1.1138	0.1676	0.4921	0.064
H(4a2)	1.0968	0.1938	0.5947	0.064
H(4a3)	1.0659	0.2097	0.4642	0.064
H(5a1)	0.6046	0.1572	0.5049	0.051
H(5a2)	0.6893	0.1331	0.6083	0.051
H(5a3)	0.6368	0.1147	0.4819	0.051
H(6ba)	0.6418	0.1266	0.4632	0.025
H(2ba)	0.9480	0.1698	0.6281	0.033
H(4b1)	0.6683	0.1424	0.6829	0.049
H(4b2)	0.8015	0.1473	0.7598	0.049
H(4b3)	0.7558	0.1072	0.7039	0.049
H(5b1)	0.9371	0.1636	0.3157	0.049
H(5b2)	1.0197	0.1807	0.4349	0.049
H(5b3)	0.9139	0.2052	0.3554	0.049
H(2Sa)	0.1510	0.0087	0.3874	0.035
H(3Sa)	0.3229	−0.0035	0.5329	0.038
H(4Sa)	0.4673	−0.0411	0.4952	0.037
H(5Sa)	0.4354	−0.0682	0.3111	0.036
H(6Sa)	0.2610	−0.0570	0.1659	0.035
H(7S1)	0.0225	−0.0010	0.1984	0.058
H(7S2)	0.0463	−0.0359	0.1238	0.058
H(7S3)	0.0989	0.0047	0.1100	0.058

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor the estimated standard deviations of the least significant digits are given in parentheses.

Table S13. Mössbauer Parameters for [Fe(TPP)(Hdmpz)] at variable temperatures.

Complex	ΔE_Q, mm/s	δ_{Fe}, mm/s	T, K	M	ref.
[Fe(TPP)(Hdmpz)]	1.86	0.78	298	500G	tw
	2.03	0.82	250	500G	
	2.20	0.85	200	500G	
	2.31	0.87	150	500G	
	2.41	0.89	100	500G	
	2.47	0.90	50	500G	
	2.51	0.90	20	500G	
	2.54	0.91	16	500G	

Table S14. Fits for applied field Mössbauer measurements.

Complex	Fe(TPP)(Hdmpz)
D, cm^{-1}	9.4
E/D	0.29
ΔE_Q, mm/s	−2.54
η	0.74
δ_{Fe}, mm/s	0.91
$A^*_{xx}/g^*_N\beta_N$, T	−6.8
$A^*_{yy}/g^*_N\beta_N$, T	−6.8
$A^*_{zz}/g^*_N\beta_N$, T	−2.2
α^a	−58
β^a	36
γ^a	31

[a] Euler angles for rotation of the electric field gradient with respect to the g tensor. See Tinkham, M. "Group Theory and Quantum Mechanics," McGraw-Hill Book Company, New York, NY, 1964, p102.

Table S15. Out-of-Plane Displacements (Å) of the Minimal Basis for the X-ray Crystal Structures of Five-Coordinate High-Spin Iron(II) Porphyrinates

porphyrin	Doop[a]	δ_{oop}[b]	*sad*	*ruf*	*dom*	*wav(x)*	*wav(y)*	*pro*	ΔN_4[c]	Δ[d]	ref
[Fe(TPP)(Hdmpz)]	0.243	0.010	-0.042	-0.051	0.199	0.031	0.1208	-0.003	0.32	0.38	tw
[Fe(T*p*-OCH_3PP)(Hdmpz)]	0.165	0.011	0.030	0.034	-0.102	-0.081	0.090	0.010	0.31	0.34	tw

[a] Observed total distortion. [b] The mean deviation as a measure of the goodness-of-fit. [c] Displacement of iron from the mean plane of the four pyrrole nitrogen atoms.[d] Displacement of iron from the 24-atom mean plane