Supporting Information

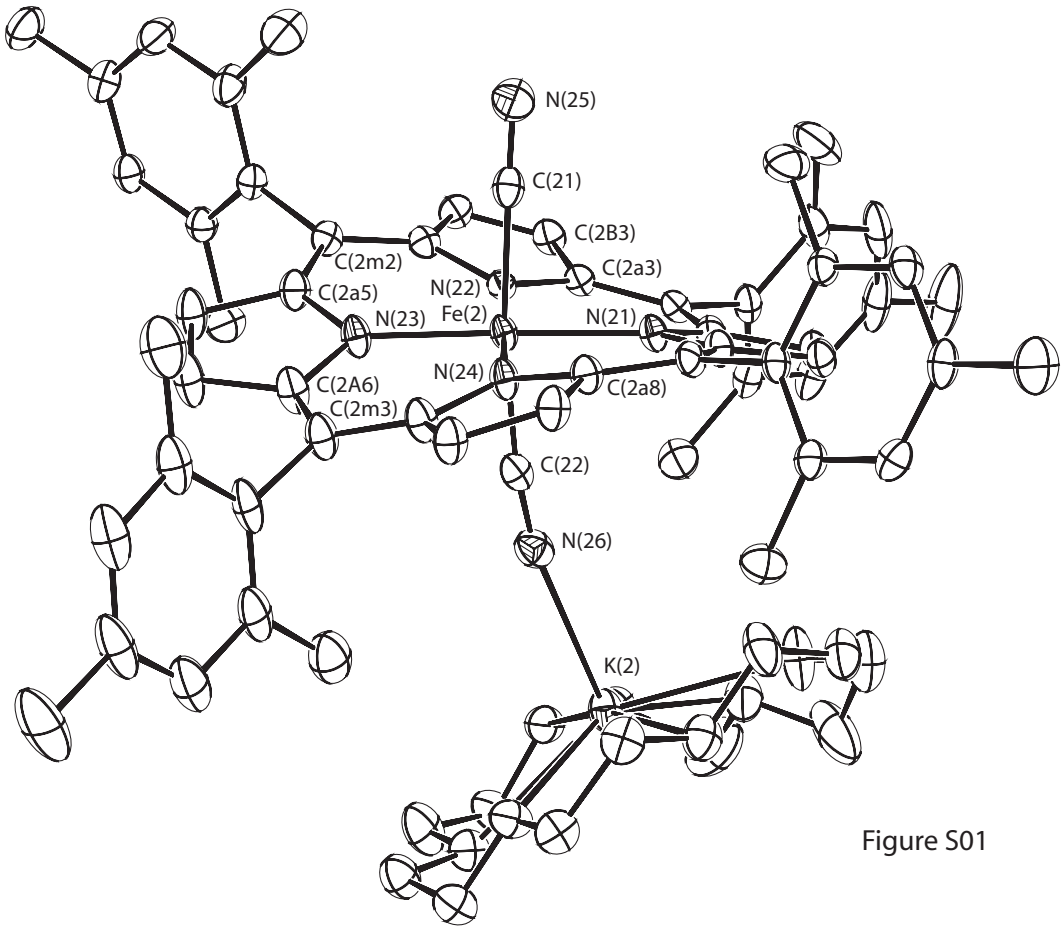


Figure S1. ORTEP diagram of the second unit in the cell of [K(18-C-6)][Fe(TMP)$(CN)_2$] displaying the atom labeling scheme. Thermal ellipsoids of all atoms are contoured at the 50% probability level. Hydrogen atoms have been omitted for clarity.

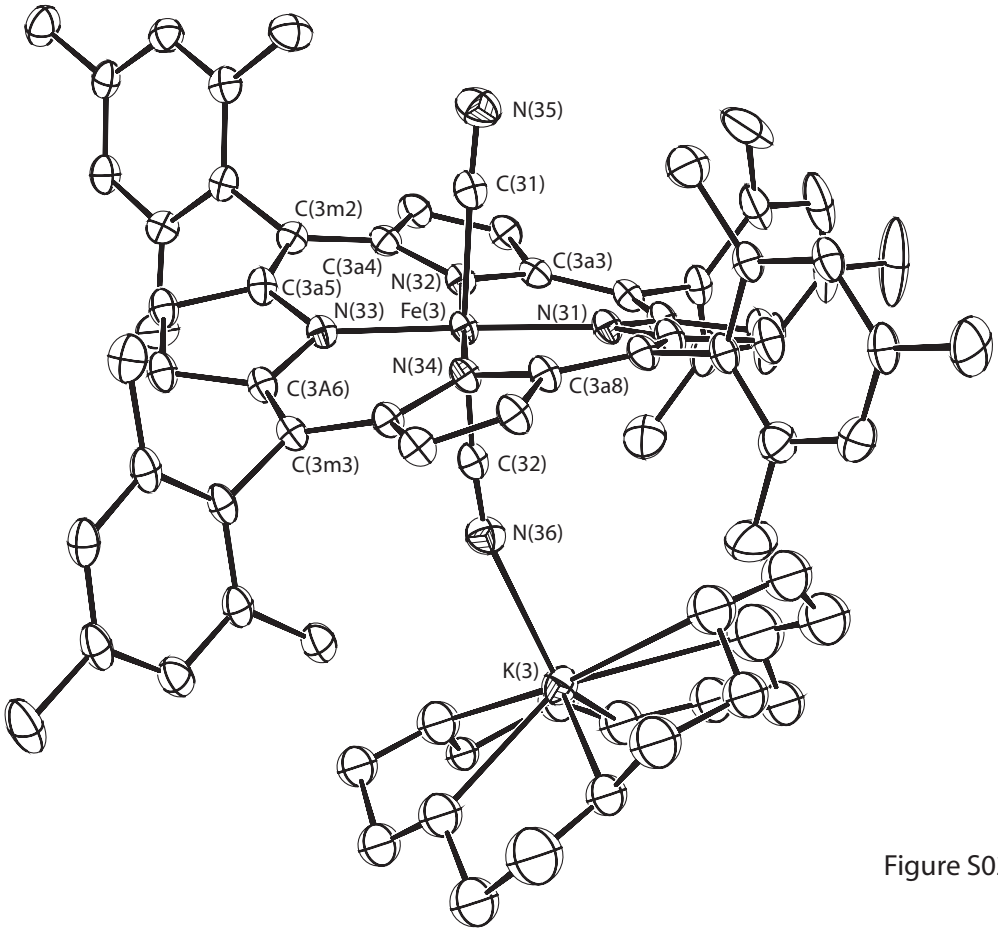


Figure S2. ORTEP diagram of the third unit in [K(18-C-6)][Fe(TMP)$(CN)_2$] displaying the atom labeling scheme. Thermal ellipsoids of all atoms are contoured at the 50% probability level. Hydrogen atoms have been omitted for clarity.

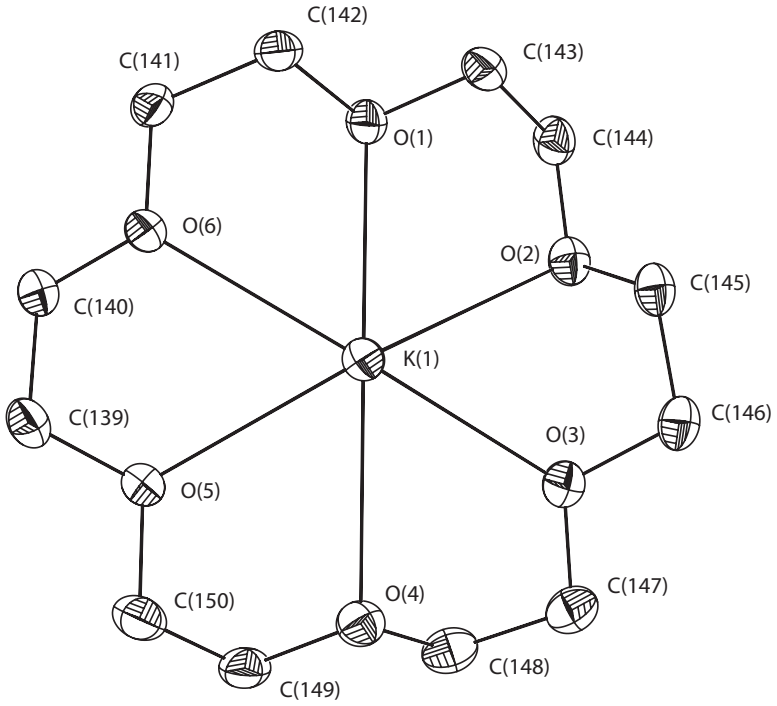


Figure S3. ORTEP diagram of the ordered 18-crown-6 ring in the first [K(18-C-6)][Fe(TMP)$(CN)_2$] unit displaying the atom labeling scheme. 50% probablity countours are shown.

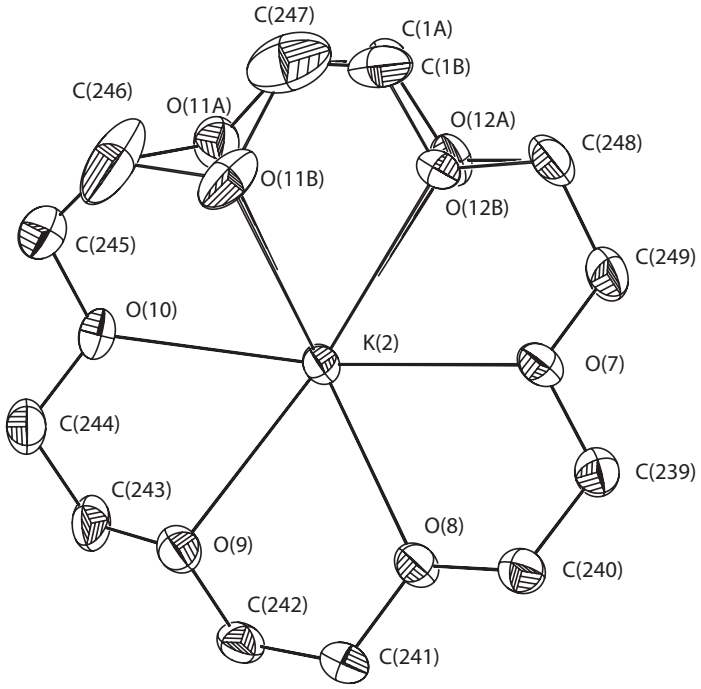


Figure S04

Figure S4. ORTEP diagram of the disordered 18-crown-6 ring in the second [K(18-C-6)][Fe(TMP)$(CN)_2$] unit displaying the atom labeling scheme. 50% probablity countours are shown.

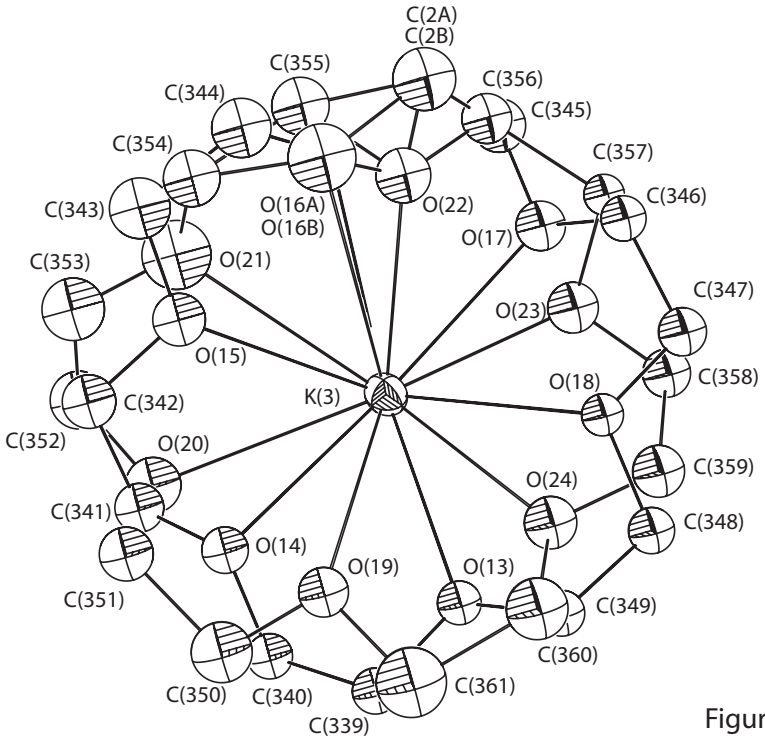


Figure S05

Figure S5. ORTEP diagram of the disordered 18-crown-6 ring in the third [K(18-C-6)][Fe(TMP)$(CN)_2$] unit displaying the atom labeling scheme. 50% probablity countours are shown.

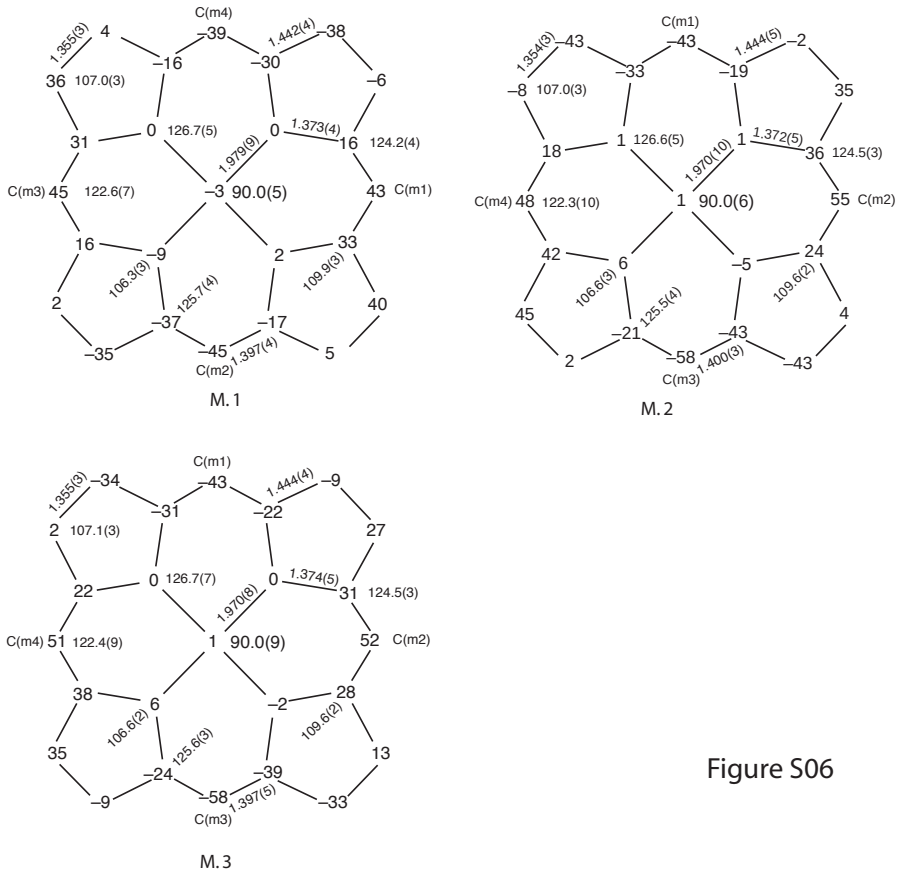


Figure S6. Formal diagrams of the porphyrin cores for all entities (1, 2, 3) of [K(18-C-6)][Fe(TMP)$(CN)_2$]. Averaged values of the chemically unique bond distances (in 0.01 Å) and angles (in degrees) are shown. Positive values of displacements are toward the cyanide ligand that is not also coordinated to the [K(18-crown-6)] cation.

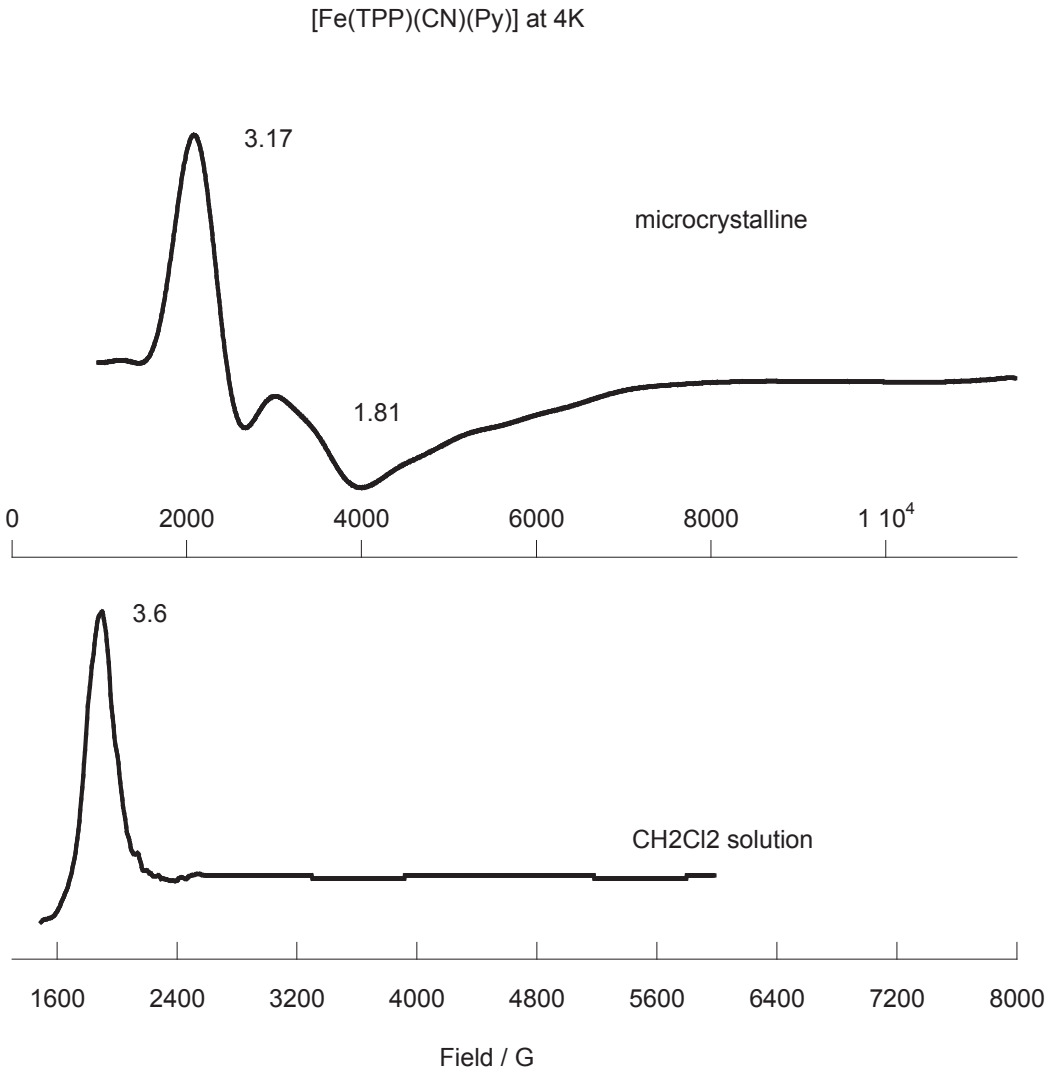


Figure S7. EPR spectra for [Fe(TPP)(CN)(Py)] in the solid state and in a frozen CH_2Cl_2 solution.

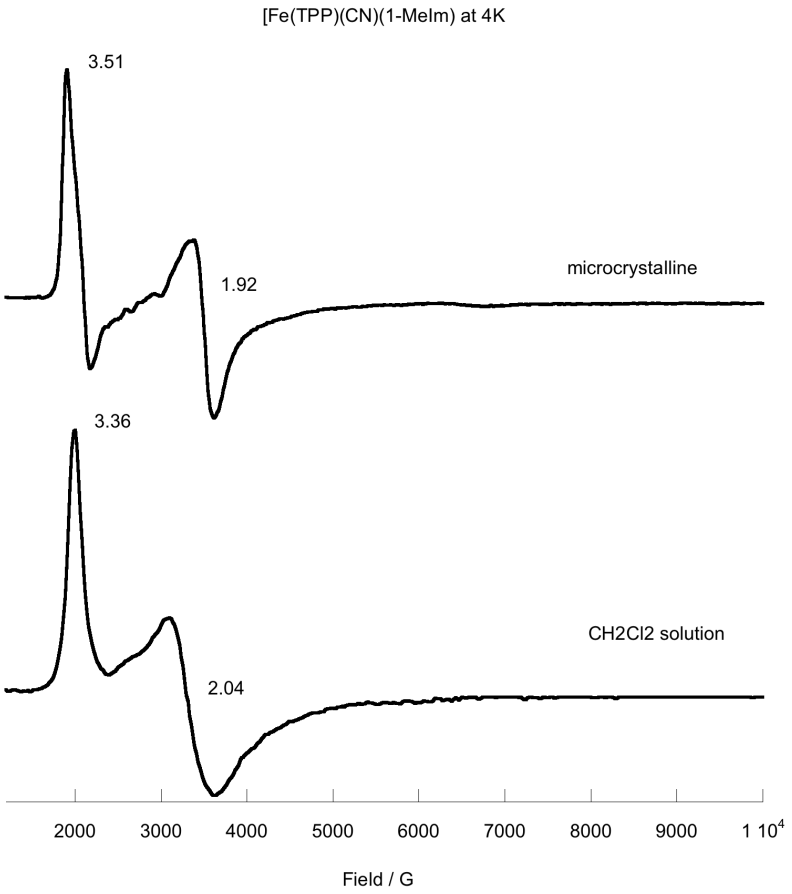


Figure S8. EPR spectra for [Fe(TPP)(CN)(1-MeIm)] in the solid state and in a frozen CH_2Cl_2 solution.

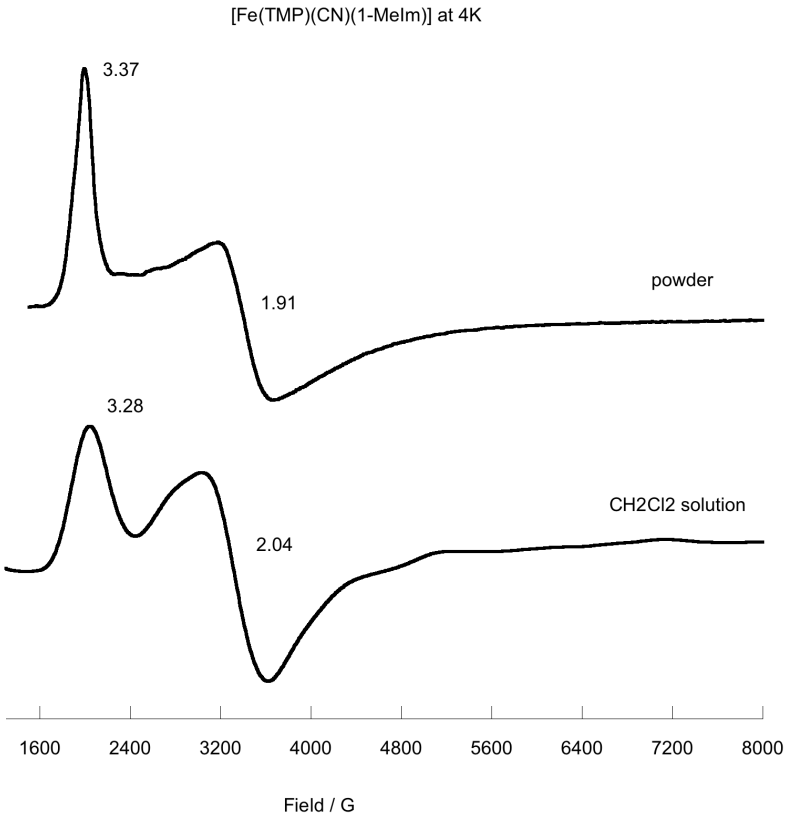


Figure S9. EPR spectra for [Fe(TMP)(CN)(1-MeIm)] in the solid state and in a frozen CH_2Cl_2 solution.

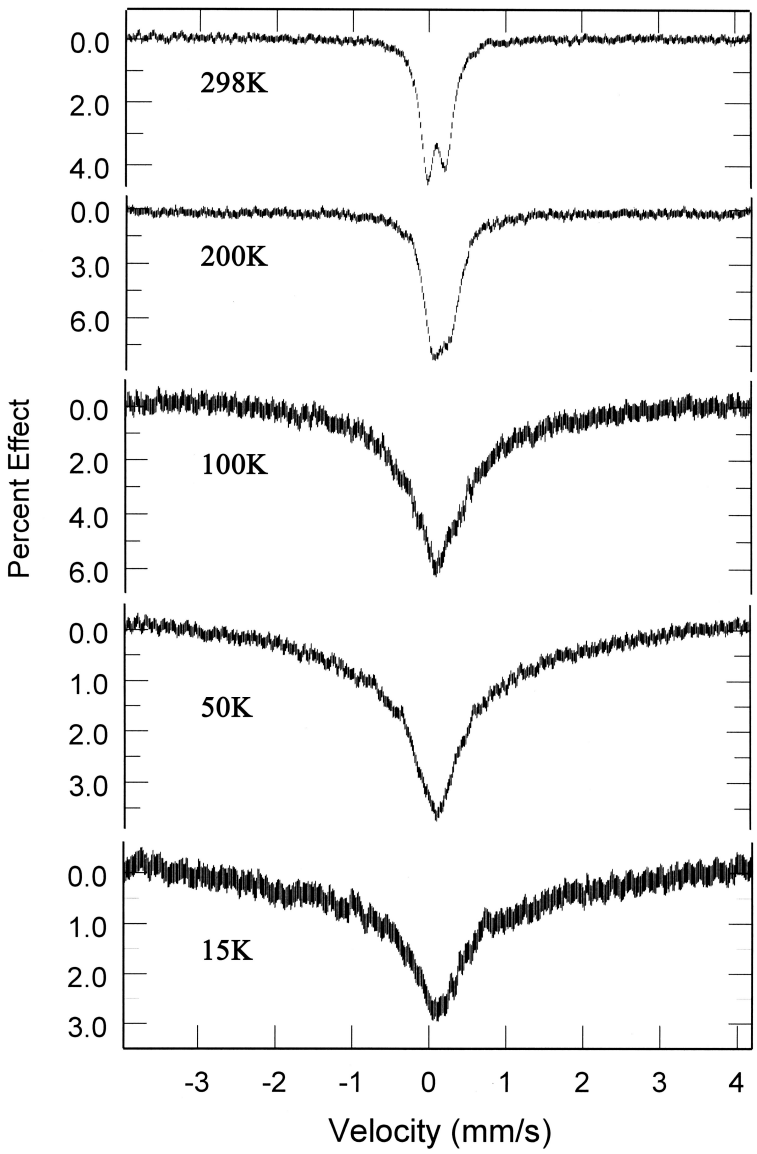


Figure S10. Mössbauer spectra for $[K((CH_3)_2CO)_2][Fe(TPP)(CN)_2]$ over the temperature range of 298 – 15 K.

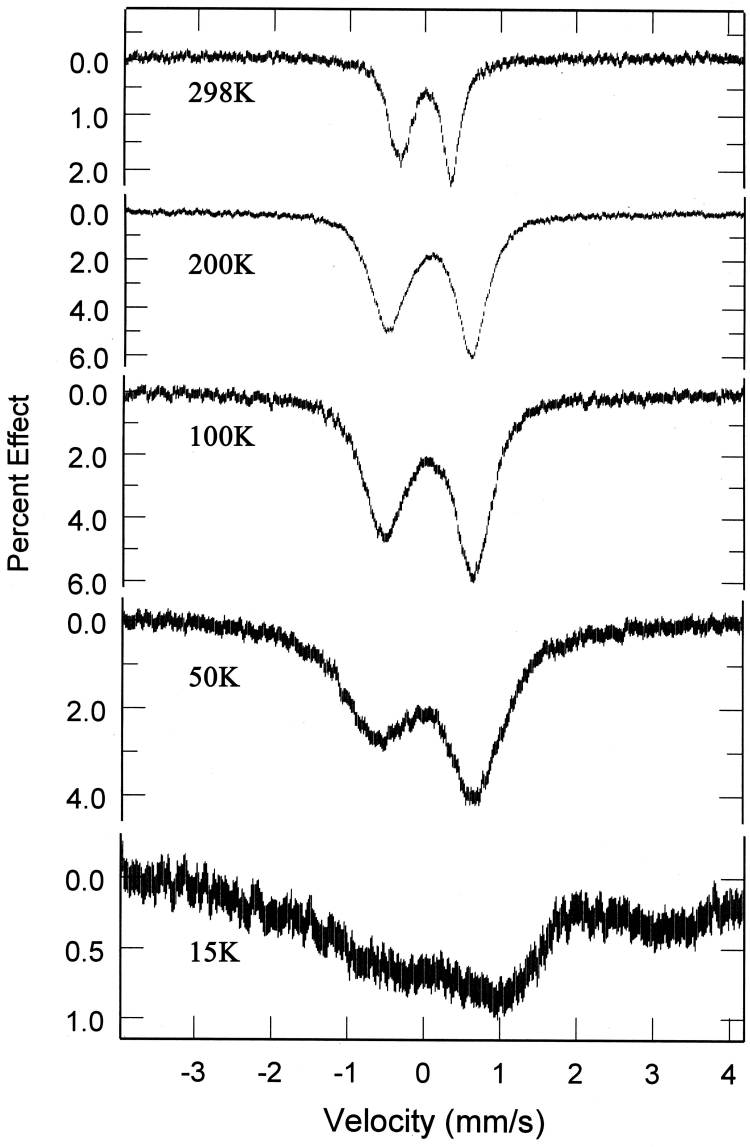


Figure S11. Mössbauer spectra for [K(18-C-6)][Fe(TMP)$(CN)_2$] over the temperature range of 298 – 15 K.

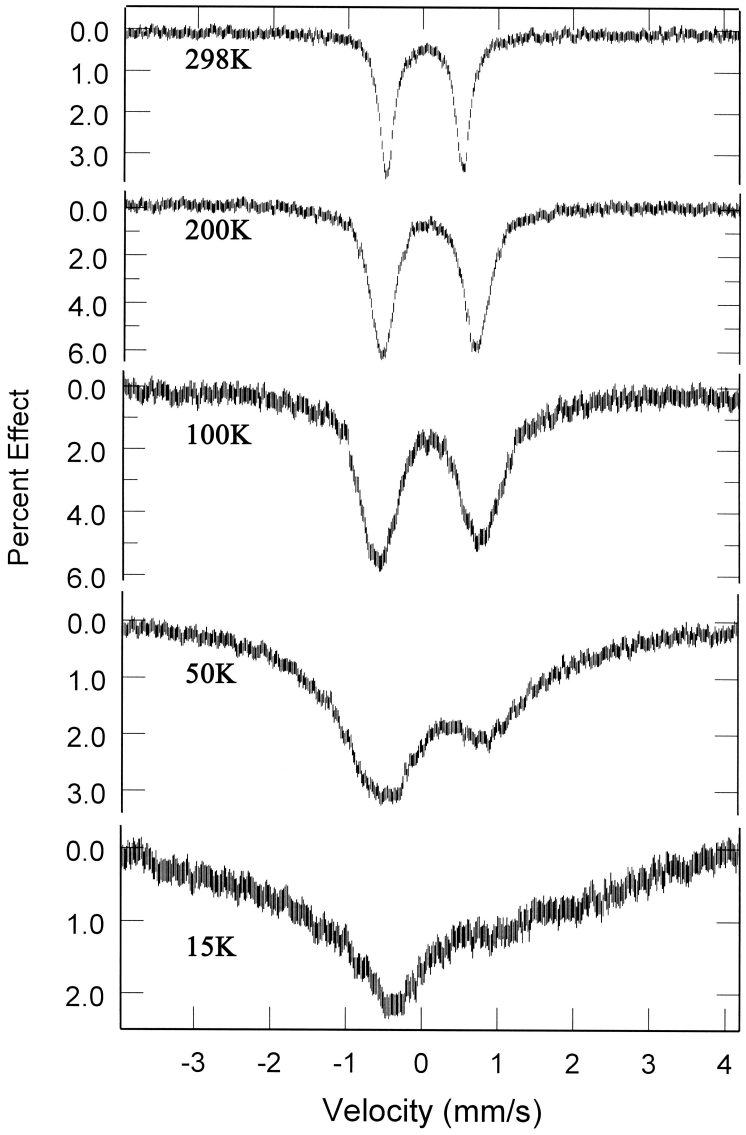


Figure S12. Mössbauer spectra for [Fe(TMP)(CN)(1-MeIm)] over the temperature range of 298 – 15 K.

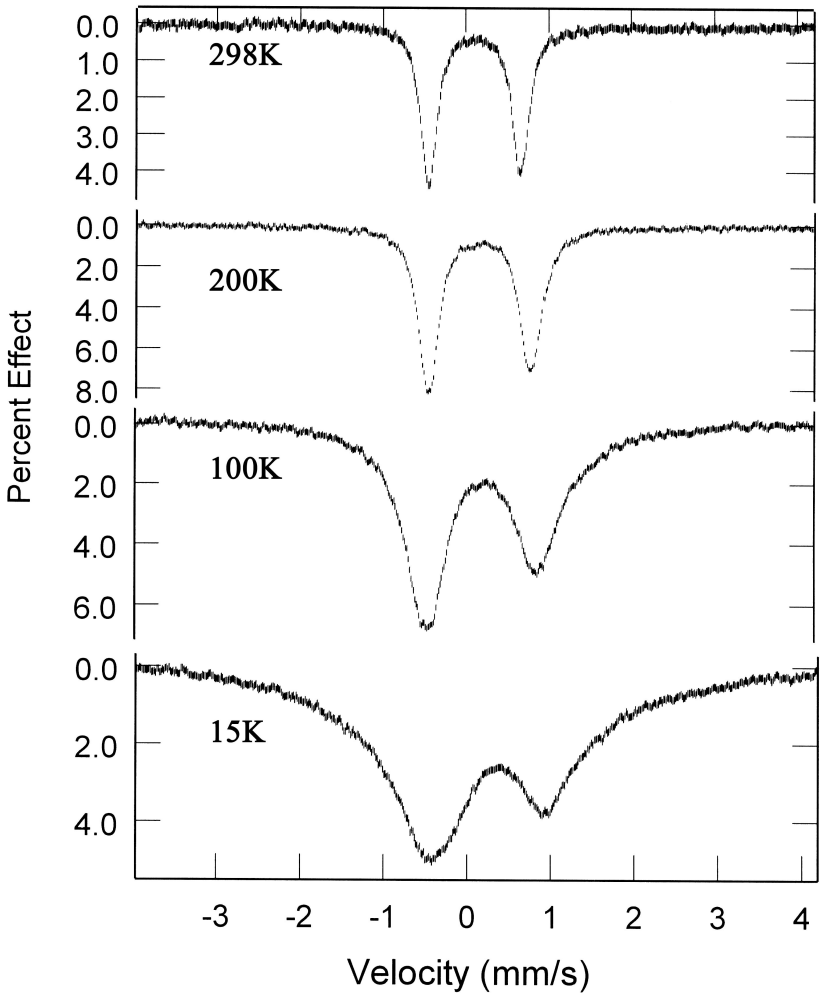


Figure S13. Mössbauer spectra for [Fe(TPP)(CN)(1-MeIm)] over the temperature range of 298 – 15 K.

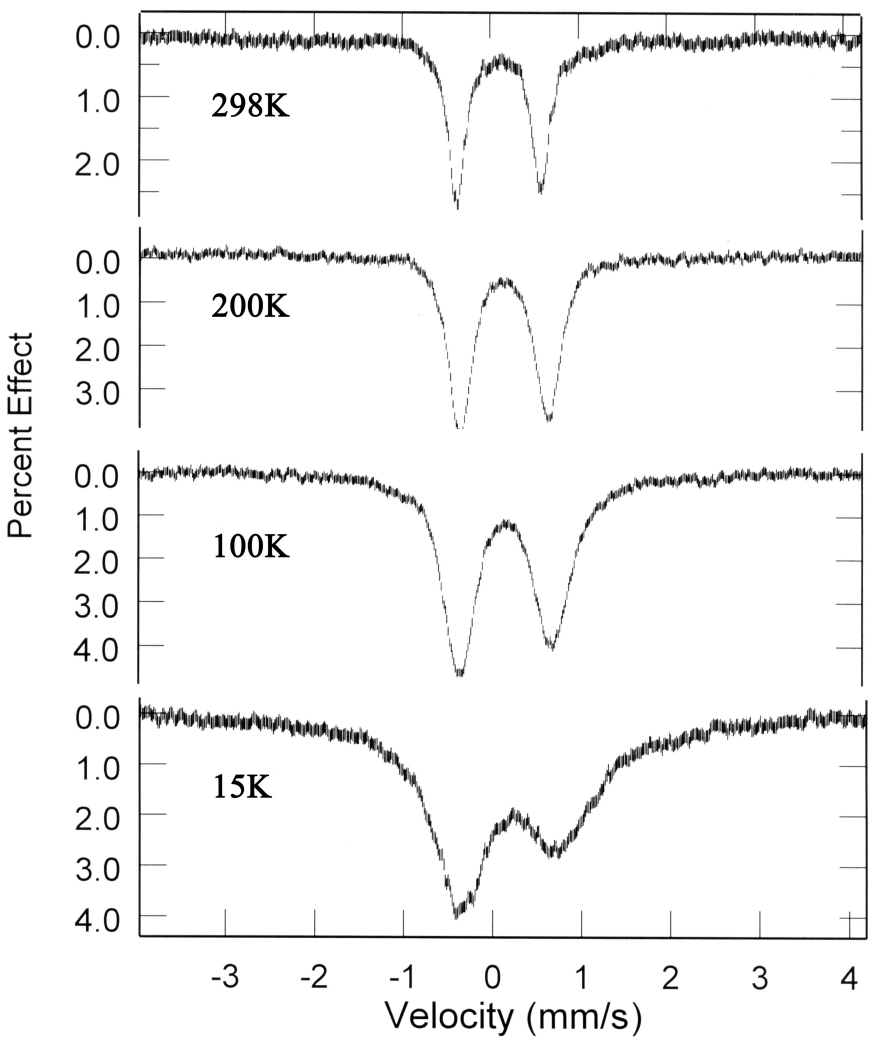
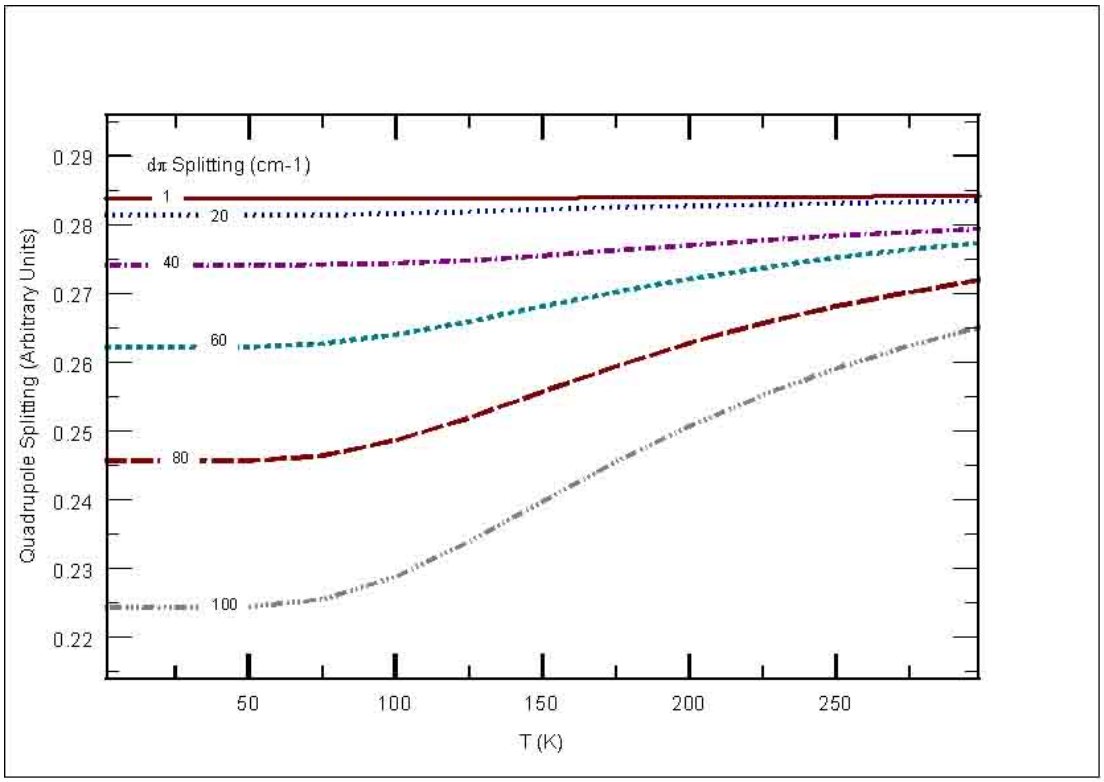


Figure S14. Mössbauer spectra for [Fe(TPP)(CN)(Py)] over the temperature range of 298 – 15 K.



The above graph shows the expected temperature dependence of the quadrupole splitting for various values of the splitting between d_{xz} and d_{yz}. The calculation uses a spin-orbit coupling of 250cm^{-1} and a splitting of 2000 cm^{-1} to the d_{xy} orbital.

Figure S15. Mössbauer QS calculations.

Table S1. Details for fitting high-field (5, 9 T) Mössbauer for $[K((CH_3)_2CO)_2][Fe(TPP)(CN)_2]$

Temperature	4.2 K
Quadrupole splitting	−0.40 mm/s
Isomer shift	0.19 mm/s
Eta	0.7
Gamma,	0.40 mm/s
g	(0.52, 1.05, 3.7)
A	(−1.8, −2.2, 90.3) T
Euler ($g \rightarrow Q$)	(102, 64, −11)°
Euler ($g \rightarrow A$)	(105, 19, 33)°

Table S2. Complete Crystallographic Details for [Fe(TPP)(CN)(Py)]·0.65Py

formula	$C_{53.25}H_{36.25}FeN_{6.65}$
FW, amu	825.09
a, Å	13.1214(2)
b, Å	23.5538(4)
c, Å	14.0324(2)
β, deg	102.606(1)
V, Å^3	4232.29(11)
space group	P21/n
Z	4
D_c, g/cm^3	1.295
F(000)	1713
μ, mm^{-1}	0.402
crystal dimensions, mm	0.55 × 0.53 × 0.40
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.11–26.00
index range	$-16 \leq h \leq 16$
	$-29 \leq k \leq 29$
	$-15 \leq l \leq 17$
total data collected	48079
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.8557 and 0.8091
unique data	8310 (R_{int} = 0.0221)
unique observed data [I > 2σ(I)]	7789
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	8310/173/583
goodness-of-fit (pased on F^2)	1.044
final R indices [I > 2σ(I)]	R_1 = 0.0515, wR_2 = 0.1511
final R indices (all data)	R_1 = 0.0543, wR_2 = 0.1531

Table S3. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CN)(Py)]·0.65Py[a]

atom	x	y	z	U(eq)
Fe(1)	0.65769(2)	0.19879(1)	0.88166(2)	0.0141(1)
N(1)	0.76691(15)	0.22118(8)	0.81296(14)	0.0164(4)
N(2)	0.56883(15)	0.26340(8)	0.82145(15)	0.0176(4)
N(3)	0.54834(15)	0.17632(8)	0.95108(14)	0.0162(4)
N(4)	0.74838(15)	0.13625(8)	0.94467(14)	0.0160(4)
N(5)	0.57302(18)	0.12149(10)	0.70487(17)	0.0279(5)
N(6)	0.72526(16)	0.25307(9)	0.99390(15)	0.0195(4)
C(a1)	0.84814(18)	0.18812(10)	0.79687(17)	0.0175(5)
C(a2)	0.77011(18)	0.27041(10)	0.76150(17)	0.0185(5)
C(a3)	0.60194(19)	0.30969(10)	0.77640(18)	0.0188(5)
C(a4)	0.46737(19)	0.27516(10)	0.82747(18)	0.0195(5)
C(a5)	0.44636(19)	0.19530(10)	0.93390(18)	0.0187(5)
C(a6)	0.55507(18)	0.13350(10)	1.01965(17)	0.0169(5)
C(a7)	0.73485(18)	0.10378(10)	1.02285(17)	0.0165(4)
C(a8)	0.84013(18)	0.11777(10)	0.92293(17)	0.0167(5)
C(b1)	0.89963(19)	0.21654(11)	0.72998(19)	0.0224(5)
C(b2)	0.85464(19)	0.26806(11)	0.71162(19)	0.0227(5)
C(b3)	0.5197(2)	0.35139(11)	0.75430(19)	0.0235(5)
C(b4)	0.4367(2)	0.32991(11)	0.7840(2)	0.0238(5)
C(b5)	0.38844(19)	0.16244(10)	0.99017(18)	0.0206(5)
C(b6)	0.45585(19)	0.12531(10)	1.04431(18)	0.0191(5)
C(b7)	0.82364(19)	0.06726(10)	1.05434(17)	0.0187(5)
C(b8)	0.88755(18)	0.07512(10)	0.99208(18)	0.0183(5)
C(m1)	0.69851(19)	0.31481(10)	0.75120(18)	0.0193(5)
C(m2)	0.40683(19)	0.24235(10)	0.87656(18)	0.0200(5)
C(m3)	0.64404(19)	0.10126(10)	1.05822(17)	0.0173(5)
C(m4)	0.88380(18)	0.13854(10)	0.84762(18)	0.0179(5)
C(1)	0.72670(19)	0.36998(10)	0.71031(19)	0.0208(5)
C(2)	0.6826(2)	0.38709(11)	0.61553(19)	0.0240(5)
C(3)	0.7103(2)	0.43909(11)	0.5808(2)	0.0269(6)
C(4)	0.7817(2)	0.47396(11)	0.6404(2)	0.0278(6)
C(5)	0.8268(2)	0.45688(12)	0.7344(2)	0.0329(6)
C(6)	0.7999(2)	0.40510(12)	0.7694(2)	0.0309(6)
C(7)	0.2978(2)	0.26179(11)	0.8753(2)	0.0243(5)

Table S3. Continued

atom	x	y	z	U(eq)
C(8)	0.2236(2)	0.26606(11)	0.7877(2)	0.0272(6)
C(9)	0.1233(2)	0.28544(12)	0.7870(3)	0.0335(7)
C(10)	0.0960(2)	0.30068(13)	0.8732(3)	0.0417(8)
C(11)	0.1685(3)	0.29671(14)	0.9603(3)	0.0421(8)
C(12)	0.2692(2)	0.27732(13)	0.9613(2)	0.0338(6)
C(13)	0.63550(18)	0.05871(10)	1.13572(17)	0.0177(5)
C(14)	0.6034(2)	0.00332(11)	1.11029(19)	0.0222(5)
C(15)	0.5833(2)	−0.03424(11)	1.1805(2)	0.0248(5)
C(16)	0.5977(2)	−0.01712(11)	1.2768(2)	0.0267(6)
C(17)	0.6334(2)	0.03716(12)	1.3035(2)	0.0298(6)
C(18)	0.6524(2)	0.07493(11)	1.23300(19)	0.0258(5)
C(19)	0.97368(19)	0.10734(10)	0.82327(17)	0.0193(5)
C(20)	0.9571(2)	0.05294(11)	0.7831(2)	0.0250(5)
C(21)	1.0381(2)	0.02394(12)	0.7548(2)	0.0286(6)
C(22)	1.1365(2)	0.04833(12)	0.7677(2)	0.0271(6)
C(23)	1.1540(2)	0.10156(12)	0.80968(19)	0.0253(5)
C(24)	1.07306(19)	0.13124(11)	0.83712(19)	0.0224(5)
C(25)	0.60222(18)	0.14984(10)	0.77263(18)	0.0190(5)
C(26)	0.6699(2)	0.29375(11)	1.0266(2)	0.0263(6)
C(27)	0.7161(3)	0.33480(13)	1.0934(2)	0.0357(7)
C(28)	0.8228(3)	0.33371(13)	1.1279(2)	0.0365(7)
C(29)	0.8805(2)	0.29148(13)	1.0962(2)	0.0315(6)
C(30)	0.8294(2)	0.25225(11)	1.02929(19)	0.0237(5)
N(7)	0.9800(7)	0.0313(6)	0.4954(7)	0.104(3)
C(32)	0.9417(9)	−0.0206(5)	0.5097(8)	0.123(4)
C(33)	0.8463(10)	−0.0274(4)	0.5358(9)	0.114(4)
C(34)	0.7873(7)	0.0196(6)	0.5467(7)	0.113(3)
C(35)	0.8270(9)	0.0730(5)	0.5341(8)	0.106(3)
C(36)	0.9220(9)	0.0769(5)	0.5081(7)	0.130(4)
N(8)	0.4947(8)	0.0747(4)	0.4971(6)	0.0705(12)
C(31)	0.5814(8)	0.0379(4)	0.5444(6)	0.0686(14)
C(37)	0.4292(9)	0.0256(4)	0.4749(8)	0.0875(15)
C(39)	0.4947(8)	0.0747(4)	0.4971(6)	0.0705(12)
C(40)	0.5814(8)	0.0379(4)	0.5444(6)	0.0686(14)

Table S3. Continued

atom	x	y	z	U(eq)
C(38)	0.4292(9)	0.0256(4)	0.4749(8)	0.0875(15)

[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 S4. Bond Lengths for [Fe(TPP)(CN)(Py)]·0.65Py[a]

bond	length (Å)	bond	length (Å)
Fe(1)–C(25)	1.927(3)	C(7)–C(8)	1.395(4)
Fe(1)–N(1)	1.966(2)	C(8)–C(9)	1.392(4)
Fe(1)–N(3)	1.974(2)	C(8)–H(8a)	0.9500
Fe(1)–N(4)	1.977(2)	C(9)–C(10)	1.382(5)
Fe(1)–N(2)	1.990(2)	C(9)–H(9a)	0.9500
Fe(1)–N(6)	2.072(2)	C(10)–C(11)	1.378(5)
N(1)–C(a2)	1.371(3)	C(10)–H(10a)	0.9500
N(1)–C(a1)	1.378(3)	C(11)–C(12)	1.395(4)
N(2)–C(a3)	1.377(3)	C(11)–H(11a)	0.9500
N(2)–C(a4)	1.380(3)	C(12)–H(12a)	0.9500
N(3)–C(a5)	1.381(3)	C(13)–C(18)	1.388(4)
N(3)–C(a6)	1.383(3)	C(13)–C(14)	1.393(3)
N(4)–C(a8)	1.376(3)	C(14)–C(15)	1.391(4)
N(4)–C(a7)	1.380(3)	C(14)–H(14a)	0.9500
N(5)–C(25)	1.157(3)	C(15)–C(16)	1.384(4)
N(6)–C(26)	1.343(3)	C(15)–H(15a)	0.9500
N(6)–C(30)	1.348(3)	C(16)–C(17)	1.385(4)
C(a1)–C(m4)	1.394(3)	C(16)–H(16a)	0.9500
C(a1)–C(b1)	1.436(3)	C(17)–C(18)	1.392(4)
C(a2)–C(m1)	1.392(3)	C(17)–H(17a)	0.9500
C(a2)–C(b2)	1.436(3)	C(18)–H(18a)	0.9500
C(a3)–C(m1)	1.393(3)	C(19)–C(24)	1.394(4)
C(a3)–C(b3)	1.441(3)	C(19)–C(20)	1.398(4)
C(a4)–C(m2)	1.393(3)	C(20)–C(21)	1.392(4)
C(a4)–C(b4)	1.445(3)	C(20)–H(20a)	0.9500
C(a5)–C(m2)	1.401(3)	C(21)–C(22)	1.388(4)
C(a5)–C(b5)	1.436(3)	C(21)–H(21a)	0.9500
C(a6)–C(m3)	1.399(3)	C(22)–C(23)	1.383(4)
C(a6)–C(b6)	1.431(3)	C(22)–H(22a)	0.9500
C(a7)–C(m3)	1.389(3)	C(23)–C(24)	1.394(4)
C(a7)–C(b7)	1.438(3)	C(23)–H(23a)	0.9500
C(a8)–C(m4)	1.396(3)	C(24)–H(24a)	0.9500
C(a8)–C(b8)	1.440(3)	C(26)–C(27)	1.391(4)
C(b1)–C(b2)	1.349(4)	C(26)–H(26a)	0.9500

Table S4. Continued

bond	length (Å)	bond	length (Å)
C(b1)–H(b1)	0.9500	C(27)–C(28)	1.378(5)
C(b2)–H(b2)	0.9500	C(27)–H(27a)	0.9500
C(b3)–C(b4)	1.347(4)	C(28)–C(29)	1.382(5)
C(b3)–H(b3)	0.9500	C(28)–H(28a)	0.9500
C(b4)–H(b4)	0.9500	C(29)–C(30)	1.382(4)
C(b5)–C(b6)	1.353(4)	C(29)–H(29a)	0.9500
C(b5)–H(b5)	0.9500	C(30)–H(30a)	0.9500
C(b6)–H(b6)	0.9500	N(7)–C(32)#1)	1.076(19)
C(b7)–C(b8)	1.349(3)	N(7)–C(36)	1.3492
C(b7)–H(b7)	0.9500	N(7)–C(32)	1.3536
C(b8)–H(b8)	0.9500	N(7)–N(7)#1)	1.56(3)
C(m1)–C(1)	1.499(3)	C(32)–C(33)	1.3873
C(m2)–C(7)	1.498(3)	C(32)–H(32)	0.9500
C(m3)–C(13)	1.501(3)	C(33)–C(34)	1.3799
C(m4)–C(19)	1.491(3)	C(33)–H(43a)	0.9500
C(1)–C(2)	1.389(4)	C(34)–C(35)	1.3865
C(1)–C(6)	1.395(4)	C(34)–H(44a)	0.9500
C(2)–C(3)	1.396(4)	C(35)–C(36)	1.3767
C(2)–H(2a)	0.9500	C(35)–H(35)	0.9500
C(3)–C(4)	1.382(4)	C(36)–H(46)	0.9500
C(3)–H(3a)	0.9500	N(8)–C(37)	1.433(11)
C(4)–C(5)	1.383(4)	N(8)–C(31)	1.469(12)
C(4)–H(4a)	0.9500	C(31)–C(37)#2)	1.523(10)
C(5)–C(6)	1.389(4)	C(31)–H(31)	0.9500
C(5)–H(5a)	0.9500	C(37)–C(31)#2)	1.523(10)
C(6)–H(6a)	0.9500	C(37)–H(37)	0.9500
C(7)–C(12)	1.390(4)		

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

Table S5. Bond Angles for [Fe(TPP)(CN)(Py)]·0.65Py[a]

angle	degree	angle	degree
C(25)–Fe(1)–N(1)	87.74(9)	C(4)–C(5)–H(5a)	119.9
C(25)–Fe(1)–N(3)	92.41(9)	C(6)–C(5)–H(5a)	119.9
N(1)–Fe(1)–N(3)	179.80(9)	C(5)–C(6)–C(1)	120.4(3)
C(25)–Fe(1)–N(4)	89.74(9)	C(5)–C(6)–H(6a)	119.8
N(1)–Fe(1)–N(4)	89.26(8)	C(1)–C(6)–H(6a)	119.8
N(3)–Fe(1)–N(4)	90.62(8)	C(12)–C(7)–C(8)	118.5(3)
C(25)–Fe(1)–N(2)	92.05(9)	C(12)–C(7)–C(m2)	120.5(3)
N(1)–Fe(1)–N(2)	90.51(8)	C(8)–C(7)–C(m2)	120.9(2)
N(3)–Fe(1)–N(2)	89.60(8)	C(9)–C(8)–C(7)	120.5(3)
N(4)–Fe(1)–N(2)	178.19(8)	C(9)–C(8)–H(8a)	119.8
C(25)–Fe(1)–N(6)	176.05(9)	C(7)–C(8)–H(8a)	119.8
N(1)–Fe(1)–N(6)	88.30(8)	C(10)–C(9)–C(8)	120.3(3)
N(3)–Fe(1)–N(6)	91.54(8)	C(10)–C(9)–H(9a)	119.9
N(4)–Fe(1)–N(6)	90.22(8)	C(8)–C(9)–H(9a)	119.9
N(2)–Fe(1)–N(6)	87.98(8)	C(11)–C(10)–C(9)	119.8(3)
C(a2)–N(1)–C(a1)	106.13(19)	C(11)–C(10)–H(10a)	120.1
C(a2)–N(1)–Fe(1)	126.47(16)	C(9)–C(10)–H(10a)	120.1
C(a1)–N(1)–Fe(1)	126.98(16)	C(10)–C(11)–C(12)	120.1(3)
C(a3)–N(2)–C(a4)	105.91(19)	C(10)–C(11)–H(11a)	120.0
C(a3)–N(2)–Fe(1)	125.88(16)	C(12)–C(11)–H(11a)	120.0
C(a4)–N(2)–Fe(1)	127.67(16)	C(7)–C(12)–C(11)	120.8(3)
C(a5)–N(3)–C(a6)	105.65(19)	C(7)–C(12)–H(12a)	119.6
C(a5)–N(3)–Fe(1)	127.43(16)	C(11)–C(12)–H(12a)	119.6
C(a6)–N(3)–Fe(1)	126.57(16)	C(18)–C(13)–C(14)	119.0(2)
C(a8)–N(4)–C(a7)	105.76(19)	C(18)–C(13)–C(m3)	120.5(2)
C(a8)–N(4)–Fe(1)	127.38(16)	C(14)–C(13)–C(m3)	120.4(2)
C(a7)–N(4)–Fe(1)	126.81(16)	C(15)–C(14)–C(13)	120.5(2)
C(26)–N(6)–C(30)	117.7(2)	C(15)–C(14)–H(14a)	119.8
C(26)–N(6)–Fe(1)	121.77(18)	C(13)–C(14)–H(14a)	119.8
C(30)–N(6)–Fe(1)	120.16(17)	C(16)–C(15)–C(14)	120.0(2)
N(1)–C(a1)–C(m4)	125.1(2)	C(16)–C(15)–H(15a)	120.0
N(1)–C(a1)–C(b1)	109.6(2)	C(14)–C(15)–H(15a)	120.0
C(m4)–C(a1)–C(b1)	124.8(2)	C(15)–C(16)–C(17)	119.9(2)
N(1)–C(a2)–C(m1)	126.3(2)	C(15)–C(16)–H(16a)	120.0

Table S5. Continued

angle	degree	angle	degree
N(1)–C(a2)–C(b2)	109.9(2)	C(17)–C(16)–H(16a)	120.0
C(m1)–C(a2)–C(b2)	123.6(2)	C(16)–C(17)–C(18)	120.0(3)
N(2)–C(a3)–C(m1)	125.5(2)	C(16)–C(17)–H(17a)	120.0
N(2)–C(a3)–C(b3)	110.0(2)	C(18)–C(17)–H(17a)	120.0
C(m1)–C(a3)–C(b3)	124.4(2)	C(13)–C(18)–C(17)	120.5(2)
N(2)–C(a4)–C(m2)	125.5(2)	C(13)–C(18)–H(18a)	119.7
N(2)–C(a4)–C(b4)	109.7(2)	C(17)–C(18)–H(18a)	119.7
C(m2)–C(a4)–C(b4)	124.5(2)	C(24)–C(19)–C(20)	119.0(2)
N(3)–C(a5)–C(m2)	125.4(2)	C(24)–C(19)–C(m4)	122.1(2)
N(3)–C(a5)–C(b5)	109.8(2)	C(20)–C(19)–C(m4)	118.9(2)
C(m2)–C(a5)–C(b5)	124.6(2)	C(21)–C(20)–C(19)	120.2(2)
N(3)–C(a6)–C(m3)	125.9(2)	C(21)–C(20)–H(20a)	119.9
N(3)–C(a6)–C(b6)	110.1(2)	C(19)–C(20)–H(20a)	119.9
C(m3)–C(a6)–C(b6)	124.0(2)	C(22)–C(21)–C(20)	120.4(3)
N(4)–C(a7)–C(m3)	125.2(2)	C(22)–C(21)–H(21a)	119.8
N(4)–C(a7)–C(b7)	109.9(2)	C(20)–C(21)–H(21a)	119.8
C(m3)–C(a7)–C(b7)	124.4(2)	C(23)–C(22)–C(21)	119.6(2)
N(4)–C(a8)–C(m4)	125.5(2)	C(23)–C(22)–H(22a)	120.2
N(4)–C(a8)–C(b8)	110.0(2)	C(21)–C(22)–H(22a)	120.2
C(m4)–C(a8)–C(b8)	124.5(2)	C(22)–C(23)–C(24)	120.5(2)
C(b2)–C(b1)–C(a1)	107.2(2)	C(22)–C(23)–H(23a)	119.8
C(b2)–C(b1)–H(b1)	126.4	C(24)–C(23)–H(23a)	119.8
C(a1)–C(b1)–H(b1)	126.4	C(23)–C(24)–C(19)	120.3(2)
C(b1)–C(b2)–C(a2)	107.1(2)	C(23)–C(24)–H(24a)	119.9
C(b1)–C(b2)–H(b2)	126.5	C(19)–C(24)–H(24a)	119.9
C(a2)–C(b2)–H(b2)	126.5	N(5)–C(25)–Fe(1)	176.4(2)
C(b4)–C(b3)–C(a3)	107.2(2)	N(6)–C(26)–C(27)	122.5(3)
C(b4)–C(b3)–H(b3)	126.4	N(6)–C(26)–H(26a)	118.7
C(a3)–C(b3)–H(b3)	126.4	C(27)–C(26)–H(26a)	118.7
C(b3)–C(b4)–C(a4)	107.2(2)	C(28)–C(27)–C(26)	119.0(3)
C(b3)–C(b4)–H(b4)	126.4	C(28)–C(27)–H(27a)	120.5
C(a4)–C(b4)–H(b4)	126.4	C(26)–C(27)–H(27a)	120.5
C(b6)–C(b5)–C(a5)	107.3(2)	C(27)–C(28)–C(29)	119.1(3)
C(b6)–C(b5)–H(b5)	126.3	C(27)–C(28)–H(28a)	120.4

Table S5. Continued

angle	degree	angle	degree
C(a5)–C(b5)–H(b5)	126.3	C(29)–C(28)–H(28a)	120.4
C(b5)–C(b6)–C(a6)	107.1(2)	C(28)–C(29)–C(30)	118.8(3)
C(b5)–C(b6)–H(b6)	126.4	C(28)–C(29)–H(29a)	120.6
C(a6)–C(b6)–H(b6)	126.4	C(30)–C(29)–H(29a)	120.6
C(b8)–C(b7)–C(a7)	107.2(2)	N(6)–C(30)–C(29)	122.9(3)
C(b8)–C(b7)–H(b7)	126.4	N(6)–C(30)–H(30a)	118.5
C(a7)–C(b7)–H(b7)	126.4	C(29)–C(30)–H(30a)	118.5
C(b7)–C(b8)–C(a8)	107.1(2)	C(32)#1–N(7)–C(36)	140(2)
C(b7)–C(b8)–H(b8)	126.5	C(32)#1–N(7)–C(32)	101(2)
C(a8)–C(b8)–H(b8)	126.5	C(36)–N(7)–C(32)	117.4
C(a2)–C(m1)–C(a3)	122.6(2)	C(36)–N(7)–N(7)#1	158.4(9)
C(a2)–C(m1)–C(1)	118.3(2)	N(7)–C(32)–C(33)	121.9
C(a3)–C(m1)–C(1)	119.1(2)	N(7)–C(32)–H(32)	119.0
C(a4)–C(m2)–C(a5)	122.9(2)	C(33)–C(32)–H(32)	119.0
C(a4)–C(m2)–C(7)	118.0(2)	C(34)–C(33)–C(32)	119.7
C(a5)–C(m2)–C(7)	118.8(2)	C(34)–C(33)–H(43a)	120.1
C(a7)–C(m3)–C(a6)	123.2(2)	C(32)–C(33)–H(43a)	120.1
C(a7)–C(m3)–C(13)	119.5(2)	C(33)–C(34)–C(35)	118.7
C(a6)–C(m3)–C(13)	117.1(2)	C(33)–C(34)–H(44a)	120.7
C(a1)–C(m4)–C(a8)	122.2(2)	C(35)–C(34)–H(44a)	120.7
C(a1)–C(m4)–C(19)	119.3(2)	C(36)–C(35)–C(34)	118.7
C(a8)–C(m4)–C(19)	118.5(2)	C(36)–C(35)–H(35)	120.7
C(2)–C(1)–C(6)	119.1(2)	C(34)–C(35)–H(35)	120.7
C(2)–C(1)–C(m1)	122.1(2)	N(7)–C(36)–C(35)	123.5
C(6)–C(1)–C(m1)	118.8(2)	N(7)–C(36)–H(46)	118.3
C(1)–C(2)–C(3)	120.2(3)	C(35)–C(36)–H(46)	118.3
C(1)–C(2)–H(2a)	119.9	C(37)–N(8)–C(31)	89.5(7)
C(3)–C(2)–H(2a)	119.9	N(8)–C(31)–C(37)#2	117.9(9)
C(4)–C(3)–C(2)	120.2(3)	N(8)–C(31)–H(31)	121.0
C(4)–C(3)–H(3a)	119.9	C(37)#2–C(31)–H(31)	121.0
C(2)–C(3)–H(3a)	119.9	N(8)–C(37)–C(31)#2	149.2(11)
C(3)–C(4)–C(5)	119.8(2)	N(8)–C(37)–H(37)	105.4
C(3)–C(4)–H(4a)	120.1	C(31)#2–C(37)–H(37)	105.4
C(5)–C(4)–H(4a)	120.1		

Table S5. Continued

angle	degree	angle	degree
C(4)–C(5)–C(6)	120.2(3)		

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

Table S6. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(CN)(Py)]·0.65Py[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0132(2)	0.0118(2)	0.0171(2)	0.0017(1)	0.0030(1)	0.0002(1)
N(1)	0.0144(9)	0.0147(9)	0.0194(9)	0.0024(7)	0.0019(7)	0.0006(7)
N(2)	0.0164(9)	0.0149(9)	0.0213(10)	0.0021(8)	0.0039(8)	0.0002(7)
N(3)	0.0160(9)	0.0137(9)	0.0189(9)	0.0013(7)	0.0039(7)	0.0013(7)
N(4)	0.0152(9)	0.0138(9)	0.0188(9)	0.0016(7)	0.0035(7)	−0.0012(7)
N(5)	0.0256(11)	0.0270(12)	0.0289(12)	−0.0047(10)	0.0013(9)	−0.0035(9)
N(6)	0.0220(10)	0.0158(10)	0.0208(10)	0.0022(8)	0.0046(8)	−0.0016(8)
C(A1)	0.0156(11)	0.0171(11)	0.0198(11)	0.0011(9)	0.0038(9)	0.0000(9)
C(A2)	0.0176(11)	0.0173(11)	0.0200(11)	0.0032(9)	0.0027(9)	−0.0026(9)
C(A3)	0.0198(12)	0.0144(11)	0.0215(12)	0.0027(9)	0.0031(9)	0.0006(9)
C(A4)	0.0177(11)	0.0167(12)	0.0236(12)	0.0015(9)	0.0033(9)	0.0033(9)
C(A5)	0.0172(11)	0.0173(11)	0.0222(12)	−0.0017(9)	0.0054(9)	0.0003(9)
C(A6)	0.0195(11)	0.0133(11)	0.0186(11)	−0.0009(8)	0.0055(9)	−0.0016(9)
C(A7)	0.0190(11)	0.0120(10)	0.0177(11)	0.0006(8)	0.0023(9)	−0.0009(9)
C(A8)	0.0153(10)	0.0132(11)	0.0210(11)	0.0002(9)	0.0028(9)	−0.0001(8)
C(B1)	0.0185(11)	0.0243(13)	0.0256(12)	0.0071(10)	0.0078(10)	0.0030(10)
C(B2)	0.0193(12)	0.0234(12)	0.0259(12)	0.0087(10)	0.0067(10)	0.0013(10)
C(B3)	0.0233(12)	0.0159(11)	0.0317(13)	0.0067(10)	0.0065(10)	0.0040(10)
C(B4)	0.0195(12)	0.0190(12)	0.0333(14)	0.0058(10)	0.0065(10)	0.0049(10)
C(B5)	0.0188(11)	0.0187(12)	0.0259(12)	−0.0001(9)	0.0083(9)	0.0009(9)
C(B6)	0.0206(12)	0.0160(11)	0.0224(11)	−0.0002(9)	0.0087(9)	−0.0010(9)
C(B7)	0.0193(11)	0.0149(11)	0.0207(11)	0.0018(9)	0.0020(9)	0.0003(9)
C(B8)	0.0165(11)	0.0135(11)	0.0240(12)	0.0011(9)	0.0028(9)	0.0013(9)
C(M1)	0.0193(11)	0.0164(11)	0.0213(11)	0.0045(9)	0.0026(9)	0.0002(9)
C(M2)	0.0172(11)	0.0177(11)	0.0250(12)	0.0003(9)	0.0045(9)	0.0019(9)
C(M3)	0.0210(11)	0.0129(11)	0.0180(11)	0.0001(9)	0.0040(9)	−0.0005(9)
C(M4)	0.0156(11)	0.0160(11)	0.0217(11)	0.0008(9)	0.0035(9)	−0.0003(9)
C(1)	0.0173(11)	0.0169(11)	0.0294(13)	0.0060(10)	0.0076(10)	0.0028(9)
C(2)	0.0265(13)	0.0184(12)	0.0280(13)	0.0032(10)	0.0081(10)	0.0035(10)
C(3)	0.0332(14)	0.0203(13)	0.0298(13)	0.0082(10)	0.0130(11)	0.0067(11)
C(4)	0.0260(13)	0.0178(12)	0.0438(16)	0.0091(11)	0.0164(12)	0.0028(10)
C(5)	0.0265(14)	0.0242(14)	0.0457(17)	0.0060(12)	0.0027(12)	−0.0069(11)
C(6)	0.0269(14)	0.0273(14)	0.0354(15)	0.0104(11)	−0.0001(11)	−0.0045(11)
C(7)	0.0197(12)	0.0176(12)	0.0372(14)	0.0067(10)	0.0095(10)	0.0032(9)

Table S6. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(8)	0.0207(12)	0.0192(12)	0.0417(15)	0.0069(11)	0.0066(11)	0.0003(10)
C(9)	0.0201(13)	0.0228(13)	0.0568(19)	0.0118(13)	0.0064(12)	0.0010(11)
C(10)	0.0255(15)	0.0294(16)	0.074(2)	0.0140(15)	0.0201(16)	0.0103(12)
C(11)	0.0405(18)	0.0369(17)	0.056(2)	0.0043(14)	0.0266(16)	0.0118(14)
C(12)	0.0327(15)	0.0309(15)	0.0408(16)	0.0042(12)	0.0144(13)	0.0082(12)
C(13)	0.0165(11)	0.0159(11)	0.0219(11)	0.0032(9)	0.0066(9)	0.0018(9)
C(14)	0.0231(12)	0.0187(12)	0.0246(12)	0.0015(10)	0.0051(10)	0.0003(9)
C(15)	0.0251(13)	0.0166(12)	0.0335(14)	0.0047(10)	0.0079(11)	−0.0007(10)
C(16)	0.0292(13)	0.0226(13)	0.0319(14)	0.0113(11)	0.0147(11)	0.0052(10)
C(17)	0.0430(16)	0.0267(14)	0.0224(13)	0.0022(10)	0.0127(11)	0.0025(12)
C(18)	0.0364(14)	0.0170(12)	0.0253(13)	−0.0002(10)	0.0096(11)	−0.0013(10)
C(19)	0.0195(12)	0.0185(11)	0.0207(11)	0.0065(9)	0.0060(9)	0.0038(9)
C(20)	0.0244(13)	0.0198(12)	0.0324(14)	0.0025(10)	0.0099(11)	−0.0004(10)
C(21)	0.0340(14)	0.0197(12)	0.0347(14)	0.0020(11)	0.0129(12)	0.0058(11)
C(22)	0.0280(13)	0.0272(13)	0.0294(13)	0.0104(11)	0.0135(11)	0.0128(11)
C(23)	0.0192(12)	0.0298(14)	0.0280(13)	0.0085(11)	0.0079(10)	0.0037(10)
C(24)	0.0206(12)	0.0207(12)	0.0260(12)	0.0052(10)	0.0057(10)	0.0023(10)
C(25)	0.0145(11)	0.0173(11)	0.0251(12)	0.0047(10)	0.0037(9)	0.0008(9)
C(26)	0.0303(14)	0.0222(13)	0.0258(13)	−0.0019(10)	0.0047(11)	0.0039(11)
C(27)	0.0477(18)	0.0255(14)	0.0330(15)	−0.0084(12)	0.0068(13)	0.0038(13)
C(28)	0.0482(18)	0.0267(15)	0.0325(15)	−0.0100(12)	0.0044(13)	−0.0117(13)
C(29)	0.0291(14)	0.0319(15)	0.0317(14)	−0.0045(12)	0.0028(12)	−0.0107(12)
C(30)	0.0225(12)	0.0226(12)	0.0255(12)	−0.0013(10)	0.0039(10)	−0.0034(10)
N(7)	0.121(6)	0.138(6)	0.046(4)	−0.026(5)	−0.001(5)	−0.014(5)
C(32)	0.135(7)	0.150(6)	0.077(6)	−0.028(6)	0.004(6)	−0.014(6)
C(33)	0.122(6)	0.126(6)	0.085(6)	−0.023(6)	0.003(5)	−0.008(5)
C(34)	0.132(6)	0.112(6)	0.078(6)	−0.002(5)	−0.016(5)	−0.009(5)
C(35)	0.114(6)	0.109(6)	0.076(5)	0.008(5)	−0.023(5)	−0.014(5)
C(36)	0.137(6)	0.146(6)	0.097(6)	0.008(6)	0.003(6)	−0.001(6)
N(8)	0.102(3)	0.070(2)	0.044(2)	−0.020(2)	0.026(2)	−0.016(2)
C(31)	0.102(3)	0.065(3)	0.044(2)	−0.023(2)	0.027(2)	−0.019(3)
C(37)	0.113(3)	0.086(3)	0.064(3)	−0.013(2)	0.020(2)	−0.009(3)
C(39)	0.102(3)	0.070(2)	0.044(2)	−0.020(2)	0.026(2)	−0.016(2)
C(40)	0.102(3)	0.065(3)	0.044(2)	−0.023(2)	0.027(2)	−0.019(3)

Table S6. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(38)	0.113(3)	0.086(3)	0.064(3)	−0.013(2)	0.020(2)	−0.009(3)

[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 S7. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(CN)(Py)]·0.65Py[a]

atom	x	y	z	U(eq)
H(B1	0.9550	0.2018	0.7036	0.027
H(B2	0.8750	0.2973	0.6730	0.027
H(B3	0.5234	0.3873	0.7244	0.028
H(B4	0.3704	0.3475	0.7776	0.029
H(B5	0.3162	0.1661	0.9895	0.025
H(B6	0.4402	0.0988	1.0901	0.023
H(B7	0.8351	0.0423	1.1088	0.022
H(B8	0.9517	0.0561	0.9936	0.022
H(2A)	0.6334	0.3633	0.5743	0.029
H(3A)	0.6800	0.4506	0.5159	0.032
H(4A)	0.7997	0.5096	0.6168	0.033
H(5A)	0.8763	0.4807	0.7753	0.040
H(6A)	0.8315	0.3935	0.8339	0.037
H(8A)	0.2418	0.2557	0.7281	0.033
H(9A)	0.0733	0.2882	0.7270	0.040
H(10A)	0.0274	0.3139	0.8725	0.050
H(11A)	0.1499	0.3072	1.0196	0.051
H(12A)	0.3188	0.2747	1.0216	0.041
H(14A)	0.5952	−0.0089	1.0445	0.027
H(15A)	0.5597	−0.0716	1.1623	0.030
H(16A)	0.5830	−0.0426	1.3246	0.032
H(17A)	0.6449	0.0486	1.3699	0.036
H(18A)	0.6771	0.1121	1.2517	0.031
H(20A)	0.8903	0.0357	0.7750	0.030
H(21A)	1.0260	−0.0128	0.7266	0.034
H(22A)	1.1915	0.0286	0.7478	0.033
H(23A)	1.2216	0.1180	0.8199	0.030
H(24A)	1.0857	0.1679	0.8654	0.027
H(26A)	0.5963	0.2945	1.0032	0.032
H(27A)	0.6748	0.3632	1.1149	0.043
H(28A)	0.8562	0.3616	1.1729	0.044
H(29A)	0.9540	0.2894	1.1198	0.038
H(30A)	0.8694	0.2234	1.0073	0.028
H(32)	0.9812	−0.0533	0.5016	0.148

Table S7. Continued

atom	x	y	z	U(eq)
H(43A)	0.8218	−0.0644	0.5461	0.137
H(44A)	0.7209	0.0156	0.5625	0.136
H(35)	0.7893	0.1063	0.5433	0.128
H(46)	0.9482	0.1136	0.4986	0.156
H(31)	0.6423	0.0533	0.5856	0.082
H(37)	0.3600	0.0391	0.4697	0.105
H(39)	0.4857	0.1144	0.4860	0.085
H(40)	0.6423	0.0533	0.5856	0.082
H(38)	0.3600	0.0391	0.4697	0.105

[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 S8. Complete Crystallographic Details for [Fe(TPP)(CN)(1-MeIm)]·1-MeIm·$CHCl_3$

formula	$C_{54}H_{41}Cl_3FeN_9$
FW, amu	978.16
a, Å	20.7612(3)
b, Å	9.7535(1)
c, Å	26.5363(4)
β, deg	121.109(1)
V, Å^3	4600.67(11)
space group	P21/c
Z	4
D_c, g/cm^3	1.412
F(000)	2020
μ, mm^{-1}	0.552
crystal dimensions, mm	0.42 × 0.23 × 0.07
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.15–34.35
index range	$-32 \leq h \leq 23$
	$-9 \leq k \leq 15$
	$-39 \leq l \leq 42$
total data collected	79823
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.962 and 0.858
unique data	19164 (R_{int} = 0.031)
unique observed data [I > 2σ(I)]	13118
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	19164/0/606
goodness-of-fit (pased on F^2)	1.111
final R indices [I > 2σ(I)]	R_1 = 0.0462, wR_2 = 0.1281
final R indices (all data)	R_1 = 0.0765, wR_2 = 0.1380

Table S9. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CN)(1-MeIm)]·1-MeIm·$CHCl_3$[a]

atom	x	y	z	U(eq)
Fe(1)	0.28494(1)	0.78715(2)	0.02497(1)	0.0102(1)
N(1)	0.39374(6)	0.78304(12)	0.05054(5)	0.0116(2)
N(2)	0.25716(6)	0.73905(12)	−0.05667(5)	0.0121(2)
N(3)	0.17621(6)	0.79680(12)	−0.00082(5)	0.0117(2)
N(4)	0.31334(6)	0.82403(12)	0.10788(5)	0.0121(2)
N(5)	0.28177(6)	0.98782(12)	0.00578(5)	0.0139(2)
N(6)	0.24233(7)	1.19056(12)	−0.03510(5)	0.0157(2)
N(7)	0.28377(7)	0.48097(14)	0.05269(5)	0.0200(3)
N(8)	0.27580(7)	0.43456(16)	0.29593(6)	0.0257(3)
N(9)	0.28239(10)	0.2151(2)	0.31728(9)	0.0510(5)
C(a1)	0.45469(8)	0.80098(14)	0.10670(6)	0.0122(2)
C(a2)	0.42363(7)	0.76953(14)	0.01506(6)	0.0122(2)
C(a3)	0.30605(8)	0.71232(14)	−0.07581(6)	0.0134(3)
C(a4)	0.18621(8)	0.71197(15)	−0.10378(6)	0.0132(3)
C(a5)	0.11563(8)	0.78016(14)	−0.05698(6)	0.0126(2)
C(a6)	0.14657(7)	0.83387(14)	0.03316(6)	0.0123(2)
C(a7)	0.26488(8)	0.83512(14)	0.12855(6)	0.0121(2)
C(a8)	0.38458(8)	0.81485(14)	0.15744(6)	0.0119(2)
C(b1)	0.52331(8)	0.80470(15)	0.10560(6)	0.0145(3)
C(b2)	0.50404(8)	0.78667(15)	0.04883(6)	0.0152(3)
C(b3)	0.26489(8)	0.66479(16)	−0.13583(6)	0.0168(3)
C(b4)	0.19126(8)	0.66347(16)	−0.15294(6)	0.0175(3)
C(b5)	0.04706(8)	0.81572(15)	−0.05881(6)	0.0142(3)
C(b6)	0.06599(8)	0.85015(15)	−0.00357(6)	0.0143(3)
C(b7)	0.30643(8)	0.83018(15)	0.19187(6)	0.0142(3)
C(b8)	0.38008(8)	0.81681(15)	0.20967(6)	0.0141(3)
C(m1)	0.38359(8)	0.73280(14)	−0.04402(6)	0.0125(3)
C(m2)	0.11892(8)	0.73472(15)	−0.10532(6)	0.0134(3)
C(m3)	0.18682(8)	0.84816(14)	0.09423(6)	0.0124(2)
C(m4)	0.45206(8)	0.80843(14)	0.15793(6)	0.0128(3)
C(1)	0.42666(8)	0.71062(15)	−0.07431(6)	0.0134(3)
C(2)	0.45405(9)	0.58162(17)	−0.07577(7)	0.0237(3)
C(3)	0.49712(10)	0.56355(19)	−0.10145(8)	0.0290(4)
C(4)	0.51187(9)	0.67297(19)	−0.12706(7)	0.0231(3)

Table S9. Continued

atom	x	y	z	U(eq)
C(5)	0.48367(9)	0.80101(18)	−0.12654(6)	0.0214(3)
C(6)	0.44171(8)	0.81982(16)	−0.09993(6)	0.0180(3)
C(7)	0.04644(8)	0.71124(15)	−0.16209(6)	0.0143(3)
C(8)	−0.00122(8)	0.60426(16)	−0.16742(6)	0.0187(3)
C(9)	−0.06909(9)	0.58430(18)	−0.22011(7)	0.0223(3)
C(10)	−0.09004(9)	0.67117(18)	−0.26732(7)	0.0226(3)
C(11)	−0.04276(9)	0.77758(17)	−0.26220(6)	0.0203(3)
C(12)	0.02519(8)	0.79747(16)	−0.21003(6)	0.0172(3)
C(13)	0.14416(7)	0.87241(15)	0.12473(6)	0.0129(3)
C(14)	0.09103(8)	0.77694(16)	0.12014(7)	0.0180(3)
C(15)	0.05212(9)	0.79843(16)	0.14896(7)	0.0203(3)
C(16)	0.06540(8)	0.91566(17)	0.18285(6)	0.0202(3)
C(17)	0.11741(8)	1.01057(17)	0.18778(6)	0.0191(3)
C(18)	0.15700(8)	0.98968(16)	0.15886(6)	0.0161(3)
C(19)	0.52403(8)	0.80767(15)	0.21596(6)	0.0129(3)
C(20)	0.56113(8)	0.68436(15)	0.24031(6)	0.0175(3)
C(21)	0.62502(8)	0.68077(16)	0.29607(6)	0.0197(3)
C(22)	0.65379(8)	0.80113(16)	0.32806(6)	0.0181(3)
C(23)	0.61950(8)	0.92513(16)	0.30351(6)	0.0169(3)
C(24)	0.55448(8)	0.92814(15)	0.24788(6)	0.0156(3)
C(25)	0.28587(7)	0.59593(15)	0.04219(6)	0.0134(3)
C(26)	0.34109(9)	1.07874(17)	0.03042(8)	0.0269(4)
C(27)	0.31703(9)	1.20367(17)	0.00548(8)	0.0260(4)
C(28)	0.22328(8)	1.05971(15)	−0.03384(6)	0.0153(3)
C(29)	0.19211(9)	1.29906(16)	−0.07329(7)	0.0205(3)
C(30)	0.26906(12)	0.5636(2)	0.26556(9)	0.0362(4)
C(31)	0.28600(9)	0.4194(2)	0.35105(8)	0.0354(5)
C(32)	0.29017(9)	0.2890(2)	0.36468(7)	0.0275(4)
C(33)	0.27252(9)	0.30417(16)	0.27405(7)	0.0203(3)
C(34)	0.14203(9)	0.36611(17)	0.05029(7)	0.0215(3)
Cl(1)	0.13120(3)	0.19128(4)	0.03148(2)	0.0311(1)
Cl(2)	0.07682(2)	0.46734(5)	−0.00922(2)	0.0314(1)
Cl(3)	0.13157(3)	0.39090(5)	0.11184(2)	0.0306(1)

[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 S10. Bond Lengths for [Fe(TPP)(CN)(1-MeIm)]·1-MeIm·$CHCl_3$[a]

bond	length (Å)	bond	length (Å)
Fe(1)–C(25)	1.9179(15)	C(2)–H(29)	0.9500
Fe(1)–N(2)	1.9889(11)	C(3)–C(4)	1.382(2)
Fe(1)–N(3)	1.9941(12)	C(3)–H(30)	0.9500
Fe(1)–N(4)	1.9943(11)	C(4)–C(5)	1.382(2)
Fe(1)–N(1)	1.9952(11)	C(4)–H(31)	0.9500
Fe(1)–N(5)	2.0149(12)	C(5)–C(6)	1.388(2)
N(1)–C(a2)	1.3758(17)	C(5)–H(32)	0.9500
N(1)–C(a1)	1.3800(17)	C(6)–H(33)	0.9500
N(2)–C(a3)	1.3742(17)	C(7)–C(12)	1.393(2)
N(2)–C(a4)	1.3782(17)	C(7)–C(8)	1.394(2)
N(3)–C(a5)	1.3757(17)	C(8)–C(9)	1.394(2)
N(3)–C(a6)	1.3768(17)	C(8)–H(18)	0.9500
N(4)–C(a7)	1.3763(17)	C(9)–C(10)	1.383(2)
N(4)–C(a8)	1.3839(17)	C(9)–H(19)	0.9500
N(5)–C(28)	1.3237(18)	C(10)–C(11)	1.386(2)
N(5)–C(26)	1.378(2)	C(10)–H(20)	0.9500
N(6)–C(28)	1.3416(19)	C(11)–C(12)	1.388(2)
N(6)–C(27)	1.362(2)	C(11)–H(21)	0.9500
N(6)–C(29)	1.4635(19)	C(12)–H(22)	0.9500
N(7)–C(25)	1.1616(19)	C(13)–C(18)	1.396(2)
N(8)–C(31)	1.373(2)	C(13)–C(14)	1.400(2)
N(8)–C(33)	1.385(2)	C(14)–C(15)	1.385(2)
N(8)–C(30)	1.462(2)	C(14)–H(11)	0.9500
N(9)–C(33)	1.367(2)	C(15)–C(16)	1.391(2)
N(9)–C(32)	1.385(3)	C(15)–H(10)	0.9500
C(a1)–C(m4)	1.3901(19)	C(16)–C(17)	1.376(2)
C(a1)–C(b1)	1.4405(19)	C(16)–H(9)	0.9500
C(a2)–C(m1)	1.3894(19)	C(17)–C(18)	1.399(2)
C(a2)–C(b2)	1.4395(19)	C(17)–H(8)	0.9500
C(a3)–C(m1)	1.3927(19)	C(18)–H(7)	0.9500
C(a3)–C(b3)	1.4407(19)	C(19)–C(20)	1.394(2)
C(a4)–C(m2)	1.3942(19)	C(19)–C(24)	1.394(2)
C(a4)–C(b4)	1.4414(19)	C(20)–C(21)	1.386(2)
C(a5)–C(m2)	1.3917(19)	C(20)–H(44)	0.9500

Table S10. Continued

bond	length (Å)	bond	length (Å)
C(a5)–C(b5)	1.442(2)	C(21)–C(22)	1.390(2)
C(a6)–C(m3)	1.3945(18)	C(21)–H(43)	0.9500
C(a6)–C(b6)	1.4454(19)	C(22)–C(23)	1.384(2)
C(a7)–C(m3)	1.3953(19)	C(22)–H(42)	0.9500
C(a7)–C(b7)	1.4395(18)	C(23)–C(24)	1.3939(19)
C(a8)–C(m4)	1.3957(19)	C(23)–H(41)	0.9500
C(a8)–C(b8)	1.4368(19)	C(24)–H(40)	0.9500
C(b1)–C(b2)	1.3555(19)	C(26)–C(27)	1.353(2)
C(b1)–H(36)	0.9500	C(26)–H(49)	0.9500
C(b2)–H(35)	0.9500	C(27)–H(48)	0.9500
C(b3)–C(b4)	1.351(2)	C(28)–H(46)	0.9500
C(b3)–H(25)	0.9500	C(29)–H(47a)	0.9800
C(b4)–H(24)	0.9500	C(29)–H(47b)	0.9800
C(b5)–C(b6)	1.3493(19)	C(29)–H(47C)	0.9800
C(b5)–H(14)	0.9500	C(30)–H(50a)	0.9800
C(b6)–H(13)	0.9500	C(30)–H(50b)	0.9800
C(b7)–C(b8)	1.354(2)	C(30)–H(50C)	0.9800
C(b7)–H(3)	0.9500	C(31)–C(32)	1.313(3)
C(b8)–H(2)	0.9500	C(31)–H(51)	0.9500
C(m1)–C(1)	1.4952(19)	C(32)–H(52)	0.9500
C(m2)–C(7)	1.4979(19)	C(33)–H(53)	0.9500
C(m3)–C(13)	1.4956(19)	C(34)–Cl(1)	1.7582(17)
C(m4)–C(19)	1.4921(19)	C(34)–Cl(2)	1.7584(16)
C(1)–C(6)	1.383(2)	C(34)–Cl(3)	1.7722(16)
C(1)–C(2)	1.389(2)	C(34)–H(54)	1.0000
C(2)–C(3)	1.387(2)		

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

Table S11. Bond Angles for [Fe(TPP)(CN)(1-MeIm)]·1-MeIm·$CHCl_3$[a]

angle	degree	angle	degree
C(25)–Fe(1)–N(2)	89.52(5)	C(4)–C(3)–H(30)	119.8
C(25)–Fe(1)–N(3)	89.89(5)	C(2)–C(3)–H(30)	119.8
N(2)–Fe(1)–N(3)	89.86(5)	C(3)–C(4)–C(5)	119.36(14)
C(25)–Fe(1)–N(4)	87.24(5)	C(3)–C(4)–H(31)	120.3
N(2)–Fe(1)–N(4)	176.75(5)	C(5)–C(4)–H(31)	120.3
N(3)–Fe(1)–N(4)	90.41(5)	C(4)–C(5)–C(6)	120.31(15)
C(25)–Fe(1)–N(1)	91.67(5)	C(4)–C(5)–H(32)	119.8
N(2)–Fe(1)–N(1)	90.33(5)	C(6)–C(5)–H(32)	119.8
N(3)–Fe(1)–N(1)	178.43(5)	C(1)–C(6)–C(5)	120.57(15)
N(4)–Fe(1)–N(1)	89.49(5)	C(1)–C(6)–H(33)	119.7
C(25)–Fe(1)–N(5)	178.88(6)	C(5)–C(6)–H(33)	119.7
N(2)–Fe(1)–N(5)	90.03(5)	C(12)–C(7)–C(8)	119.07(13)
N(3)–Fe(1)–N(5)	89.08(5)	C(12)–C(7)–C(m2)	120.38(13)
N(4)–Fe(1)–N(5)	93.22(5)	C(8)–C(7)–C(m2)	120.54(13)
N(1)–Fe(1)–N(5)	89.36(5)	C(9)–C(8)–C(7)	120.21(14)
C(a2)–N(1)–C(a1)	105.38(11)	C(9)–C(8)–H(18)	119.9
C(a2)–N(1)–Fe(1)	126.94(9)	C(7)–C(8)–H(18)	119.9
C(a1)–N(1)–Fe(1)	127.58(9)	C(10)–C(9)–C(8)	120.32(15)
C(a3)–N(2)–C(a4)	106.01(11)	C(10)–C(9)–H(19)	119.8
C(a3)–N(2)–Fe(1)	126.41(9)	C(8)–C(9)–H(19)	119.8
C(a4)–N(2)–Fe(1)	127.28(9)	C(9)–C(10)–C(11)	119.63(14)
C(a5)–N(3)–C(a6)	105.83(11)	C(9)–C(10)–H(20)	120.2
C(a5)–N(3)–Fe(1)	127.26(9)	C(11)–C(10)–H(20)	120.2
C(a6)–N(3)–Fe(1)	126.68(9)	C(10)–C(11)–C(12)	120.39(14)
C(a7)–N(4)–C(a8)	105.60(11)	C(10)–C(11)–H(21)	119.8
C(a7)–N(4)–Fe(1)	126.40(9)	C(12)–C(11)–H(21)	119.8
C(a8)–N(4)–Fe(1)	126.74(9)	C(11)–C(12)–C(7)	120.38(14)
C(28)–N(5)–C(26)	105.32(13)	C(11)–C(12)–H(22)	119.8
C(28)–N(5)–Fe(1)	127.74(10)	C(7)–C(12)–H(22)	119.8
C(26)–N(5)–Fe(1)	126.92(10)	C(18)–C(13)–C(14)	118.62(13)
C(28)–N(6)–C(27)	107.42(12)	C(18)–C(13)–C(m3)	120.83(12)
C(28)–N(6)–C(29)	126.25(13)	C(14)–C(13)–C(m3)	120.54(12)
C(27)–N(6)–C(29)	126.32(13)	C(15)–C(14)–C(13)	120.61(14)
C(31)–N(8)–C(33)	107.15(16)	C(15)–C(14)–H(11)	119.7

Table S11. Continued

angle	degree	angle	degree
C(31)–N(8)–C(30)	126.72(17)	C(13)–C(14)–H(11)	119.7
C(33)–N(8)–C(30)	126.13(14)	C(14)–C(15)–C(16)	120.25(14)
C(33)–N(9)–C(32)	109.16(18)	C(14)–C(15)–H(10)	119.9
N(1)–C(a1)–C(m4)	125.84(12)	C(16)–C(15)–H(10)	119.9
N(1)–C(a1)–C(b1)	110.23(11)	C(17)–C(16)–C(15)	119.86(13)
C(m4)–C(a1)–C(b1)	123.88(12)	C(17)–C(16)–H(9)	120.1
N(1)–C(a2)–C(m1)	125.34(12)	C(15)–C(16)–H(9)	120.1
N(1)–C(a2)–C(b2)	110.54(11)	C(16)–C(17)–C(18)	120.29(14)
C(m1)–C(a2)–C(b2)	123.91(13)	C(16)–C(17)–H(8)	119.9
N(2)–C(a3)–C(m1)	126.31(12)	C(18)–C(17)–H(8)	119.9
N(2)–C(a3)–C(b3)	109.88(12)	C(13)–C(18)–C(17)	120.37(14)
C(m1)–C(a3)–C(b3)	123.75(13)	C(13)–C(18)–H(7)	119.8
N(2)–C(a4)–C(m2)	125.55(12)	C(17)–C(18)–H(7)	119.8
N(2)–C(a4)–C(b4)	109.89(12)	C(20)–C(19)–C(24)	118.49(13)
C(m2)–C(a4)–C(b4)	124.47(13)	C(20)–C(19)–C(m4)	120.10(13)
N(3)–C(a5)–C(m2)	125.69(12)	C(24)–C(19)–C(m4)	121.38(13)
N(3)–C(a5)–C(b5)	110.01(12)	C(21)–C(20)–C(19)	120.75(14)
C(m2)–C(a5)–C(b5)	124.30(12)	C(21)–C(20)–H(44)	119.6
N(3)–C(a6)–C(m3)	125.81(12)	C(19)–C(20)–H(44)	119.6
N(3)–C(a6)–C(b6)	109.91(11)	C(20)–C(21)–C(22)	120.19(14)
C(m3)–C(a6)–C(b6)	124.23(12)	C(20)–C(21)–H(43)	119.9
N(4)–C(a7)–C(m3)	126.06(12)	C(22)–C(21)–H(43)	119.9
N(4)–C(a7)–C(b7)	110.00(12)	C(23)–C(22)–C(21)	119.77(14)
C(m3)–C(a7)–C(b7)	123.94(12)	C(23)–C(22)–H(42)	120.1
N(4)–C(a8)–C(m4)	125.93(12)	C(21)–C(22)–H(42)	120.1
N(4)–C(a8)–C(b8)	110.21(12)	C(22)–C(23)–C(24)	119.88(14)
C(m4)–C(a8)–C(b8)	123.84(12)	C(22)–C(23)–H(41)	120.1
C(b2)–C(b1)–C(a1)	107.00(12)	C(24)–C(23)–H(41)	120.1
C(b2)–C(b1)–H(36)	126.5	C(23)–C(24)–C(19)	120.84(14)
C(a1)–C(b1)–H(36)	126.5	C(23)–C(24)–H(40)	119.6
C(b1)–C(b2)–C(a2)	106.76(12)	C(19)–C(24)–H(40)	119.6
C(b1)–C(b2)–H(35)	126.6	N(7)–C(25)–Fe(1)	177.18(13)
C(a2)–C(b2)–H(35)	126.6	C(27)–C(26)–N(5)	109.51(14)
C(b4)–C(b3)–C(a3)	107.23(12)	C(27)–C(26)–H(49)	125.2

Table S11. Continued

angle	degree	angle	degree
C(b4)–C(b3)–H(25)	126.4	N(5)–C(26)–H(49)	125.2
C(a3)–C(b3)–H(25)	126.4	C(26)–C(27)–N(6)	106.50(14)
C(b3)–C(b4)–C(a4)	106.95(12)	C(26)–C(27)–H(48)	126.8
C(b3)–C(b4)–H(24)	126.5	N(6)–C(27)–H(48)	126.8
C(a4)–C(b4)–H(24)	126.5	N(5)–C(28)–N(6)	111.25(13)
C(b6)–C(b5)–C(a5)	107.16(12)	N(5)–C(28)–H(46)	124.4
C(b6)–C(b5)–H(14)	126.4	N(6)–C(28)–H(46)	124.4
C(a5)–C(b5)–H(14)	126.4	N(6)–C(29)–H(47a)	109.5
C(b5)–C(b6)–C(a6)	106.93(12)	N(6)–C(29)–H(47b)	109.5
C(b5)–C(b6)–H(13)	126.5	H(47a)–C(29)–H(47b)	109.5
C(a6)–C(b6)–H(13)	126.5	N(6)–C(29)–H(47C)	109.5
C(b8)–C(b7)–C(a7)	107.35(12)	H(47a)–C(29)–H(47C)	109.5
C(b8)–C(b7)–H(3)	126.3	H(47b)–C(29)–H(47C)	109.5
C(a7)–C(b7)–H(3)	126.3	N(8)–C(30)–H(50a)	109.5
C(b7)–C(b8)–C(a8)	106.82(12)	N(8)–C(30)–H(50b)	109.5
C(b7)–C(b8)–H(2)	126.6	H(50a)–C(30)–H(50b)	109.5
C(a8)–C(b8)–H(2)	126.6	N(8)–C(30)–H(50C)	109.5
C(a2)–C(m1)–C(a3)	123.43(12)	H(50a)–C(30)–H(50C)	109.5
C(a2)–C(m1)–C(1)	117.94(12)	H(50b)–C(30)–H(50C)	109.5
C(a3)–C(m1)–C(1)	118.61(12)	C(32)–C(31)–N(8)	110.47(18)
C(a5)–C(m2)–C(a4)	123.32(12)	C(32)–C(31)–H(51)	124.8
C(a5)–C(m2)–C(7)	118.26(12)	N(8)–C(31)–H(51)	124.8
C(a4)–C(m2)–C(7)	118.42(12)	C(31)–C(32)–N(9)	107.08(16)
C(a6)–C(m3)–C(a7)	123.09(12)	C(31)–C(32)–H(52)	126.5
C(a6)–C(m3)–C(13)	118.55(12)	N(9)–C(32)–H(52)	126.5
C(a7)–C(m3)–C(13)	118.30(11)	N(9)–C(33)–N(8)	106.13(15)
C(a1)–C(m4)–C(a8)	122.65(12)	N(9)–C(33)–H(53)	126.9
C(a1)–C(m4)–C(19)	119.00(12)	N(8)–C(33)–H(53)	126.9
C(a8)–C(m4)–C(19)	118.35(12)	Cl(1)–C(34)–Cl(2)	111.32(9)
C(6)–C(1)–C(2)	118.95(13)	Cl(1)–C(34)–Cl(3)	109.59(9)
C(6)–C(1)–C(m1)	120.16(13)	Cl(2)–C(34)–Cl(3)	110.30(9)
C(2)–C(1)–C(m1)	120.87(13)	Cl(1)–C(34)–H(54)	108.5
C(3)–C(2)–C(1)	120.38(15)	Cl(2)–C(34)–H(54)	108.5
C(3)–C(2)–H(29)	119.8	Cl(3)–C(34)–H(54)	108.5

Table S11. Continued

angle	degree	angle	degree
C(1)–C(2)–H(29)	119.8		
C(4)–C(3)–C(2)	120.41(16)		

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

Table S12. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(CN)(1-MeIm)]·1-MeIm·$CHCl_3$[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0093(1)	0.0119(1)	0.0094(1)	−0.0004(1)	0.0047(1)	−0.0001(1)
N(1)	0.0106(5)	0.0134(5)	0.0106(5)	−0.0008(4)	0.0053(4)	−0.0007(4)
N(2)	0.0112(5)	0.0148(6)	0.0104(5)	−0.0012(4)	0.0056(4)	0.0001(4)
N(3)	0.0103(5)	0.0138(5)	0.0105(5)	−0.0003(4)	0.0051(4)	0.0003(4)
N(4)	0.0101(5)	0.0151(5)	0.0112(5)	−0.0007(4)	0.0054(4)	0.0001(4)
N(5)	0.0138(5)	0.0141(6)	0.0130(5)	−0.0009(4)	0.0064(4)	−0.0004(4)
N(6)	0.0173(6)	0.0135(6)	0.0160(5)	0.0009(4)	0.0083(5)	0.0016(5)
N(7)	0.0212(6)	0.0188(6)	0.0183(6)	0.0022(5)	0.0090(5)	−0.0003(5)
N(8)	0.0205(7)	0.0342(8)	0.0234(7)	−0.0051(6)	0.0122(6)	−0.0046(6)
N(9)	0.0327(10)	0.0719(15)	0.0454(11)	0.0095(10)	0.0180(9)	−0.0050(9)
C(A1)	0.0102(6)	0.0133(6)	0.0119(5)	0.0005(5)	0.0048(5)	0.0002(5)
C(A2)	0.0106(6)	0.0133(6)	0.0130(6)	0.0003(5)	0.0063(5)	−0.0002(5)
C(A3)	0.0133(6)	0.0153(6)	0.0115(5)	0.0002(5)	0.0064(5)	0.0010(5)
C(A4)	0.0112(6)	0.0164(7)	0.0107(5)	−0.0008(5)	0.0046(5)	−0.0008(5)
C(A5)	0.0111(6)	0.0131(6)	0.0123(5)	−0.0001(5)	0.0052(5)	−0.0006(5)
C(A6)	0.0111(6)	0.0129(6)	0.0132(6)	−0.0007(5)	0.0066(5)	−0.0002(5)
C(A7)	0.0134(6)	0.0114(6)	0.0124(5)	−0.0009(5)	0.0073(5)	−0.0008(5)
C(A8)	0.0111(6)	0.0135(6)	0.0107(5)	−0.0012(5)	0.0053(5)	−0.0004(5)
C(B1)	0.0097(6)	0.0192(7)	0.0130(6)	−0.0004(5)	0.0048(5)	0.0000(5)
C(B2)	0.0118(6)	0.0198(7)	0.0153(6)	0.0000(5)	0.0079(5)	−0.0002(5)
C(B3)	0.0172(7)	0.0223(7)	0.0129(6)	−0.0035(5)	0.0092(5)	0.0004(6)
C(B4)	0.0165(7)	0.0235(8)	0.0117(6)	−0.0042(5)	0.0067(5)	−0.0012(6)
C(B5)	0.0101(6)	0.0172(7)	0.0135(6)	0.0003(5)	0.0048(5)	0.0001(5)
C(B6)	0.0104(6)	0.0171(7)	0.0150(6)	−0.0010(5)	0.0062(5)	0.0013(5)
C(B7)	0.0147(6)	0.0169(7)	0.0123(6)	−0.0001(5)	0.0079(5)	−0.0006(5)
C(B8)	0.0138(6)	0.0173(7)	0.0098(5)	−0.0006(5)	0.0051(5)	−0.0007(5)
C(M1)	0.0138(6)	0.0132(6)	0.0126(6)	0.0006(5)	0.0082(5)	0.0003(5)
C(M2)	0.0113(6)	0.0156(7)	0.0111(5)	0.0008(5)	0.0042(5)	−0.0008(5)
C(M3)	0.0124(6)	0.0126(6)	0.0130(6)	−0.0018(5)	0.0072(5)	−0.0010(5)
C(M4)	0.0108(6)	0.0145(6)	0.0110(5)	−0.0007(5)	0.0041(5)	−0.0009(5)
C(1)	0.0112(6)	0.0171(7)	0.0121(5)	−0.0008(5)	0.0062(5)	−0.0004(5)
C(2)	0.0315(9)	0.0183(7)	0.0326(8)	0.0007(7)	0.0246(8)	0.0014(7)
C(3)	0.0347(9)	0.0245(9)	0.0394(10)	−0.0030(8)	0.0273(8)	0.0056(7)
C(4)	0.0178(7)	0.0372(10)	0.0196(7)	−0.0058(7)	0.0134(6)	−0.0034(7)

Table S12. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(5)	0.0188(7)	0.0308(9)	0.0157(6)	0.0017(6)	0.0097(6)	−0.0049(6)
C(6)	0.0171(7)	0.0201(7)	0.0166(6)	0.0020(6)	0.0086(6)	0.0007(6)
C(7)	0.0107(6)	0.0196(7)	0.0113(5)	−0.0031(5)	0.0049(5)	0.0004(5)
C(8)	0.0172(7)	0.0215(7)	0.0152(6)	−0.0009(6)	0.0068(6)	−0.0018(6)
C(9)	0.0171(7)	0.0271(8)	0.0197(7)	−0.0077(6)	0.0074(6)	−0.0077(6)
C(10)	0.0137(7)	0.0338(9)	0.0153(6)	−0.0069(6)	0.0041(6)	0.0021(6)
C(11)	0.0171(7)	0.0294(9)	0.0115(6)	−0.0001(6)	0.0052(5)	0.0054(6)
C(12)	0.0146(7)	0.0225(8)	0.0138(6)	−0.0004(5)	0.0068(5)	0.0006(6)
C(13)	0.0113(6)	0.0153(6)	0.0117(5)	0.0010(5)	0.0055(5)	0.0020(5)
C(14)	0.0181(7)	0.0186(7)	0.0207(7)	−0.0019(6)	0.0125(6)	−0.0013(6)
C(15)	0.0188(7)	0.0221(8)	0.0257(7)	0.0021(6)	0.0155(6)	−0.0004(6)
C(16)	0.0191(7)	0.0287(8)	0.0174(6)	0.0036(6)	0.0126(6)	0.0057(6)
C(17)	0.0204(7)	0.0223(8)	0.0158(6)	−0.0027(6)	0.0102(6)	0.0031(6)
C(18)	0.0143(6)	0.0192(7)	0.0145(6)	−0.0018(5)	0.0073(5)	−0.0003(5)
C(19)	0.0097(6)	0.0175(7)	0.0117(5)	−0.0005(5)	0.0057(5)	−0.0002(5)
C(20)	0.0156(7)	0.0156(7)	0.0172(6)	−0.0027(5)	0.0056(6)	−0.0010(5)
C(21)	0.0167(7)	0.0186(7)	0.0185(7)	0.0010(6)	0.0053(6)	0.0045(6)
C(22)	0.0126(6)	0.0251(8)	0.0134(6)	−0.0022(6)	0.0045(5)	−0.0009(6)
C(23)	0.0166(7)	0.0192(7)	0.0130(6)	−0.0028(5)	0.0062(5)	−0.0048(6)
C(24)	0.0169(7)	0.0146(6)	0.0139(6)	0.0004(5)	0.0069(5)	−0.0005(5)
C(25)	0.0109(6)	0.0183(7)	0.0110(5)	−0.0011(5)	0.0057(5)	−0.0008(5)
C(26)	0.0154(7)	0.0174(8)	0.0322(9)	0.0003(7)	0.0012(7)	−0.0013(6)
C(27)	0.0157(7)	0.0165(7)	0.0338(9)	0.0008(7)	0.0043(7)	−0.0029(6)
C(28)	0.0151(6)	0.0147(7)	0.0148(6)	−0.0002(5)	0.0067(5)	−0.0009(5)
C(29)	0.0239(8)	0.0163(7)	0.0169(6)	0.0029(5)	0.0074(6)	0.0048(6)
C(30)	0.0476(12)	0.0272(9)	0.0393(10)	−0.0068(8)	0.0263(9)	−0.0134(9)
C(31)	0.0171(8)	0.0664(14)	0.0232(8)	−0.0053(9)	0.0107(7)	−0.0149(9)
C(32)	0.0162(7)	0.0491(12)	0.0162(7)	0.0027(7)	0.0077(6)	−0.0096(7)
C(33)	0.0165(7)	0.0251(8)	0.0185(7)	−0.0017(6)	0.0084(6)	0.0010(6)
C(34)	0.0187(7)	0.0216(8)	0.0248(7)	0.0044(6)	0.0117(6)	0.0023(6)
Cl(1)	0.0430(3)	0.0216(2)	0.0420(2)	0.0003(2)	0.0315(2)	0.0022(2)
Cl(2)	0.0265(2)	0.0350(2)	0.0303(2)	0.0128(2)	0.0130(2)	0.0106(2)
Cl(3)	0.0361(2)	0.0317(2)	0.0248(2)	−0.0029(2)	0.0162(2)	0.0002(2)

[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 S13. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CN)(1-MeIm)]·1-MeIm·$CHCl_3$[a]

atom	x	y	z	U(eq)
H(36)	0.5727	0.8174	0.1384	0.017
H(35)	0.5372	0.7856	0.0342	0.018
H(25)	0.2856	0.6391	−0.1591	0.020
H(24)	0.1506	0.6358	−0.1903	0.021
H(14)	−0.0022	0.8150	−0.0926	0.017
H(13)	0.0327	0.8795	0.0088	0.017
H(3)	0.2859	0.8354	0.2166	0.017
H(2)	0.4210	0.8100	0.2491	0.017
H(29)	0.4432	0.5054	−0.0591	0.028
H(30)	0.5166	0.4754	−0.1014	0.035
H(31)	0.5411	0.6603	−0.1448	0.028
H(32)	0.4930	0.8765	−0.1445	0.026
H(33)	0.4232	0.9085	−0.0993	0.022
H(18)	0.0126	0.5448	−0.1350	0.022
H(19)	−0.1011	0.5107	−0.2236	0.027
H(20)	−0.1366	0.6580	−0.3031	0.027
H(21)	−0.0570	0.8372	−0.2946	0.024
H(22)	0.0574	0.8703	−0.2070	0.021
H(11)	0.0816	0.6967	0.0971	0.022
H(10)	0.0162	0.7329	0.1456	0.024
H(9)	0.0386	0.9302	0.2025	0.024
H(8)	0.1265	1.0906	0.2109	0.023
H(7)	0.1928	1.0557	0.1625	0.019
H(44)	0.5424	0.6018	0.2184	0.021
H(43)	0.6492	0.5958	0.3125	0.024
H(42)	0.6969	0.7983	0.3666	0.022
H(41)	0.6402	1.0081	0.3245	0.020
H(40)	0.5306	1.0133	0.2315	0.019
H(49)	0.3912	1.0570	0.0603	0.032
H(48)	0.3465	1.2846	0.0145	0.031
H(46)	0.1742	1.0234	−0.0582	0.018
H(47A)	0.1402	1.2650	−0.0947	0.031
H(47B)	0.2069	1.3266	−0.1014	0.031
H(47C)	0.1955	1.3782	−0.0493	0.031

Table S13. Continued

atom	x	y	z	U(eq)
H(50A)	0.2209	0.5657	0.2281	0.054
H(50B)	0.3104	0.5712	0.2580	0.054
H(50C)	0.2714	0.6405	0.2902	0.054
H(51)	0.2895	0.4930	0.3758	0.042
H(52)	0.2972	0.2523	0.4003	0.033
H(53)	0.2649	0.2812	0.2366	0.024
H(54)	0.1939	0.3951	0.0613	0.026

[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 S14. Complete Crystallographic Details for [Fe(TMP)(CN)(1-MeIm)]·1.8$CHCl_3$

formula	$C_{62.80}H_{59.80}Cl_{5.40}FeN_7$
FW, amu	1159.86
a, Å	16.4839(2)
b, Å	17.6960(3)
c, Å	20.0081(3)
β, deg	99.032(1)
V, Å^3	5763.98(15)
space group	P21/n
Z	4
D_c, g/cm^3	1.337
F(000)	2414
μ, mm^{-1}	0.558
crystal dimensions, mm	0.31 × 0.24 × 0.17
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.49–26.62
index range	$-20 \leq h \leq 19$
	$-20 \leq k \leq 22$
	$-24 \leq l \leq 25$
total data collected	51896
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9110 and 0.8459
unique data	12045 (R_{int} = 0.067)
unique observed data [I > 2σ(I)]	6964
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	12045/160/728
goodness-of-fit (pased on F^2)	0.923
final R indices [I > 2σ(I)]	R_1 = 0.0513, wR_2 = 0.1221
final R indices (all data)	R_1 = 0.0896, wR_2 = 0.1292

Table S15. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TMP)(CN)(1-MeIm)]·1.8$CHCl_3$[a]

atom	x	y	z	U(eq)
Fe(1)	0.65255(2)	0.71570(2)	0.64925(2)	0.0129(1)
N(1)	0.56209(14)	0.75419(13)	0.69374(12)	0.0133(6)
N(2)	0.71171(14)	0.68403(13)	0.73937(12)	0.0134(6)
N(3)	0.74335(14)	0.67751(13)	0.60472(12)	0.0130(6)
N(4)	0.59433(13)	0.74836(13)	0.55933(12)	0.0124(6)
N(5)	0.56549(16)	0.56103(15)	0.64080(13)	0.0228(7)
N(6)	0.70771(14)	0.81828(14)	0.65964(12)	0.0153(6)
N(7)	0.77196(15)	0.91915(14)	0.70597(12)	0.0171(6)
C(a1)	0.49600(17)	0.79671(17)	0.66437(15)	0.0158(7)
C(a2)	0.54897(17)	0.74028(17)	0.75917(15)	0.0160(7)
C(a3)	0.68089(18)	0.67932(17)	0.79955(15)	0.0152(7)
C(a4)	0.79194(17)	0.65987(16)	0.75359(15)	0.0138(7)
C(a5)	0.81865(17)	0.65229(17)	0.63655(15)	0.0154(7)
C(a6)	0.74492(17)	0.66921(17)	0.53621(15)	0.0150(7)
C(a7)	0.61637(17)	0.73517(16)	0.49674(14)	0.0127(7)
C(a8)	0.52515(17)	0.79302(17)	0.54811(15)	0.0142(7)
C(b1)	0.44278(17)	0.81217(18)	0.71287(15)	0.0174(7)
C(b2)	0.47420(17)	0.77594(17)	0.77072(16)	0.0189(7)
C(b3)	0.74350(17)	0.65250(17)	0.85211(15)	0.0166(7)
C(b4)	0.81192(18)	0.64216(17)	0.82410(15)	0.0179(7)
C(b5)	0.86747(18)	0.62786(18)	0.58739(15)	0.0185(7)
C(b6)	0.82107(18)	0.63585(17)	0.52588(16)	0.0190(7)
C(b7)	0.55901(17)	0.77261(17)	0.44520(15)	0.0174(7)
C(b8)	0.50401(18)	0.80860(17)	0.47719(15)	0.0173(7)
C(m1)	0.60264(17)	0.70245(17)	0.80898(15)	0.0144(7)
C(m2)	0.84439(17)	0.64767(16)	0.70647(15)	0.0143(7)
C(m3)	0.68513(17)	0.69544(16)	0.48411(14)	0.0130(7)
C(m4)	0.47925(17)	0.81822(17)	0.59671(15)	0.0159(7)
C(1)	0.57497(18)	0.68825(18)	0.87612(15)	0.0176(7)
C(2)	0.53484(18)	0.62146(18)	0.88736(16)	0.0218(7)
C(3)	0.5201(2)	0.5604(2)	0.83364(18)	0.0364(9)
C(4)	0.50684(19)	0.61038(19)	0.94909(16)	0.0247(8)
C(5)	0.51724(19)	0.6645(2)	0.99906(17)	0.0266(8)
C(6)	0.4849(2)	0.6525(2)	1.06509(18)	0.0420(10)

Table S15. Continued

atom	x	y	z	U(eq)
C(7)	0.55648(19)	0.7311(2)	0.98719(16)	0.0278(9)
C(8)	0.58589(18)	0.74421(19)	0.92609(16)	0.0220(8)
C(9)	0.6275(2)	0.8181(2)	0.91557(17)	0.0339(9)
C(10)	0.93300(17)	0.62926(18)	0.73125(14)	0.0164(7)
C(11)	0.96045(18)	0.55450(18)	0.73785(15)	0.0195(7)
C(12)	0.90172(19)	0.48915(18)	0.72335(18)	0.0292(9)
C(13)	1.04329(19)	0.54067(19)	0.75934(16)	0.0249(8)
C(14)	1.09976(19)	0.5988(2)	0.77326(16)	0.0260(8)
C(15)	1.19048(19)	0.5826(2)	0.7953(2)	0.0394(10)
C(16)	1.07141(18)	0.67255(19)	0.76689(15)	0.0229(8)
C(17)	0.98871(18)	0.68915(18)	0.74596(15)	0.0187(7)
C(18)	0.96018(19)	0.77007(18)	0.74075(17)	0.0252(8)
C(19)	0.69567(17)	0.68167(17)	0.41183(15)	0.0146(7)
C(20)	0.64464(18)	0.62866(17)	0.37346(15)	0.0173(7)
C(21)	0.5804(2)	0.58541(19)	0.40334(16)	0.0268(8)
C(22)	0.65258(18)	0.61746(18)	0.30549(16)	0.0217(8)
C(23)	0.70843(18)	0.6577(2)	0.27453(15)	0.0229(8)
C(24)	0.7129(2)	0.6458(2)	0.20051(16)	0.0397(10)
C(25)	0.75867(18)	0.70911(19)	0.31379(16)	0.0225(8)
C(26)	0.75372(17)	0.72192(18)	0.38144(15)	0.0177(7)
C(27)	0.81066(19)	0.77924(19)	0.42055(16)	0.0268(8)
C(28)	0.40671(17)	0.86840(18)	0.57489(14)	0.0148(7)
C(29)	0.32747(18)	0.83736(18)	0.55855(15)	0.0177(7)
C(30)	0.31303(19)	0.75340(18)	0.56132(17)	0.0268(8)
C(31)	0.26120(18)	0.88585(18)	0.54088(15)	0.0189(7)
C(32)	0.27124(18)	0.96387(19)	0.53865(15)	0.0197(7)
C(33)	0.19634(19)	1.01487(19)	0.52441(17)	0.0276(8)
C(34)	0.35052(19)	0.99317(19)	0.55369(16)	0.0224(8)
C(35)	0.41855(18)	0.94666(18)	0.57178(15)	0.0183(7)
C(36)	0.50330(18)	0.97986(18)	0.58767(17)	0.0239(8)
C(37)	0.59850(18)	0.61868(18)	0.64166(15)	0.0157(7)
C(38)	0.74130(17)	0.85153(17)	0.71702(15)	0.0158(7)
C(39)	0.7179(2)	0.86891(19)	0.60984(17)	0.0281(9)
C(40)	0.7569(2)	0.9310(2)	0.63763(17)	0.0309(9)

Table S15. Continued

atom	x	y	z	U(eq)
C(41)	0.8158(2)	0.97084(18)	0.75680(16)	0.0246(8)
C(42)	0.37385(18)	0.57772(18)	0.43698(16)	0.0222(8)
Cl(1)	0.35260(5)	0.66591(5)	0.39492(4)	0.0270(2)
Cl(2)	0.28106(5)	0.53141(5)	0.44616(5)	0.0308(2)
Cl(3)	0.43556(5)	0.59150(5)	0.51589(4)	0.0245(2)
C(43a)	0.8965(7)	0.4781(5)	0.4064(5)	0.086(3)
Cl(4a)	0.9688(3)	0.4844(3)	0.4781(2)	0.0936(12)
Cl(5a)	0.8891(6)	0.5620(4)	0.3688(4)	0.161(3)
Cl(6a)	0.8180(5)	0.4243(4)	0.4017(3)	0.168(2)
C(43b)	0.8097(10)	0.4623(8)	0.3941(11)	0.086(3)
Cl(4b)	0.8511(4)	0.5351(4)	0.3680(3)	0.0936(12)
Cl(5b)	0.7107(5)	0.4297(4)	0.3578(4)	0.161(3)
Cl(6b)	0.8760(6)	0.3791(6)	0.3904(7)	0.168(2)
Cl(4C)	0.9502(5)	0.5455(6)	0.4047(4)	0.0936(12)
Cl(5C)	0.7877(7)	0.4967(7)	0.3863(7)	0.161(3)
Cl(6C)	0.9078(11)	0.3857(8)	0.3925(13)	0.168(2)

[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 S16. Bond Lengths for [Fe(TMP)(CN)(1-MeIm)]·1.8$CHCl_3$[a]

bond	length (Å)	bond	length (Å)
Fe(1)–C(37)	1.929(3)	C(12)–H(12C)	0.9800
Fe(1)–N(1)	1.974(2)	C(13)–C(14)	1.386(4)
Fe(1)–N(3)	1.977(2)	C(13)–H(13)	0.9500
Fe(1)–N(4)	1.987(2)	C(14)–C(16)	1.385(4)
Fe(1)–N(2)	1.991(2)	C(14)–C(15)	1.518(4)
Fe(1)–N(6)	2.026(2)	C(15)–H(15a)	0.9800
N(1)–C(a1)	1.377(3)	C(15)–H(15b)	0.9800
N(1)–C(a2)	1.382(4)	C(15)–H(15C)	0.9800
N(2)–C(a4)	1.376(3)	C(16)–C(17)	1.393(4)
N(2)–C(a3)	1.381(4)	C(16)–H(16)	0.9500
N(3)–C(a5)	1.377(3)	C(17)–C(18)	1.506(4)
N(3)–C(a6)	1.383(4)	C(18)–H(18a)	0.9800
N(4)–C(a8)	1.377(3)	C(18)–H(18b)	0.9800
N(4)–C(a7)	1.378(4)	C(18)–H(18C)	0.9800
N(5)–C(37)	1.155(4)	C(19)–C(20)	1.405(4)
N(6)–C(38)	1.331(4)	C(19)–C(26)	1.406(4)
N(6)–C(39)	1.370(4)	C(20)–C(22)	1.401(4)
N(7)–C(38)	1.331(4)	C(20)–C(21)	1.504(4)
N(7)–C(40)	1.367(4)	C(21)–H(21a)	0.9800
N(7)–C(41)	1.471(4)	C(21)–H(21b)	0.9800
C(a1)–C(m4)	1.391(4)	C(21)–H(21C)	0.9800
C(a1)–C(b1)	1.433(4)	C(22)–C(23)	1.384(4)
C(a2)–C(m1)	1.395(4)	C(22)–H(22)	0.9500
C(a2)–C(b2)	1.435(4)	C(23)–C(25)	1.388(4)
C(a3)–C(m1)	1.394(4)	C(23)–C(24)	1.509(4)
C(a3)–C(b3)	1.434(4)	C(24)–H(24a)	0.9800
C(a4)–C(m2)	1.392(4)	C(24)–H(24b)	0.9800
C(a4)–C(b4)	1.432(4)	C(24)–H(24C)	0.9800
C(a5)–C(m2)	1.399(4)	C(25)–C(26)	1.387(4)
C(a5)–C(b5)	1.432(4)	C(25)–H(25)	0.9500
C(a6)–C(m3)	1.397(4)	C(26)–C(27)	1.514(4)
C(a6)–C(b6)	1.431(4)	C(27)–H(27a)	0.9800
C(a7)–C(m3)	1.390(4)	C(27)–H(27b)	0.9800
C(a7)–C(b7)	1.446(4)	C(27)–H(27C)	0.9800

Table S16. Continued

bond	length (Å)	bond	length (Å)
C(a8)–C(m4)	1.396(4)	C(28)–C(35)	1.401(4)
C(a8)–C(b8)	1.434(4)	C(28)–C(29)	1.407(4)
C(b1)–C(b2)	1.353(4)	C(29)–C(31)	1.391(4)
C(b1)–H(b1)	0.9500	C(29)–C(30)	1.507(4)
C(b2)–H(b2)	0.9500	C(30)–H(30a)	0.9800
C(b3)–C(b4)	1.348(4)	C(30)–H(30b)	0.9800
C(b3)–H(b3)	0.9500	C(30)–H(30C)	0.9800
C(b4)–H(b4)	0.9500	C(31)–C(32)	1.392(4)
C(b5)–C(b6)	1.351(4)	C(31)–H(31)	0.9500
C(b5)–H(b5)	0.9500	C(32)–C(34)	1.394(4)
C(b6)–H(b6)	0.9500	C(32)–C(33)	1.520(4)
C(b7)–C(b8)	1.349(4)	C(33)–H(33a)	0.9800
C(b7)–H(b7)	0.9500	C(33)–H(33b)	0.9800
C(b8)–H(b8)	0.9500	C(33)–H(33C)	0.9800
C(m1)–C(1)	1.506(4)	C(34)–C(35)	1.392(4)
C(m2)–C(10)	1.503(4)	C(34)–H(34)	0.9500
C(m3)–C(19)	1.503(4)	C(35)–C(36)	1.503(4)
C(m4)–C(28)	1.498(4)	C(36)–H(36a)	0.9800
C(1)–C(2)	1.390(4)	C(36)–H(36b)	0.9800
C(1)–C(8)	1.399(4)	C(36)–H(36C)	0.9800
C(2)–C(4)	1.399(4)	C(38)–H(38)	0.9500
C(2)–C(3)	1.516(5)	C(39)–C(40)	1.347(4)
C(3)–H(3a)	0.9800	C(39)–H(39)	0.9500
C(3)–H(3b)	0.9800	C(40)–H(40)	0.9500
C(3)–H(3C)	0.9800	C(41)–H(41a)	0.9800
C(4)–C(5)	1.375(4)	C(41)–H(41b)	0.9800
C(4)–H(4)	0.9500	C(41)–H(41C)	0.9800
C(5)–C(7)	1.382(5)	C(42)–Cl(3)	1.756(3)
C(5)–C(6)	1.515(5)	C(42)–Cl(2)	1.770(3)
C(6)–H(6a)	0.9800	C(42)–Cl(1)	1.782(3)
C(6)–H(6b)	0.9800	C(42)–H(42)	1.0000
C(6)–H(6C)	0.9800	C(43a)–Cl(4C)	1.490(11)
C(7)–C(8)	1.403(4)	C(43a)–Cl(6a)	1.597(11)
C(7)–H(7)	0.9500	C(43a)–Cl(5a)	1.661(10)

Table S16. Continued

bond	length (Å)	bond	length (Å)
C(8)–C(9)	1.506(5)	C(43a)–Cl(6C)	1.674(14)
C(9)–H(9a)	0.9800	C(43a)–Cl(4a)	1.719(10)
C(9)–H(9b)	0.9800	C(43a)–Cl(5C)	1.806(13)
C(9)–H(9C)	0.9800	Cl(4a)–Cl(4a)#1)	1.360(8)
C(10)–C(11)	1.398(4)	C(43b)–Cl(4b)	1.584(15)
C(10)–C(17)	1.403(4)	C(43b)–Cl(5b)	1.775(16)
C(11)–C(13)	1.388(4)	C(43b)–Cl(6b)	1.842(15)
C(11)–C(12)	1.507(4)	C(43b)–H(43b)	1.0000
C(12)–H(12a)	0.9800		
C(12)–H(12b)	0.9800		

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

Table S17. Bond Angles for [Fe(TMP)(CN)(1-MeIm)]·1.8$CHCl_3$[a]

angle	degree	angle	degree
C(37)–Fe(1)–N(1)	88.30(11)	C(14)–C(13)–C(11)	121.9(3)
C(37)–Fe(1)–N(3)	91.90(11)	C(14)–C(13)–H(13)	119.0
N(1)–Fe(1)–N(3)	179.80(11)	C(11)–C(13)–H(13)	119.0
C(37)–Fe(1)–N(4)	92.07(11)	C(16)–C(14)–C(13)	118.3(3)
N(1)–Fe(1)–N(4)	90.93(10)	C(16)–C(14)–C(15)	120.5(3)
N(3)–Fe(1)–N(4)	89.06(10)	C(13)–C(14)–C(15)	121.2(3)
C(37)–Fe(1)–N(2)	88.58(11)	C(14)–C(15)–H(15a)	109.5
N(1)–Fe(1)–N(2)	89.20(10)	C(14)–C(15)–H(15b)	109.5
N(3)–Fe(1)–N(2)	90.81(10)	H(15a)–C(15)–H(15b)	109.5
N(4)–Fe(1)–N(2)	179.34(10)	C(14)–C(15)–H(15C)	109.5
C(37)–Fe(1)–N(6)	178.30(11)	H(15a)–C(15)–H(15C)	109.5
N(1)–Fe(1)–N(6)	90.18(10)	H(15b)–C(15)–H(15C)	109.5
N(3)–Fe(1)–N(6)	89.62(10)	C(14)–C(16)–C(17)	121.8(3)
N(4)–Fe(1)–N(6)	88.71(10)	C(14)–C(16)–H(16)	119.1
N(2)–Fe(1)–N(6)	90.64(10)	C(17)–C(16)–H(16)	119.1
C(a1)–N(1)–C(a2)	105.7(2)	C(16)–C(17)–C(10)	118.8(3)
C(a1)–N(1)–Fe(1)	126.8(2)	C(16)–C(17)–C(18)	120.1(3)
C(a2)–N(1)–Fe(1)	127.40(19)	C(10)–C(17)–C(18)	121.1(3)
C(a4)–N(2)–C(a3)	105.9(2)	C(17)–C(18)–H(18a)	109.5
C(a4)–N(2)–Fe(1)	126.35(19)	C(17)–C(18)–H(18b)	109.5
C(a3)–N(2)–Fe(1)	127.72(19)	H(18a)–C(18)–H(18b)	109.5
C(a5)–N(3)–C(a6)	105.6(2)	C(17)–C(18)–H(18C)	109.5
C(a5)–N(3)–Fe(1)	126.4(2)	H(18a)–C(18)–H(18C)	109.5
C(a6)–N(3)–Fe(1)	128.05(19)	H(18b)–C(18)–H(18C)	109.5
C(a8)–N(4)–C(a7)	106.2(2)	C(20)–C(19)–C(26)	119.5(3)
C(a8)–N(4)–Fe(1)	125.8(2)	C(20)–C(19)–C(m3)	119.0(3)
C(a7)–N(4)–Fe(1)	127.95(19)	C(26)–C(19)–C(m3)	121.6(3)
C(38)–N(6)–C(39)	104.9(3)	C(22)–C(20)–C(19)	119.1(3)
C(38)–N(6)–Fe(1)	127.1(2)	C(22)–C(20)–C(21)	119.5(3)
C(39)–N(6)–Fe(1)	128.0(2)	C(19)–C(20)–C(21)	121.4(3)
C(38)–N(7)–C(40)	106.8(3)	C(20)–C(21)–H(21a)	109.5
C(38)–N(7)–C(41)	127.1(3)	C(20)–C(21)–H(21b)	109.5
C(40)–N(7)–C(41)	126.1(3)	H(21a)–C(21)–H(21b)	109.5
N(1)–C(a1)–C(m4)	126.0(3)	C(20)–C(21)–H(21C)	109.5

Table S17. Continued

angle	degree	angle	degree
N(1)–C(a1)–C(b1)	110.0(3)	H(21a)–C(21)–H(21C)	109.5
C(m4)–C(a1)–C(b1)	123.9(3)	H(21b)–C(21)–H(21C)	109.5
N(1)–C(a2)–C(m1)	125.9(3)	C(23)–C(22)–C(20)	122.1(3)
N(1)–C(a2)–C(b2)	109.9(3)	C(23)–C(22)–H(22)	118.9
C(m1)–C(a2)–C(b2)	124.1(3)	C(20)–C(22)–H(22)	118.9
N(2)–C(a3)–C(m1)	125.1(3)	C(22)–C(23)–C(25)	117.6(3)
N(2)–C(a3)–C(b3)	109.8(2)	C(22)–C(23)–C(24)	120.4(3)
C(m1)–C(a3)–C(b3)	124.9(3)	C(25)–C(23)–C(24)	122.0(3)
N(2)–C(a4)–C(m2)	125.9(3)	C(23)–C(24)–H(24a)	109.5
N(2)–C(a4)–C(b4)	109.7(3)	C(23)–C(24)–H(24b)	109.5
C(m2)–C(a4)–C(b4)	124.2(3)	H(24a)–C(24)–H(24b)	109.5
N(3)–C(a5)–C(m2)	126.2(3)	C(23)–C(24)–H(24C)	109.5
N(3)–C(a5)–C(b5)	110.1(3)	H(24a)–C(24)–H(24C)	109.5
C(m2)–C(a5)–C(b5)	123.7(3)	H(24b)–C(24)–H(24C)	109.5
N(3)–C(a6)–C(m3)	125.7(3)	C(26)–C(25)–C(23)	122.5(3)
N(3)–C(a6)–C(b6)	109.9(3)	C(26)–C(25)–H(25)	118.7
C(m3)–C(a6)–C(b6)	124.1(3)	C(23)–C(25)–H(25)	118.7
N(4)–C(a7)–C(m3)	126.1(3)	C(25)–C(26)–C(19)	119.2(3)
N(4)–C(a7)–C(b7)	109.5(2)	C(25)–C(26)–C(27)	119.2(3)
C(m3)–C(a7)–C(b7)	124.2(3)	C(19)–C(26)–C(27)	121.7(3)
N(4)–C(a8)–C(m4)	126.6(3)	C(26)–C(27)–H(27a)	109.5
N(4)–C(a8)–C(b8)	109.8(3)	C(26)–C(27)–H(27b)	109.5
C(m4)–C(a8)–C(b8)	123.6(3)	H(27a)–C(27)–H(27b)	109.5
C(b2)–C(b1)–C(a1)	107.2(3)	C(26)–C(27)–H(27C)	109.5
C(b2)–C(b1)–H(b1)	126.4	H(27a)–C(27)–H(27C)	109.5
C(a1)–C(b1)–H(b1)	126.4	H(27b)–C(27)–H(27C)	109.5
C(b1)–C(b2)–C(a2)	107.1(3)	C(35)–C(28)–C(29)	120.4(3)
C(b1)–C(b2)–H(b2)	126.5	C(35)–C(28)–C(m4)	119.2(3)
C(a2)–C(b2)–H(b2)	126.5	C(29)–C(28)–C(m4)	120.4(3)
C(b4)–C(b3)–C(a3)	107.0(3)	C(31)–C(29)–C(28)	118.8(3)
C(b4)–C(b3)–H(b3)	126.5	C(31)–C(29)–C(30)	119.7(3)
C(a3)–C(b3)–H(b3)	126.5	C(28)–C(29)–C(30)	121.5(3)
C(b3)–C(b4)–C(a4)	107.6(3)	C(29)–C(30)–H(30a)	109.5
C(b3)–C(b4)–H(b4)	126.2	C(29)–C(30)–H(30b)	109.5

Table S17. Continued

angle	degree	angle	degree
C(a4)–C(b4)–H(b4)	126.2	H(30a)–C(30)–H(30b)	109.5
C(b6)–C(b5)–C(a5)	107.2(3)	C(29)–C(30)–H(30C)	109.5
C(b6)–C(b5)–H(b5)	126.4	H(30a)–C(30)–H(30C)	109.5
C(a5)–C(b5)–H(b5)	126.4	H(30b)–C(30)–H(30C)	109.5
C(b5)–C(b6)–C(a6)	107.2(3)	C(29)–C(31)–C(32)	121.8(3)
C(b5)–C(b6)–H(b6)	126.4	C(29)–C(31)–H(31)	119.1
C(a6)–C(b6)–H(b6)	126.4	C(32)–C(31)–H(31)	119.1
C(b8)–C(b7)–C(a7)	106.9(3)	C(31)–C(32)–C(34)	118.3(3)
C(b8)–C(b7)–H(b7)	126.5	C(31)–C(32)–C(33)	119.9(3)
C(a7)–C(b7)–H(b7)	126.5	C(34)–C(32)–C(33)	121.7(3)
C(b7)–C(b8)–C(a8)	107.6(3)	C(32)–C(33)–H(33a)	109.5
C(b7)–C(b8)–H(b8)	126.2	C(32)–C(33)–H(33b)	109.5
C(a8)–C(b8)–H(b8)	126.2	H(33a)–C(33)–H(33b)	109.5
C(a3)–C(m1)–C(a2)	122.7(3)	C(32)–C(33)–H(33C)	109.5
C(a3)–C(m1)–C(1)	119.2(3)	H(33a)–C(33)–H(33C)	109.5
C(a2)–C(m1)–C(1)	118.1(3)	H(33b)–C(33)–H(33C)	109.5
C(a4)–C(m2)–C(a5)	123.0(3)	C(35)–C(34)–C(32)	121.7(3)
C(a4)–C(m2)–C(10)	119.0(3)	C(35)–C(34)–H(34)	119.1
C(a5)–C(m2)–C(10)	118.0(3)	C(32)–C(34)–H(34)	119.1
C(a7)–C(m3)–C(a6)	122.2(3)	C(34)–C(35)–C(28)	118.9(3)
C(a7)–C(m3)–C(19)	118.5(3)	C(34)–C(35)–C(36)	120.5(3)
C(a6)–C(m3)–C(19)	119.3(3)	C(28)–C(35)–C(36)	120.5(3)
C(a1)–C(m4)–C(a8)	123.0(3)	C(35)–C(36)–H(36a)	109.5
C(a1)–C(m4)–C(28)	118.2(3)	C(35)–C(36)–H(36b)	109.5
C(a8)–C(m4)–C(28)	118.8(3)	H(36a)–C(36)–H(36b)	109.5
C(2)–C(1)–C(8)	119.8(3)	C(35)–C(36)–H(36C)	109.5
C(2)–C(1)–C(m1)	120.3(3)	H(36a)–C(36)–H(36C)	109.5
C(8)–C(1)–C(m1)	119.8(3)	H(36b)–C(36)–H(36C)	109.5
C(1)–C(2)–C(4)	119.6(3)	N(5)–C(37)–Fe(1)	176.2(3)
C(1)–C(2)–C(3)	121.2(3)	N(6)–C(38)–N(7)	111.8(3)
C(4)–C(2)–C(3)	119.2(3)	N(6)–C(38)–H(38)	124.1
C(2)–C(3)–H(3a)	109.5	N(7)–C(38)–H(38)	124.1
C(2)–C(3)–H(3b)	109.5	C(40)–C(39)–N(6)	109.7(3)
H(3a)–C(3)–H(3b)	109.5	C(40)–C(39)–H(39)	125.1

Table S17. Continued

angle	degree	angle	degree
C(2)–C(3)–H(3C)	109.5	N(6)–C(39)–H(39)	125.1
H(3a)–C(3)–H(3C)	109.5	C(39)–C(40)–N(7)	106.8(3)
H(3b)–C(3)–H(3C)	109.5	C(39)–C(40)–H(40)	126.6
C(5)–C(4)–C(2)	121.6(3)	N(7)–C(40)–H(40)	126.6
C(5)–C(4)–H(4)	119.2	N(7)–C(41)–H(41a)	109.5
C(2)–C(4)–H(4)	119.2	N(7)–C(41)–H(41b)	109.5
C(4)–C(5)–C(7)	118.5(3)	H(41a)–C(41)–H(41b)	109.5
C(4)–C(5)–C(6)	121.1(3)	N(7)–C(41)–H(41C)	109.5
C(7)–C(5)–C(6)	120.5(3)	H(41a)–C(41)–H(41C)	109.5
C(5)–C(6)–H(6a)	109.5	H(41b)–C(41)–H(41C)	109.5
C(5)–C(6)–H(6b)	109.5	Cl(3)–C(42)–Cl(2)	111.04(17)
H(6a)–C(6)–H(6b)	109.5	Cl(3)–C(42)–Cl(1)	110.26(17)
C(5)–C(6)–H(6C)	109.5	Cl(2)–C(42)–Cl(1)	110.21(17)
H(6a)–C(6)–H(6C)	109.5	Cl(3)–C(42)–H(42)	108.4
H(6b)–C(6)–H(6C)	109.5	Cl(2)–C(42)–H(42)	108.4
C(5)–C(7)–C(8)	121.7(3)	Cl(1)–C(42)–H(42)	108.4
C(5)–C(7)–H(7)	119.1	Cl(4C)–C(43a)–Cl(6a)	162.8(8)
C(8)–C(7)–H(7)	119.1	Cl(6a)–C(43a)–Cl(5a)	120.4(8)
C(1)–C(8)–C(7)	118.8(3)	Cl(4C)–C(43a)–Cl(6C)	134.1(10)
C(1)–C(8)–C(9)	121.6(3)	Cl(6a)–C(43a)–Cl(6C)	61.2(7)
C(7)–C(8)–C(9)	119.5(3)	Cl(5a)–C(43a)–Cl(6C)	143.1(11)
C(8)–C(9)–H(9a)	109.5	Cl(4C)–C(43a)–Cl(4a)	68.3(6)
C(8)–C(9)–H(9b)	109.5	Cl(6a)–C(43a)–Cl(4a)	122.5(7)
H(9a)–C(9)–H(9b)	109.5	Cl(5a)–C(43a)–Cl(4a)	108.2(7)
C(8)–C(9)–H(9C)	109.5	Cl(6C)–C(43a)–Cl(4a)	97.0(9)
H(9a)–C(9)–H(9C)	109.5	Cl(4C)–C(43a)–Cl(5C)	114.9(7)
H(9b)–C(9)–H(9C)	109.5	Cl(6a)–C(43a)–Cl(5C)	47.8(5)
C(11)–C(10)–C(17)	120.2(3)	Cl(5a)–C(43a)–Cl(5C)	74.8(6)
C(11)–C(10)–C(m2)	121.3(3)	Cl(6C)–C(43a)–Cl(5C)	105.9(9)
C(17)–C(10)–C(m2)	118.4(3)	Cl(4a)–C(43a)–Cl(5C)	135.1(8)
C(13)–C(11)–C(10)	119.0(3)	Cl(4a)#1–Cl(4a)–C(43a)	156.8(7)
C(13)–C(11)–C(12)	119.7(3)	Cl(4b)–C(43b)–Cl(5b)	123.1(12)
C(10)–C(11)–C(12)	121.3(3)	Cl(4b)–C(43b)–Cl(6b)	110.3(11)
C(11)–C(12)–H(12a)	109.5	Cl(5b)–C(43b)–Cl(6b)	103.7(9)

Table S17. Continued

angle	degree	angle	degree
C(11)–C(12)–H(12b)	109.5	Cl(4b)–C(43b)–H(43b)	106.2
H(12a)–C(12)–H(12b)	109.5	Cl(5b)–C(43b)–H(43b)	106.2
C(11)–C(12)–H(12C)	109.5	Cl(6b)–C(43b)–H(43b)	106.2
H(12a)–C(12)–H(12C)	109.5		
H(12b)–C(12)–H(12C)	109.5		

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

Table S18. Anisotropic Displacement Parameters (Å^2) for [Fe(TMP)(CN)(1-MeIm)]·1.8$CHCl_3$[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0113(2)	0.0153(3)	0.0121(2)	−0.0005(2)	0.0014(2)	0.0001(2)
N(1)	0.0134(13)	0.0130(14)	0.0137(14)	0.0011(11)	0.0026(11)	−0.0007(11)
N(2)	0.0118(12)	0.0166(15)	0.0118(14)	−0.0013(11)	0.0019(10)	−0.0009(11)
N(3)	0.0126(12)	0.0150(15)	0.0113(14)	−0.0006(11)	0.0016(10)	0.0007(11)
N(4)	0.0110(12)	0.0148(15)	0.0111(14)	−0.0008(11)	0.0006(10)	−0.0015(11)
N(5)	0.0220(15)	0.0186(17)	0.0266(17)	0.0013(13)	−0.0006(12)	−0.0017(13)
N(6)	0.0151(13)	0.0163(15)	0.0149(15)	−0.0007(12)	0.0037(11)	−0.0010(11)
N(7)	0.0189(14)	0.0154(15)	0.0160(15)	0.0016(12)	0.0000(11)	−0.0025(11)
C(A1)	0.0149(15)	0.0181(18)	0.0145(17)	−0.0020(14)	0.0026(13)	−0.0005(13)
C(A2)	0.0164(15)	0.0175(18)	0.0145(18)	0.0011(14)	0.0037(13)	−0.0020(13)
C(A3)	0.0182(16)	0.0142(18)	0.0139(17)	0.0003(14)	0.0045(13)	−0.0022(13)
C(A4)	0.0139(15)	0.0133(17)	0.0135(17)	0.0023(14)	0.0000(13)	−0.0026(13)
C(A5)	0.0127(15)	0.0176(18)	0.0159(17)	0.0014(14)	0.0023(13)	0.0004(13)
C(A6)	0.0163(15)	0.0144(18)	0.0149(18)	−0.0020(14)	0.0044(13)	−0.0025(13)
C(A7)	0.0131(15)	0.0143(18)	0.0107(17)	−0.0010(13)	0.0020(12)	−0.0024(13)
C(A8)	0.0131(15)	0.0153(18)	0.0140(17)	−0.0004(14)	0.0018(13)	−0.0025(13)
C(B1)	0.0130(15)	0.0228(19)	0.0166(18)	−0.0015(15)	0.0034(13)	0.0026(13)
C(B2)	0.0156(15)	0.026(2)	0.0163(18)	−0.0005(15)	0.0066(13)	0.0003(14)
C(B3)	0.0189(16)	0.0187(18)	0.0121(17)	0.0021(14)	0.0026(13)	0.0016(14)
C(B4)	0.0150(15)	0.0220(19)	0.0149(18)	−0.0013(15)	−0.0031(13)	−0.0004(14)
C(B5)	0.0135(15)	0.025(2)	0.0176(18)	−0.0003(15)	0.0042(13)	0.0037(14)
C(B6)	0.0180(16)	0.024(2)	0.0158(18)	−0.0037(15)	0.0044(14)	0.0023(14)
C(B7)	0.0190(16)	0.023(2)	0.0094(17)	0.0014(14)	0.0015(13)	0.0003(14)
C(B8)	0.0167(16)	0.0193(18)	0.0150(17)	0.0015(14)	−0.0009(13)	0.0033(14)
C(M1)	0.0150(15)	0.0188(19)	0.0105(16)	0.0001(14)	0.0046(12)	−0.0026(13)
C(M2)	0.0131(15)	0.0144(17)	0.0146(17)	−0.0039(14)	−0.0005(13)	0.0002(13)
C(M3)	0.0128(15)	0.0142(17)	0.0121(17)	−0.0022(13)	0.0027(12)	−0.0031(12)
C(M4)	0.0147(15)	0.0151(18)	0.0176(18)	−0.0004(14)	0.0019(13)	0.0001(13)
C(1)	0.0159(10)	0.0197(11)	0.0173(11)	0.0022(9)	0.0028(8)	0.0016(8)
C(2)	0.0207(10)	0.0232(11)	0.0217(11)	0.0032(9)	0.0039(8)	0.0017(9)
C(3)	0.0389(16)	0.0331(17)	0.0391(17)	0.0016(14)	0.0122(14)	−0.0048(14)
C(4)	0.0225(11)	0.0259(11)	0.0261(11)	0.0058(9)	0.0050(9)	0.0007(9)
C(5)	0.0241(11)	0.0311(12)	0.0252(11)	0.0047(9)	0.0054(9)	0.0015(9)
C(6)	0.0408(17)	0.0522(18)	0.0349(17)	0.0087(15)	0.0115(14)	−0.0004(15)

Table S18. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(7)	0.0218(17)	0.046(3)	0.0158(19)	−0.0037(17)	0.0036(14)	0.0034(17)
C(8)	0.0157(16)	0.033(2)	0.0176(19)	0.0079(16)	0.0032(14)	0.0009(15)
C(9)	0.040(2)	0.044(3)	0.020(2)	−0.0114(18)	0.0107(17)	−0.0121(19)
C(10)	0.0138(15)	0.027(2)	0.0090(16)	−0.0008(14)	0.0029(13)	0.0020(14)
C(11)	0.0181(16)	0.024(2)	0.0158(18)	−0.0023(15)	0.0005(14)	0.0012(14)
C(12)	0.0239(18)	0.025(2)	0.037(2)	−0.0024(17)	−0.0006(16)	0.0040(16)
C(13)	0.0221(17)	0.028(2)	0.025(2)	0.0010(17)	0.0043(15)	0.0058(16)
C(14)	0.0175(17)	0.038(2)	0.022(2)	0.0012(17)	0.0010(15)	0.0038(16)
C(15)	0.0153(18)	0.050(3)	0.050(3)	0.002(2)	−0.0029(17)	0.0045(17)
C(16)	0.0164(16)	0.032(2)	0.0197(19)	−0.0004(16)	0.0018(14)	−0.0051(15)
C(17)	0.0177(16)	0.027(2)	0.0115(17)	0.0007(15)	0.0032(13)	0.0000(14)
C(18)	0.0214(17)	0.029(2)	0.026(2)	−0.0013(16)	0.0057(15)	−0.0034(15)
C(19)	0.0129(15)	0.0181(18)	0.0129(17)	0.0014(14)	0.0017(13)	0.0054(13)
C(20)	0.0167(16)	0.0212(19)	0.0142(18)	0.0004(14)	0.0027(13)	0.0018(14)
C(21)	0.0305(19)	0.030(2)	0.0197(19)	−0.0002(16)	0.0028(15)	−0.0113(16)
C(22)	0.0190(17)	0.026(2)	0.0189(19)	−0.0062(15)	−0.0011(14)	0.0031(15)
C(23)	0.0169(16)	0.039(2)	0.0134(18)	−0.0007(16)	0.0041(14)	0.0078(15)
C(24)	0.029(2)	0.072(3)	0.019(2)	−0.002(2)	0.0077(16)	0.001(2)
C(25)	0.0120(15)	0.034(2)	0.023(2)	0.0055(16)	0.0062(14)	0.0029(15)
C(26)	0.0132(15)	0.0218(19)	0.0175(18)	0.0016(15)	0.0009(13)	0.0018(14)
C(27)	0.0253(18)	0.029(2)	0.025(2)	0.0014(17)	0.0018(15)	−0.0109(16)
C(28)	0.0165(16)	0.022(2)	0.0062(16)	0.0003(14)	0.0040(12)	0.0056(14)
C(29)	0.0193(16)	0.024(2)	0.0101(17)	−0.0028(14)	0.0038(13)	0.0040(14)
C(30)	0.0193(17)	0.027(2)	0.032(2)	−0.0064(17)	−0.0012(15)	0.0022(15)
C(31)	0.0147(16)	0.028(2)	0.0138(17)	−0.0013(15)	0.0019(13)	−0.0007(14)
C(32)	0.0197(17)	0.026(2)	0.0137(17)	0.0015(15)	0.0046(13)	0.0055(15)
C(33)	0.0198(17)	0.032(2)	0.030(2)	0.0026(17)	0.0018(15)	0.0080(15)
C(34)	0.0231(18)	0.022(2)	0.0226(19)	0.0033(15)	0.0050(15)	0.0050(15)
C(35)	0.0198(16)	0.022(2)	0.0136(17)	0.0026(15)	0.0042(13)	0.0033(14)
C(36)	0.0195(17)	0.023(2)	0.029(2)	0.0037(16)	0.0024(15)	0.0027(14)
C(37)	0.0154(15)	0.021(2)	0.0106(17)	0.0006(14)	0.0013(13)	0.0072(14)
C(38)	0.0164(16)	0.0179(19)	0.0130(17)	0.0046(14)	0.0018(13)	−0.0014(14)
C(39)	0.044(2)	0.027(2)	0.0138(19)	−0.0014(16)	0.0069(16)	−0.0148(17)
C(40)	0.047(2)	0.026(2)	0.020(2)	0.0050(16)	0.0060(17)	−0.0136(18)

Table S18. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	0.0291(19)	0.022(2)	0.0216(19)	−0.0058(15)	−0.0001(15)	−0.0057(15)
C(42)	0.0193(17)	0.025(2)	0.0229(19)	0.0008(16)	0.0044(14)	−0.0017(14)
Cl(1)	0.0296(4)	0.0248(5)	0.0248(5)	0.0041(4)	−0.0010(4)	−0.0010(4)
Cl(2)	0.0216(4)	0.0309(5)	0.0399(6)	0.0042(4)	0.0043(4)	−0.0040(4)
Cl(3)	0.0255(4)	0.0275(5)	0.0195(5)	0.0001(4)	0.0004(3)	0.0021(4)
C(43A)	0.127(6)	0.048(5)	0.083(6)	0.002(5)	0.016(5)	0.017(5)
Cl(4A)	0.096(2)	0.126(3)	0.062(2)	−0.023(2)	0.0244(17)	0.052(2)
Cl(5A)	0.258(6)	0.107(3)	0.155(4)	0.067(3)	0.144(4)	0.093(3)
Cl(6A)	0.230(6)	0.182(4)	0.114(3)	0.075(3)	0.091(4)	0.109(4)
C(43B)	0.127(6)	0.048(5)	0.083(6)	0.002(5)	0.016(5)	0.017(5)
Cl(4B)	0.096(2)	0.126(3)	0.062(2)	−0.023(2)	0.0244(17)	0.052(2)
Cl(5B)	0.258(6)	0.107(3)	0.155(4)	0.067(3)	0.144(4)	0.093(3)
Cl(6B)	0.230(6)	0.182(4)	0.114(3)	0.075(3)	0.091(4)	0.109(4)
Cl(4C)	0.096(2)	0.126(3)	0.062(2)	−0.023(2)	0.0244(17)	0.052(2)
Cl(5C)	0.258(6)	0.107(3)	0.155(4)	0.067(3)	0.144(4)	0.093(3)
Cl(6C)	0.230(6)	0.182(4)	0.114(3)	0.075(3)	0.091(4)	0.109(4)

[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 S19. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TMP)(CN)(1-MeIm)]·1.8$CHCl_3$[a]

atom	x	y	z	U(eq)
H(B1	0.3944	0.8422	0.7057	0.021
H(B2	0.4511	0.7744	0.8113	0.023
H(B3	0.7378	0.6437	0.8980	0.020
H(B4	0.8639	0.6261	0.8470	0.021
H(B5	0.9223	0.6095	0.5964	0.022
H(B6	0.8362	0.6219	0.4836	0.023
H(B7	0.5599	0.7720	0.3978	0.021
H(B8	0.4594	0.8388	0.4565	0.021
H(3A)	0.5692	0.5287	0.8361	0.055
H(3B)	0.5083	0.5839	0.7888	0.055
H(3C)	0.4733	0.5292	0.8413	0.055
H(4)	0.4800	0.5644	0.9567	0.030
H(6A)	0.5261	0.6695	1.1028	0.063
H(6B)	0.4734	0.5987	1.0705	0.063
H(6C)	0.4343	0.6817	1.0646	0.063
H(7)	0.5637	0.7689	1.0213	0.033
H(9A)	0.6339	0.8476	0.9575	0.051
H(9B)	0.5940	0.8465	0.8792	0.051
H(9C)	0.6817	0.8081	0.9031	0.051
H(12A)	0.9324	0.4415	0.7293	0.044
H(12B)	0.8730	0.4927	0.6767	0.044
H(12C)	0.8616	0.4907	0.7546	0.044
H(13)	1.0618	0.4899	0.7647	0.030
H(15A)	1.2229	0.6130	0.7682	0.059
H(15B)	1.2011	0.5288	0.7887	0.059
H(15C)	1.2060	0.5955	0.8432	0.059
H(16)	1.1094	0.7129	0.7771	0.027
H(18A)	0.9312	0.7818	0.7786	0.038
H(18B)	0.9230	0.7775	0.6980	0.038
H(18C)	1.0078	0.8036	0.7422	0.038
H(21A)	0.5331	0.6182	0.4057	0.040
H(21B)	0.6035	0.5684	0.4490	0.040
H(21C)	0.5630	0.5415	0.3749	0.040
H(22)	0.6185	0.5811	0.2798	0.026

Table S19. Continued

atom	x	y	z	U(eq)
H(24A)	0.7535	0.6065	0.1957	0.059
H(24B)	0.7292	0.6931	0.1809	0.059
H(24C)	0.6590	0.6302	0.1768	0.059
H(25)	0.7980	0.7366	0.2935	0.027
H(27A)	0.8594	0.7534	0.4443	0.040
H(27B)	0.7821	0.8049	0.4535	0.040
H(27C)	0.8274	0.8165	0.3891	0.040
H(30A)	0.2546	0.7427	0.5469	0.040
H(30B)	0.3297	0.7354	0.6078	0.040
H(30C)	0.3454	0.7275	0.5312	0.040
H(31)	0.2076	0.8652	0.5300	0.023
H(33A)	0.1530	0.9892	0.4935	0.041
H(33B)	0.2113	1.0619	0.5036	0.041
H(33C)	0.1765	1.0264	0.5669	0.041
H(34)	0.3583	1.0463	0.5515	0.027
H(36A)	0.5348	0.9666	0.5517	0.036
H(36B)	0.5310	0.9597	0.6309	0.036
H(36C)	0.4993	1.0350	0.5908	0.036
H(38)	0.7432	0.8296	0.7606	0.019
H(39)	0.7001	0.8614	0.5628	0.034
H(40)	0.7711	0.9745	0.6142	0.037
H(41A)	0.7939	0.9656	0.7993	0.037
H(41B)	0.8084	1.0230	0.7405	0.037
H(41C)	0.8745	0.9583	0.7644	0.037
H(42)	0.4046	0.5452	0.4086	0.027
H(43B)	0.8075	0.4712	0.4431	0.103

[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 S20. Complete Crystallographic Details for 3[K(18-crown-6)][Fe(TMP)$(CN)_2$]·5.1(THF)-·0.9H_2O

formula	$C_{230.40}H_{270.60}Fe_3K_3N_{18}O_{24}$
FW, amu	3960.90
a, Å	23.0103(9)
b, Å	20.1843(8)
c, Å	46.1854(18)
β, deg	98.535(2)
V, Å^3	21213.1(14)
space group	P21/c
Z	4
D_c, g/cm^3	1.240
F(000)	8424
μ, mm^{-1}	0.331
crystal dimensions, mm	0.49 × 0.43 × 0.22
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.10–27.50
index range	$-29 \leq h \leq 29$
	$-24 \leq k \leq 22$
	$-60 \leq l \leq 50$
total data collected	202746
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9307 and 0.8545
unique data	46934 (R_{int} = 0.051)
unique observed data [I > 2σ(I)]	36729
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	46934/654/2758
goodness-of-fit (pased on F^2)	1.100
final R indices [I > 2σ(I)]	R_1 = 0.0789, wR_2 = 0.1979
final R indices (all data)	R_1 = 0.0992, wR_2 = 0.2100

Table S21. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for 3[K(18-crown-6)][Fe(TMP)(CN)$_2$]·5.1(THF)·0.9H$_2$O^a

atom	x	y	z	U(eq)
Fe(1)	0.52721(2)	0.67297(2)	0.29907(1)	0.0154(1)
K(1)	0.46893(3)	0.41264(4)	0.34868(2)	0.0251(2)
N(11)	0.59851(11)	0.65458(14)	0.32766(6)	0.0171(5)
N(12)	0.56611(12)	0.63595(15)	0.26696(6)	0.0184(6)
N(13)	0.45584(12)	0.68960(15)	0.27091(6)	0.0188(6)
N(14)	0.48845(11)	0.71295(14)	0.33033(6)	0.0169(5)
N(15)	0.57872(14)	0.81318(17)	0.28973(7)	0.0302(7)
N(16)	0.49420(13)	0.53050(17)	0.31902(7)	0.0278(7)
C(1a1)	0.60195(13)	0.65382(18)	0.35749(7)	0.0179(6)
C(1a2)	0.65157(14)	0.63223(17)	0.32145(7)	0.0186(7)
C(1a3)	0.62508(14)	0.62362(18)	0.26813(7)	0.0193(7)
C(1a4)	0.54089(14)	0.62191(18)	0.23885(7)	0.0194(7)
C(1a5)	0.44275(14)	0.66420(19)	0.24301(7)	0.0209(7)
C(1a6)	0.40943(14)	0.73021(18)	0.27492(7)	0.0203(7)
C(1a7)	0.43993(14)	0.75321(17)	0.32681(7)	0.0185(7)
C(1a8)	0.50854(14)	0.71155(17)	0.35986(7)	0.0179(6)
C(1b1)	0.65808(14)	0.62778(19)	0.37047(7)	0.0215(7)
C(1b2)	0.68935(14)	0.61614(19)	0.34835(7)	0.0224(7)
C(1b3)	0.63739(14)	0.60420(18)	0.23972(7)	0.0211(7)
C(1b4)	0.58535(14)	0.60097(19)	0.22168(7)	0.0218(7)
C(1b5)	0.38561(15)	0.6875(2)	0.22973(7)	0.0250(8)
C(1b6)	0.36598(15)	0.7295(2)	0.24887(7)	0.0246(8)
C(1b7)	0.42931(15)	0.77818(18)	0.35473(7)	0.0218(7)
C(1b8)	0.47089(14)	0.75107(18)	0.37529(7)	0.0198(7)
C(1m1)	0.66632(14)	0.62253(18)	0.29342(7)	0.0196(7)
C(1m2)	0.48151(14)	0.63061(18)	0.22764(7)	0.0195(7)
C(1m3)	0.40289(14)	0.76477(18)	0.30035(7)	0.0193(7)
C(1m4)	0.55976(14)	0.68035(18)	0.37322(7)	0.0181(6)
C(11)	0.55868(14)	0.76126(19)	0.29225(7)	0.0202(7)
C(12)	0.50355(13)	0.58232(18)	0.30984(7)	0.0198(7)
C(13)	0.72949(14)	0.60778(19)	0.29108(7)	0.0210(7)
C(14)	0.75171(15)	0.5432(2)	0.29443(8)	0.0244(7)
C(15)	0.71296(17)	0.4849(2)	0.29892(10)	0.0355(9)
C(16)	0.81157(16)	0.5325(2)	0.29347(8)	0.0290(8)

Table S21. Continued

atom	x	y	z	U(eq)
C(17)	0.84903(15)	0.5839(2)	0.28873(8)	0.0297(8)
C(18)	0.91361(17)	0.5709(3)	0.28792(11)	0.0460(12)
C(19)	0.82590(15)	0.6473(2)	0.28478(7)	0.0272(8)
C(110)	0.76640(15)	0.6607(2)	0.28583(7)	0.0233(7)
C(111)	0.74258(17)	0.7300(2)	0.28147(10)	0.0340(9)
C(112)	0.45995(14)	0.60925(19)	0.19662(7)	0.0202(7)
C(113)	0.43667(14)	0.54561(19)	0.19128(7)	0.0220(7)
C(114)	0.43333(17)	0.4975(2)	0.21596(8)	0.0293(8)
C(115)	0.41523(15)	0.5271(2)	0.16242(8)	0.0248(7)
C(116)	0.41579(15)	0.5708(2)	0.13922(7)	0.0259(8)
C(117)	0.3893(2)	0.5510(2)	0.10832(8)	0.0382(10)
C(118)	0.43976(16)	0.6331(2)	0.14497(7)	0.0253(8)
C(119)	0.46256(14)	0.65297(19)	0.17319(7)	0.0227(7)
C(120)	0.48940(18)	0.7208(2)	0.17858(9)	0.0312(8)
C(121)	0.35677(14)	0.81789(18)	0.29841(7)	0.0194(7)
C(122)	0.29938(15)	0.80619(19)	0.30430(7)	0.0227(7)
C(123)	0.28120(18)	0.7389(2)	0.31380(11)	0.0380(10)
C(124)	0.25841(15)	0.8580(2)	0.30066(7)	0.0243(7)
C(125)	0.27214(16)	0.9199(2)	0.29138(7)	0.0252(8)
C(126)	0.22688(18)	0.9754(2)	0.28718(9)	0.0352(9)
C(127)	0.32915(16)	0.93103(19)	0.28612(8)	0.0261(8)
C(128)	0.37192(15)	0.88142(19)	0.28971(7)	0.0223(7)
C(129)	0.43360(16)	0.8969(2)	0.28486(9)	0.0310(8)
C(130)	0.57185(14)	0.67871(18)	0.40607(7)	0.0186(7)
C(131)	0.53979(14)	0.63529(18)	0.42127(7)	0.0198(7)
C(132)	0.49216(15)	0.5917(2)	0.40506(8)	0.0255(8)
C(133)	0.55169(14)	0.63271(19)	0.45190(7)	0.0219(7)
C(134)	0.59451(15)	0.6729(2)	0.46743(7)	0.0246(8)
C(135)	0.60752(17)	0.6693(2)	0.50049(8)	0.0313(9)
C(136)	0.62496(15)	0.7169(2)	0.45194(8)	0.0256(8)
C(137)	0.61474(14)	0.72071(19)	0.42150(7)	0.0221(7)
C(138)	0.64896(18)	0.7696(2)	0.40578(9)	0.0326(9)
C(139)	0.61312(16)	0.3649(2)	0.32293(8)	0.0293(8)
C(140)	0.57054(15)	0.3947(2)	0.29805(8)	0.0283(8)

Table S21. Continued

atom	x	y	z	U(eq)
C(141)	0.47086(16)	0.3893(2)	0.27567(8)	0.0278(8)
C(142)	0.41462(16)	0.3513(2)	0.27698(8)	0.0293(8)
C(143)	0.34254(16)	0.3321(2)	0.30783(8)	0.0311(9)
C(144)	0.31740(16)	0.3607(2)	0.33321(8)	0.0297(8)
C(145)	0.34128(18)	0.3790(2)	0.38451(9)	0.0344(9)
C(146)	0.38867(18)	0.3630(2)	0.40978(8)	0.0324(9)
C(147)	0.48889(18)	0.3800(2)	0.42782(8)	0.0327(9)
C(148)	0.54089(18)	0.4240(2)	0.42605(8)	0.0318(9)
C(149)	0.60695(16)	0.4509(2)	0.39243(8)	0.0305(8)
C(150)	0.61108(16)	0.4472(2)	0.36044(8)	0.0269(8)
O(1)	0.39161(11)	0.37147(15)	0.30270(5)	0.0281(6)
O(2)	0.36274(11)	0.36069(14)	0.35810(5)	0.0264(6)
O(3)	0.44016(12)	0.40215(14)	0.40747(5)	0.0279(6)
O(4)	0.55069(11)	0.42553(15)	0.39641(6)	0.0306(6)
O(5)	0.59999(11)	0.38005(14)	0.35152(6)	0.0286(6)
O(6)	0.51355(10)	0.36874(14)	0.29971(5)	0.0259(6)
Fe(2)	0.81163(2)	0.29145(3)	0.03675(1)	0.0177(1)
K(2)	0.86980(3)	0.55293(5)	−0.00766(2)	0.0282(2)
N(21)	0.73932(12)	0.31776(15)	0.01040(6)	0.0195(6)
N(22)	0.84656(11)	0.25729(14)	0.00324(6)	0.0175(6)
N(23)	0.88368(12)	0.26811(16)	0.06286(6)	0.0223(6)
N(24)	0.77673(12)	0.32278(16)	0.07072(6)	0.0208(6)
N(25)	0.76014(15)	0.14816(19)	0.03686(8)	0.0343(8)
N(26)	0.85205(14)	0.43369(17)	0.02137(7)	0.0290(7)
C(2a1)	0.68779(14)	0.33947(18)	0.01843(7)	0.0201(7)
C(2a2)	0.73451(14)	0.32559(18)	−0.01931(7)	0.0200(7)
C(2a3)	0.82543(14)	0.26646(18)	−0.02575(7)	0.0192(7)
C(2a4)	0.89318(14)	0.21418(18)	0.00436(7)	0.0198(7)
C(2a5)	0.92750(14)	0.22616(19)	0.05675(7)	0.0231(7)
C(2a6)	0.90156(15)	0.2927(2)	0.09055(7)	0.0270(8)
C(2a7)	0.80566(15)	0.3350(2)	0.09821(7)	0.0242(7)
C(2a8)	0.71813(14)	0.33487(19)	0.07173(7)	0.0217(7)
C(2b1)	0.64917(14)	0.36272(19)	−0.00704(7)	0.0220(7)
C(2b2)	0.67844(15)	0.35579(19)	−0.03017(8)	0.0239(7)

Table S21. Continued

atom	x	y	z	U(eq)
C(2b3)	0.86091(15)	0.22992(19)	−0.04346(7)	0.0223(7)
C(2b4)	0.90185(15)	0.19634(19)	−0.02492(7)	0.0226(7)
C(2b5)	0.97373(15)	0.2240(2)	0.08147(8)	0.0302(9)
C(2b6)	0.95905(16)	0.2667(2)	0.10169(8)	0.0343(10)
C(2b7)	0.76387(15)	0.3534(2)	0.11748(8)	0.0254(8)
C(2b8)	0.70984(15)	0.35089(19)	0.10116(7)	0.0235(7)
C(2m1)	0.77451(14)	0.30163(18)	−0.03685(7)	0.0196(7)
C(2m2)	0.93038(14)	0.19547(18)	0.02989(7)	0.0202(7)
C(2m3)	0.86620(15)	0.3275(2)	0.10745(8)	0.0267(8)
C(2m4)	0.67513(13)	0.34254(18)	0.04721(7)	0.0193(7)
C(21)	0.77832(14)	0.2017(2)	0.03834(7)	0.0230(7)
C(22)	0.83971(14)	0.38165(19)	0.02907(7)	0.0222(7)
C(23)	0.76053(15)	0.31131(19)	−0.06934(7)	0.0232(7)
C(24)	0.79087(16)	0.3592(2)	−0.08294(7)	0.0260(8)
C(25)	0.83751(18)	0.4018(2)	−0.06537(9)	0.0334(9)
C(26)	0.77750(18)	0.3685(2)	−0.11312(8)	0.0357(9)
C(27)	0.7347(2)	0.3314(3)	−0.13008(8)	0.0424(11)
C(28)	0.7199(3)	0.3437(3)	−0.16271(9)	0.0657(18)
C(29)	0.70498(19)	0.2838(3)	−0.11636(9)	0.0443(11)
C(210)	0.71673(16)	0.2722(2)	−0.08611(8)	0.0316(9)
C(211)	0.6834(2)	0.2200(3)	−0.07246(11)	0.0472(12)
C(212)	0.97657(14)	0.14295(18)	0.02884(7)	0.0211(7)
C(213)	1.03271(15)	0.15885(19)	0.02257(7)	0.0225(7)
C(214)	1.04788(16)	0.2279(2)	0.01398(9)	0.0318(9)
C(215)	1.07575(15)	0.10941(19)	0.02458(8)	0.0243(7)
C(216)	1.06439(16)	0.0451(2)	0.03242(8)	0.0292(8)
C(217)	1.11125(19)	−0.0077(2)	0.03509(11)	0.0400(10)
C(218)	1.00765(17)	0.0299(2)	0.03736(9)	0.0325(9)
C(219)	0.96371(16)	0.0778(2)	0.03611(9)	0.0297(8)
C(220)	0.90338(18)	0.0579(2)	0.04258(11)	0.0408(11)
C(221)	0.89120(15)	0.3585(2)	0.13622(8)	0.0304(9)
C(222)	0.90654(16)	0.4254(2)	0.13634(9)	0.0341(10)
C(223)	0.90163(19)	0.4652(3)	0.10853(10)	0.0410(10)
C(224)	0.92629(18)	0.4564(3)	0.16317(10)	0.0413(11)

Table S21. Continued

atom	x	y	z	U(eq)
C(225)	0.93104(18)	0.4218(3)	0.18946(9)	0.0443(12)
C(226)	0.9525(2)	0.4550(3)	0.21873(11)	0.0629(17)
C(227)	0.91585(17)	0.3558(3)	0.18879(9)	0.0398(11)
C(228)	0.89629(16)	0.3221(2)	0.16258(8)	0.0335(9)
C(229)	0.8810(2)	0.2507(3)	0.16316(9)	0.0442(11)
C(230)	0.61382(13)	0.35976(18)	0.05186(7)	0.0189(7)
C(231)	0.59931(14)	0.42378(18)	0.06003(7)	0.0211(7)
C(232)	0.64413(17)	0.4789(2)	0.06436(9)	0.0306(8)
C(233)	0.54156(15)	0.43696(19)	0.06425(7)	0.0241(7)
C(234)	0.49833(15)	0.3883(2)	0.06055(8)	0.0255(8)
C(235)	0.43648(17)	0.4043(3)	0.06559(11)	0.0425(11)
C(236)	0.51331(14)	0.32529(19)	0.05242(7)	0.0234(7)
C(237)	0.57073(14)	0.31023(18)	0.04786(7)	0.0207(7)
C(238)	0.58551(17)	0.2409(2)	0.03932(10)	0.0358(9)
C(239)	0.98708(18)	0.6235(2)	0.04338(9)	0.0360(9)
C(240)	0.93381(17)	0.6470(2)	0.05618(9)	0.0324(9)
C(241)	0.83744(17)	0.6142(2)	0.06223(9)	0.0311(8)
C(242)	0.78900(17)	0.5675(2)	0.05064(8)	0.0321(9)
C(243)	0.72797(18)	0.5366(3)	0.00695(10)	0.0417(11)
C(244)	0.71019(18)	0.5553(3)	−0.02437(10)	0.0400(10)
C(245)	0.7463(2)	0.5683(3)	−0.06910(10)	0.0506(13)
C(248)	1.00795(18)	0.6063(2)	−0.03324(10)	0.0387(10)
C(249)	1.02222(18)	0.6023(3)	−0.00081(10)	0.0439(11)
O(7)	0.97328(11)	0.62132(14)	0.01244(6)	0.0303(6)
O(8)	0.88730(11)	0.60143(14)	0.04805(6)	0.0304(6)
O(9)	0.77088(12)	0.58168(15)	0.02028(6)	0.0331(6)
O(10)	0.75893(13)	0.55262(19)	−0.03911(6)	0.0465(8)
C(1a)	0.9454(3)	0.5590(4)	−0.07417(13)	0.0327(14)
C(27a)	0.8967(4)	0.6051(5)	−0.0831(2)	0.047(2)
C(26a)	0.7953(4)	0.6072(5)	−0.07938(18)	0.046(2)
O(11a)	0.8457(2)	0.5740(2)	−0.07221(10)	0.0399(10)
O(12a)	0.9648(5)	0.5561(5)	−0.0434(3)	0.0327(17)
C(1b)	0.9350(7)	0.6142(10)	−0.0723(3)	0.051(4)
C(27b)	0.8749(8)	0.5998(12)	−0.0814(5)	0.047(2)

Table S21. Continued

atom	x	y	z	U(eq)
C(26b)	0.7800(8)	0.6256(10)	−0.0716(4)	0.046(2)
O(11b)	0.8448(4)	0.6285(5)	−0.0618(2)	0.0399(10)
O(12b)	0.9543(10)	0.5793(11)	−0.0428(5)	0.047(5)
Fe(3)	0.14088(2)	0.28303(3)	0.36906(1)	0.0174(1)
K(3)	0.21722(4)	0.53676(4)	0.32811(2)	0.0292(2)
N(31)	0.07236(12)	0.31289(15)	0.34098(6)	0.0201(6)
N(32)	0.17810(12)	0.24491(15)	0.33704(6)	0.0189(6)
N(33)	0.20963(12)	0.25560(15)	0.39691(6)	0.0185(6)
N(34)	0.10405(12)	0.31906(15)	0.40136(6)	0.0194(6)
N(35)	0.07653(15)	0.14648(19)	0.36853(8)	0.0359(8)
N(36)	0.19454(14)	0.42136(18)	0.35682(7)	0.0300(7)
C(3a1)	0.01985(14)	0.33613(19)	0.34737(7)	0.0230(7)
C(3a2)	0.07003(14)	0.31724(19)	0.31114(7)	0.0218(7)
C(3a3)	0.16014(15)	0.25400(18)	0.30768(7)	0.0213(7)
C(3a4)	0.22356(14)	0.19994(18)	0.33962(7)	0.0202(7)
C(3a5)	0.25193(14)	0.20986(19)	0.39263(7)	0.0203(7)
C(3a6)	0.22554(14)	0.28037(18)	0.42481(7)	0.0201(7)
C(3a7)	0.13136(14)	0.33293(18)	0.42901(7)	0.0201(7)
C(3a8)	0.04590(14)	0.33672(19)	0.40053(7)	0.0205(7)
C(3b1)	−0.01645(15)	0.3571(2)	0.32082(8)	0.0284(8)
C(3b2)	0.01487(15)	0.3470(2)	0.29857(8)	0.0285(8)
C(3b3)	0.19691(15)	0.21530(19)	0.29121(7)	0.0235(7)
C(3b4)	0.23522(15)	0.18090(19)	0.31084(7)	0.0240(7)
C(3b5)	0.29441(14)	0.20472(19)	0.41864(7)	0.0225(7)
C(3b6)	0.27987(14)	0.2497(2)	0.43805(7)	0.0232(7)
C(3b7)	0.08933(15)	0.35900(19)	0.44636(7)	0.0227(7)
C(3b8)	0.03626(15)	0.35871(19)	0.42922(7)	0.0238(7)
C(3m1)	0.11133(14)	0.29031(19)	0.29514(7)	0.0209(7)
C(3m2)	0.25715(14)	0.17970(18)	0.36600(7)	0.0204(7)
C(3m3)	0.19056(14)	0.32053(18)	0.43985(7)	0.0199(7)
C(3m4)	0.00473(14)	0.34292(18)	0.37547(7)	0.0206(7)
C(31)	0.10062(15)	0.1970(2)	0.36996(7)	0.0237(7)
C(32)	0.17641(14)	0.37044(19)	0.36277(7)	0.0213(7)
C(33)	0.09907(15)	0.29587(19)	0.26238(8)	0.0240(7)

Table S21. Continued

atom	x	y	z	U(eq)
C(34)	0.12996(17)	0.3417(2)	0.24807(8)	0.0287(8)
C(35)	0.17640(19)	0.3854(2)	0.26478(10)	0.0384(9)
C(36)	0.11722(19)	0.3473(2)	0.21772(9)	0.0369(9)
C(37)	0.0740(2)	0.3081(2)	0.20167(10)	0.0400(9)
C(38)	0.0601(3)	0.3150(3)	0.16870(12)	0.0598(14)
C(39)	0.0448(2)	0.2627(2)	0.21630(10)	0.0402(9)
C(310)	0.05598(17)	0.2551(2)	0.24637(9)	0.0328(8)
C(311)	0.0236(2)	0.2035(3)	0.26169(12)	0.0537(14)
C(312)	0.30083(14)	0.12454(18)	0.36454(7)	0.0203(7)
C(313)	0.36130(15)	0.13695(19)	0.36562(7)	0.0224(7)
C(314)	0.38701(17)	0.2055(2)	0.36960(10)	0.0344(9)
C(315)	0.39957(15)	0.0841(2)	0.36312(7)	0.0248(8)
C(316)	0.37966(16)	0.0195(2)	0.35905(7)	0.0250(8)
C(317)	0.42197(18)	−0.0368(2)	0.35710(9)	0.0345(9)
C(318)	0.31941(16)	0.0080(2)	0.35776(8)	0.0262(8)
C(319)	0.27980(15)	0.05922(19)	0.36066(7)	0.0238(7)
C(320)	0.21532(17)	0.0438(2)	0.35964(9)	0.0333(9)
C(321)	0.21546(14)	0.35249(19)	0.46844(7)	0.0224(7)
C(322)	0.22992(14)	0.4199(2)	0.46785(8)	0.0245(8)
C(323)	0.22287(16)	0.4587(2)	0.43953(8)	0.0281(8)
C(324)	0.25136(15)	0.4521(2)	0.49415(8)	0.0290(8)
C(325)	0.25869(15)	0.4183(2)	0.52087(8)	0.0286(8)
C(326)	0.28371(19)	0.4533(3)	0.54894(9)	0.0413(11)
C(327)	0.24269(15)	0.3521(2)	0.52095(8)	0.0276(8)
C(328)	0.22107(14)	0.3179(2)	0.49525(7)	0.0249(8)
C(329)	0.20490(17)	0.2460(2)	0.49692(8)	0.0316(9)
C(330)	−0.05716(14)	0.36200(19)	0.37855(7)	0.0216(7)
C(331)	−0.07446(16)	0.4287(2)	0.37884(9)	0.0294(8)
C(332)	−0.0311(2)	0.4840(2)	0.37740(13)	0.0496(12)
C(333)	−0.13318(17)	0.4436(2)	0.38124(9)	0.0341(9)
C(334)	−0.17393(15)	0.3946(2)	0.38345(8)	0.0300(9)
C(335)	−0.23669(18)	0.4124(3)	0.38718(12)	0.0478(12)
C(336)	−0.15623(15)	0.3290(2)	0.38334(7)	0.0255(8)
C(337)	−0.09828(14)	0.31195(19)	0.38111(7)	0.0220(7)

Table S21. Continued

atom	x	y	z	U(eq)
C(338)	−0.08014(17)	0.2399(2)	0.38292(10)	0.0343(9)
O(13)	0.22199(14)	0.59702(18)	0.38183(7)	0.0281(7)
O(14)	0.11388(14)	0.58211(19)	0.34595(7)	0.0323(8)
O(15)	0.12249(18)	0.5619(3)	0.28785(10)	0.0441(11)
O(17)	0.32271(17)	0.52209(19)	0.30399(9)	0.0402(9)
O(18)	0.31624(14)	0.60646(18)	0.35228(8)	0.0264(7)
C(339)	0.1675(2)	0.6125(3)	0.39205(12)	0.0311(12)
C(340)	0.1213(2)	0.5674(3)	0.37681(11)	0.0321(11)
C(341)	0.0740(4)	0.5376(7)	0.3293(2)	0.040(2)
C(342)	0.0668(2)	0.5615(4)	0.29776(12)	0.0454(15)
C(343)	0.1194(3)	0.5754(5)	0.25800(15)	0.056(2)
C(344)	0.1801(4)	0.5882(4)	0.25007(16)	0.0528(19)
C(2a)	0.2796(5)	0.5444(6)	0.25491(17)	0.046(2)
O(16a)	0.22173(19)	0.5421(2)	0.26410(10)	0.0371(16)
C(2b)	0.275(3)	0.552(3)	0.2612(11)	0.046(2)
O(16b)	0.2154(11)	0.6037(14)	0.2661(6)	0.048(9)
C(345)	0.3180(3)	0.5003(4)	0.27489(14)	0.0511(16)
C(346)	0.3571(3)	0.5797(3)	0.30965(14)	0.0311(14)
C(347)	0.3697(2)	0.5901(3)	0.34200(11)	0.0361(12)
C(348)	0.3233(2)	0.6195(3)	0.38310(12)	0.0310(12)
C(349)	0.2669(3)	0.6448(5)	0.39042(18)	0.0325(15)
O(19)	0.1557(6)	0.6176(8)	0.3634(3)	0.035(3)
O(20)	0.0882(11)	0.5292(17)	0.3241(7)	0.041(7)
O(21)	0.1320(10)	0.5493(11)	0.2725(6)	0.058(5)
O(22)	0.2536(7)	0.5780(9)	0.2773(4)	0.043(4)
O(23)	0.3263(7)	0.5352(9)	0.3270(3)	0.044(4)
O(24)	0.2774(6)	0.5958(9)	0.3723(3)	0.043(4)
C(350)	0.0985(11)	0.5939(16)	0.3677(6)	0.050(6)
C(351)	0.0652(11)	0.5846(13)	0.3375(5)	0.044(5)
C(352)	0.0593(13)	0.5070(17)	0.2972(6)	0.062(7)
C(353)	0.0727(11)	0.5505(15)	0.2746(6)	0.056(7)
C(354)	0.1541(14)	0.5986(14)	0.2557(6)	0.039(6)
C(355)	0.2133(13)	0.5801(18)	0.2498(6)	0.0528(19)
C(356)	0.3079(10)	0.5527(16)	0.2747(6)	0.0511(16)

Table S21. Continued

atom	x	y	z	U(eq)
C(357)	0.3519(14)	0.5612(18)	0.3032(6)	0.0311(14)
C(358)	0.3604(10)	0.5463(11)	0.3532(5)	0.040(5)
C(359)	0.3363(11)	0.6044(13)	0.3699(7)	0.043(6)
C(360)	0.2524(14)	0.650(2)	0.3865(9)	0.0325(15)
C(361)	0.1903(13)	0.6276(18)	0.3909(6)	0.052(8)
O(26)	0.73692(18)	0.96437(18)	0.35327(8)	0.0735(18)
C(45)	0.69771(16)	0.91361(19)	0.36036(7)	0.0183(9)
C(46)	0.7056(2)	0.85776(15)	0.33934(10)	0.0574(19)
C(47)	0.7212(2)	0.8933(2)	0.31239(8)	0.0494(17)
C(48)	0.7287(2)	0.9654(2)	0.32177(8)	0.0429(15)
O(27)	0.48460(14)	0.58858(17)	0.04256(7)	0.0439(8)
C(49)	0.4971(3)	0.6491(3)	0.05784(11)	0.0570(14)
C(50)	0.5292(3)	0.6928(3)	0.03848(11)	0.0495(12)
C(51)	0.5621(2)	0.6426(2)	0.02275(10)	0.0424(11)
C(52)	0.51842(19)	0.5854(2)	0.01870(9)	0.0376(10)
O(28)	0.1874(3)	0.8248(4)	0.19494(14)	0.089(2)
C(53)	0.1752(4)	0.8405(4)	0.22664(14)	0.059(2)
C(54)	0.1667(5)	0.7741(4)	0.23863(17)	0.065(2)
C(55)	0.1684(4)	0.7278(3)	0.21660(15)	0.063(2)
C(56)	0.1580(3)	0.7590(4)	0.19000(16)	0.0503(18)
O(30)	0.8254(3)	0.7145(3)	0.35787(13)	0.0807(17)
C(61)	0.8563(2)	0.6506(3)	0.36528(11)	0.0351(12)
C(62)	0.8484(3)	0.6389(3)	0.39759(13)	0.0462(14)
C(63)	0.8400(3)	0.7078(3)	0.40819(13)	0.0500(15)
C(64)	0.8387(2)	0.7516(3)	0.38344(10)	0.0321(11)
O(25)	0.43252(12)	0.48440(15)	0.47400(6)	0.0350(7)
C(41)	0.38232(16)	0.5037(2)	0.45319(9)	0.0304(8)
C(42)	0.37266(19)	0.5758(2)	0.46004(9)	0.0345(9)
C(43)	0.3943(2)	0.5813(2)	0.49307(9)	0.0397(10)
C(44)	0.42174(19)	0.5137(2)	0.50120(9)	0.0384(10)
O(29a)	0.8970(3)	0.0149(3)	0.37123(11)	0.0714(18)
C(57a)	0.9026(3)	−0.0345(2)	0.34954(12)	0.060(2)
C(58a)	0.9091(2)	0.0121(2)	0.32200(9)	0.0528(18)
C(59a)	0.9304(2)	0.0796(2)	0.33441(11)	0.059(2)

Table S21. Continued

atom	x	y	z	U(eq)
C(60a)	0.9353(3)	0.0672(3)	0.37075(10)	0.069(3)
O(29b)	0.9450(3)	0.0654(3)	0.30736(11)	0.0714(18)
C(57b)	0.9251(3)	0.0033(2)	0.31779(10)	0.060(2)
C(58b)	0.9199(2)	0.0039(2)	0.35012(9)	0.0528(18)
C(59b)	0.9420(3)	0.0728(3)	0.36030(10)	0.059(2)
C(60b)	0.9500(3)	0.1086(2)	0.33225(13)	0.069(3)
O(31)	0.7666(2)	0.1084(3)	−0.02445(10)	0.0414(12)
O(32)	0.5682(7)	0.8663(6)	0.3511(3)	0.063(4)

[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 S22. Bond Lengths for 3[K(18-crown-6)][Fe(TMP)$(CN)_2$]·5.1(THF)·0.9H_2O[a]

bond	length (Å)	bond	length (Å)
Fe(1)–C(11)	1.966(4)	C(248)–H(24L)	0.9411
Fe(1)–N(13)	1.967(3)	C(249)–O(7)	1.412(5)
Fe(1)–N(14)	1.978(3)	C(249)–H(18d)	0.9900
Fe(1)–N(11)	1.982(3)	C(249)–H(18e)	0.9900
Fe(1)–N(12)	1.988(3)	C(1a)–O(12a)	1.427(14)
Fe(1)–C(12)	1.993(4)	C(1a)–C(27a)	1.466(11)
K(1)–O(4)	2.690(3)	C(1a)–H(1a1)	0.9900
K(1)–O(1)	2.692(3)	C(1a)–H(1a2)	0.9900
K(1)–O(2)	2.752(3)	C(27a)–O(11a)	1.483(9)
K(1)–O(6)	2.765(3)	C(27a)–H(27a)	0.9900
K(1)–N(16)	2.848(3)	C(27a)–H(27b)	0.9900
K(1)–O(3)	2.896(3)	C(26a)–O(11a)	1.338(10)
K(1)–O(5)	3.070(3)	C(26a)–H(26b)	0.9900
N(11)–C(1a1)	1.368(4)	C(26a)–H(26C)	0.9900
N(11)–C(1a2)	1.371(4)	C(1b)–C(27b)	1.41(2)
N(12)–C(1a4)	1.371(4)	C(1b)–O(12b)	1.54(3)
N(12)–C(1a3)	1.373(4)	C(1b)–H(1b1)	0.9110
N(13)–C(1a5)	1.378(4)	C(1b)–H(1b2)	0.9110
N(13)–C(1a6)	1.380(4)	C(27b)–O(11b)	1.35(2)
N(14)–C(1a7)	1.371(4)	C(27b)–H(27C)	0.9900
N(14)–C(1a8)	1.374(4)	C(27b)–H(27d)	0.9900
N(15)–C(11)	1.158(5)	C(26b)–O(11b)	1.49(2)
N(16)–C(12)	1.161(5)	C(26b)–H(26d)	0.9900
C(1a1)–C(1m4)	1.402(4)	C(26b)–H(26e)	0.9900
C(1a1)–C(1b1)	1.440(4)	Fe(3)–N(34)	1.962(3)
C(1a2)–C(1m1)	1.400(4)	Fe(3)–N(33)	1.965(3)
C(1a2)–C(1b2)	1.444(4)	Fe(3)–C(31)	1.971(4)
C(1a3)–C(1m1)	1.392(4)	Fe(3)–N(32)	1.972(3)
C(1a3)–C(1b3)	1.437(4)	Fe(3)–N(31)	1.981(3)
C(1a4)–C(1m2)	1.398(4)	Fe(3)–C(32)	1.984(4)
C(1a4)–C(1b4)	1.447(5)	K(3)–O(23)	2.519(16)
C(1a5)–C(1m2)	1.395(5)	K(3)–O(24)	2.583(16)
C(1a5)–C(1b5)	1.444(4)	K(3)–O(15)	2.695(4)
C(1a6)–C(1m3)	1.394(5)	K(3)–O(22)	2.736(17)

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(1a6)–C(1b6)	1.446(4)	K(3)–O(13)	2.751(3)
C(1a7)–C(1m3)	1.402(4)	K(3)–N(36)	2.768(4)
C(1a7)–C(1b7)	1.439(5)	K(3)–O(18)	2.768(4)
C(1a8)–C(1m4)	1.396(4)	K(3)–O(14)	2.784(3)
C(1a8)–C(1b8)	1.441(5)	K(3)–O(19)	2.828(14)
C(1b1)–C(1b2)	1.355(5)	K(3)–O(17)	2.833(4)
C(1b1)–H(1ba)	0.9500	K(3)–O(20)	2.95(2)
C(1b2)–H(1bF)	0.9500	K(3)–O(16a)	2.976(5)
C(1b3)–C(1b4)	1.355(5)	N(31)–C(3a1)	1.368(4)
C(1b3)–H(1be)	0.9500	N(31)–C(3a2)	1.374(4)
C(1b4)–H(1bd)	0.9500	N(32)–C(3a3)	1.370(4)
C(1b5)–C(1b6)	1.351(5)	N(32)–C(3a4)	1.377(4)
C(1b5)–H(1bg)	0.9500	N(33)–C(3a5)	1.377(4)
C(1b6)–H(1bH)	0.9500	N(33)–C(3a6)	1.380(4)
C(1b7)–C(1b8)	1.359(5)	N(34)–C(3a7)	1.366(4)
C(1b7)–H(1bC)	0.9500	N(34)–C(3a8)	1.380(4)
C(1b8)–H(1bb)	0.9500	N(35)–C(31)	1.158(5)
C(1m1)–C(13)	1.503(4)	N(36)–C(32)	1.158(5)
C(1m2)–C(112)	1.508(4)	C(3a1)–C(3m4)	1.399(5)
C(1m3)–C(121)	1.502(4)	C(3a1)–C(3b1)	1.441(5)
C(1m4)–C(130)	1.502(4)	C(3a2)–C(3m1)	1.398(5)
C(13)–C(14)	1.400(5)	C(3a2)–C(3b2)	1.446(5)
C(13)–C(110)	1.408(5)	C(3a3)–C(3m1)	1.393(5)
C(14)–C(16)	1.402(5)	C(3a3)–C(3b3)	1.448(5)
C(14)–C(15)	1.509(6)	C(3a4)–C(3m2)	1.403(5)
C(15)–H(15i)	0.9800	C(3a4)–C(3b4)	1.447(5)
C(15)–H(15j)	0.9800	C(3a5)–C(3m2)	1.393(5)
C(15)–H(15K)	0.9800	C(3a5)–C(3b5)	1.435(4)
C(16)–C(17)	1.387(6)	C(3a6)–C(3m3)	1.398(5)
C(16)–H(16a)	0.9500	C(3a6)–C(3b6)	1.447(5)
C(17)–C(19)	1.388(6)	C(3a7)–C(3m3)	1.402(4)
C(17)–C(18)	1.515(5)	C(3a7)–C(3b7)	1.444(5)
C(18)–H(18a)	0.9800	C(3a8)–C(3m4)	1.388(4)
C(18)–H(18b)	0.9800	C(3a8)–C(3b8)	1.445(5)

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(18)–H(18C)	0.9800	C(3b1)–C(3b2)	1.355(5)
C(19)–C(110)	1.404(5)	C(3b1)–H(3bH)	0.9500
C(19)–H(19a)	0.9500	C(3b2)–H(3bg)	0.9500
C(110)–C(111)	1.504(6)	C(3b3)–C(3b4)	1.358(5)
C(111)–H(11C)	0.9800	C(3b3)–H(3bC)	0.9500
C(111)–H(11d)	0.9800	C(3b4)–H(3ba)	0.9500
C(111)–H(11e)	0.9800	C(3b5)–C(3b6)	1.352(5)
C(112)–C(113)	1.399(5)	C(3b5)–H(3bd)	0.9500
C(112)–C(119)	1.404(5)	C(3b6)–H(3bF)	0.9500
C(113)–C(115)	1.401(5)	C(3b7)–C(3b8)	1.353(5)
C(113)–C(114)	1.508(5)	C(3b7)–H(3bb)	0.9500
C(114)–H(11F)	0.9800	C(3b8)–H(3be)	0.9500
C(114)–H(11g)	0.9800	C(3m1)–C(33)	1.501(5)
C(114)–H(11H)	0.9800	C(3m2)–C(312)	1.508(5)
C(115)–C(116)	1.389(5)	C(3m3)–C(321)	1.504(4)
C(115)–H(11a)	0.9500	C(3m4)–C(330)	1.502(4)
C(116)–C(118)	1.384(6)	C(33)–C(34)	1.392(5)
C(116)–C(117)	1.519(5)	C(33)–C(310)	1.411(5)
C(117)–H(11i)	0.9800	C(34)–C(36)	1.393(5)
C(117)–H(11j)	0.9800	C(34)–C(35)	1.507(6)
C(117)–H(11K)	0.9800	C(35)–H(35a)	0.9800
C(118)–C(119)	1.390(5)	C(35)–H(35b)	0.9800
C(118)–H(11b)	0.9500	C(35)–H(35C)	0.9800
C(119)–C(120)	1.508(5)	C(36)–C(37)	1.395(6)
C(120)–H(12C)	0.9800	C(36)–H(36a)	0.9500
C(120)–H(12d)	0.9800	C(37)–C(39)	1.372(7)
C(120)–H(12e)	0.9800	C(37)–C(38)	1.516(7)
C(121)–C(128)	1.403(5)	C(38)–H(38a)	0.9800
C(121)–C(122)	1.407(5)	C(38)–H(38b)	0.9800
C(122)–C(124)	1.402(5)	C(38)–H(38C)	0.9800
C(122)–C(123)	1.506(6)	C(39)–C(310)	1.383(6)
C(123)–H(12i)	0.9800	C(39)–H(39a)	0.9500
C(123)–H(12j)	0.9800	C(310)–C(311)	1.514(7)
C(123)–H(12K)	0.9800	C(311)–H(31i)	0.9800

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(124)–C(125)	1.373(6)	C(311)–H(31j)	0.9800
C(124)–H(12b)	0.9500	C(311)–H(31K)	0.9800
C(125)–C(127)	1.387(5)	C(312)–C(319)	1.407(5)
C(125)–C(126)	1.521(5)	C(312)–C(313)	1.407(5)
C(126)–H(12L)	0.9800	C(313)–C(315)	1.399(5)
C(126)–H(12m)	0.9800	C(313)–C(314)	1.506(6)
C(126)–H(12N)	0.9800	C(314)–H(31F)	0.9800
C(127)–C(128)	1.396(5)	C(314)–H(31g)	0.9800
C(127)–H(12a)	0.9500	C(314)–H(31H)	0.9800
C(128)–C(129)	1.502(5)	C(315)–C(316)	1.386(6)
C(129)–H(12F)	0.9800	C(315)–H(31a)	0.9500
C(129)–H(12g)	0.9800	C(316)–C(318)	1.398(5)
C(129)–H(12H)	0.9800	C(316)–C(317)	1.507(5)
C(130)–C(131)	1.400(5)	C(317)–H(31C)	0.9800
C(130)–C(137)	1.412(5)	C(317)–H(31d)	0.9800
C(131)–C(133)	1.402(4)	C(317)–H(31e)	0.9800
C(131)–C(132)	1.514(5)	C(318)–C(319)	1.398(5)
C(132)–H(13F)	0.9800	C(318)–H(31b)	0.9500
C(132)–H(13g)	0.9800	C(319)–C(320)	1.510(5)
C(132)–H(13H)	0.9800	C(320)–H(32L)	0.9800
C(133)–C(134)	1.391(5)	C(320)–H(32m)	0.9800
C(133)–H(13a)	0.9500	C(320)–H(32N)	0.9800
C(134)–C(136)	1.393(6)	C(321)–C(322)	1.402(6)
C(134)–C(135)	1.514(5)	C(321)–C(328)	1.410(5)
C(135)–H(13C)	0.9800	C(322)–C(324)	1.401(5)
C(135)–H(13d)	0.9800	C(322)–C(323)	1.512(5)
C(135)–H(13e)	0.9800	C(323)–H(32e)	0.9800
C(136)–C(137)	1.393(5)	C(323)–H(32F)	0.9800
C(136)–H(13b)	0.9500	C(323)–H(32g)	0.9800
C(137)–C(138)	1.514(5)	C(324)–C(325)	1.398(6)
C(138)–H(13i)	0.9800	C(324)–H(32H)	0.9500
C(138)–H(13j)	0.9800	C(325)–C(327)	1.386(6)
C(138)–H(13K)	0.9800	C(325)–C(326)	1.513(5)
C(139)–O(5)	1.430(5)	C(326)–H(32i)	0.9800

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(139)–C(140)	1.519(5)	C(326)–H(32j)	0.9800
C(139)–H(13L)	0.9900	C(326)–H(32K)	0.9800
C(139)–H(13m)	0.9900	C(327)–C(328)	1.399(5)
C(140)–O(6)	1.425(4)	C(327)–H(32a)	0.9500
C(140)–H(14a)	0.9900	C(328)–C(329)	1.503(6)
C(140)–H(14b)	0.9900	C(329)–H(32b)	0.9800
C(141)–O(6)	1.431(4)	C(329)–H(32C)	0.9800
C(141)–C(142)	1.514(5)	C(329)–H(32d)	0.9800
C(141)–H(43C)	0.9900	C(330)–C(337)	1.401(5)
C(141)–H(43d)	0.9900	C(330)–C(331)	1.404(6)
C(142)–O(1)	1.430(4)	C(331)–C(333)	1.405(5)
C(142)–H(70a)	0.9900	C(331)–C(332)	1.505(6)
C(142)–H(70b)	0.9900	C(332)–H(33i)	0.9800
C(143)–O(1)	1.429(5)	C(332)–H(33j)	0.9800
C(143)–C(144)	1.497(5)	C(332)–H(33K)	0.9800
C(143)–H(43a)	0.9900	C(333)–C(334)	1.376(6)
C(143)–H(43b)	0.9900	C(333)–H(33e)	0.9500
C(144)–O(2)	1.433(4)	C(334)–C(336)	1.385(6)
C(144)–H(93a)	0.9900	C(334)–C(335)	1.522(5)
C(144)–H(93b)	0.9900	C(335)–H(33F)	0.9800
C(145)–O(2)	1.431(4)	C(335)–H(33g)	0.9800
C(145)–C(146)	1.510(6)	C(335)–H(33H)	0.9800
C(145)–H(15e)	1.0948	C(336)–C(337)	1.396(5)
C(145)–H(15F)	1.0948	C(336)–H(33a)	0.9500
C(146)–O(3)	1.442(5)	C(337)–C(338)	1.511(6)
C(146)–H(15C)	0.9900	C(338)–H(33b)	0.9800
C(146)–H(15d)	0.9900	C(338)–H(33C)	0.9800
C(147)–O(3)	1.424(5)	C(338)–H(33d)	0.9800
C(147)–C(148)	1.502(6)	O(13)–C(349)	1.426(9)
C(147)–H(94a)	0.9900	O(13)–C(339)	1.437(6)
C(147)–H(94b)	0.9900	O(14)–C(341)	1.425(12)
C(148)–O(4)	1.420(5)	O(14)–C(340)	1.441(6)
C(148)–H(14m)	0.9900	O(15)–C(343)	1.397(8)
C(148)–H(14e)	0.9900	O(15)–C(342)	1.423(7)

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(149)–O(4)	1.429(5)	O(17)–C(345)	1.403(7)
C(149)–C(150)	1.496(5)	O(17)–C(346)	1.409(7)
C(149)–H(15g)	0.9900	O(18)–C(347)	1.422(6)
C(149)–H(15H)	0.9900	O(18)–C(348)	1.433(6)
C(150)–O(5)	1.428(5)	C(339)–C(340)	1.494(8)
C(150)–H(14C)	0.9900	C(339)–H(33L)	0.9900
C(150)–H(14d)	0.9900	C(339)–H(33m)	0.9900
Fe(2)–N(23)	1.957(3)	C(340)–H(34a)	0.9900
Fe(2)–N(24)	1.970(3)	C(340)–H(34b)	0.9900
Fe(2)–N(22)	1.971(3)	C(341)–C(342)	1.517(13)
Fe(2)–C(21)	1.973(4)	C(341)–H(34C)	0.9900
Fe(2)–C(22)	1.982(4)	C(341)–H(34d)	0.9900
Fe(2)–N(21)	1.982(3)	C(342)–H(34e)	0.9900
K(2)–O(8)	2.726(3)	C(342)–H(34F)	0.9900
K(2)–O(10)	2.742(3)	C(343)–C(344)	1.516(11)
K(2)–O(12b)	2.76(2)	C(343)–H(34g)	0.9900
K(2)–O(7)	2.789(3)	C(343)–H(34H)	0.9900
K(2)–N(26)	2.814(4)	C(344)–O(16b)	1.06(2)
K(2)–O(9)	2.838(3)	C(344)–O(16a)	1.422(9)
K(2)–O(11b)	2.912(9)	C(2a)–O(16a)	1.457(11)
K(2)–O(12a)	2.928(12)	C(2a)–C(345)	1.478(11)
K(2)–O(11a)	2.981(5)	C(2a)–H(2a1)	0.9900
N(21)–C(2a1)	1.366(4)	C(2a)–H(2a2)	0.9900
N(21)–C(2a2)	1.369(4)	C(2b)–C(345)	1.512(10)
N(22)–C(2a3)	1.368(4)	C(2b)–O(16b)	1.76(3)
N(22)–C(2a4)	1.376(4)	C(2b)–H(2b1)	0.9900
N(23)–C(2a6)	1.377(4)	C(2b)–H(2b2)	0.9900
N(23)–C(2a5)	1.378(4)	C(346)–C(347)	1.494(8)
N(24)–C(2a7)	1.366(4)	C(346)–H(34m)	0.9900
N(24)–C(2a8)	1.378(4)	C(346)–H(34N)	0.9900
N(25)–C(21)	1.157(5)	C(347)–H(34O)	0.9900
N(26)–C(22)	1.158(5)	C(347)–H(34P)	0.9900
C(2a1)–C(2m4)	1.403(5)	C(348)–C(349)	1.482(9)
C(2a1)–C(2b1)	1.444(4)	C(348)–H(34Q)	0.9900

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(2a2)–C(2m1)	1.399(5)	C(348)–H(34R)	0.9900
C(2a2)–C(2b2)	1.448(4)	C(349)–H(34S)	0.9900
C(2a3)–C(2m1)	1.400(5)	C(349)–H(34T)	0.9900
C(2a3)–C(2b3)	1.441(5)	O(19)–C(361)	1.41(3)
C(2a4)–C(2m2)	1.402(5)	O(19)–C(350)	1.44(3)
C(2a4)–C(2b4)	1.442(5)	O(20)–C(352)	1.40(3)
C(2a5)–C(2m2)	1.397(5)	O(20)–C(351)	1.42(3)
C(2a5)–C(2b5)	1.441(5)	O(21)–C(353)	1.38(3)
C(2a6)–C(2m3)	1.397(5)	O(21)–C(354)	1.40(3)
C(2a6)–C(2b6)	1.445(5)	O(22)–C(356)	1.37(3)
C(2a7)–C(2m3)	1.403(5)	O(22)–C(355)	1.46(3)
C(2a7)–C(2b7)	1.452(5)	O(23)–C(358)	1.36(2)
C(2a8)–C(2m4)	1.398(4)	O(23)–C(357)	1.42(3)
C(2a8)–C(2b8)	1.437(5)	O(24)–C(359)	1.39(3)
C(2b1)–C(2b2)	1.352(5)	O(24)–C(360)	1.44(4)
C(2b1)–H(2bd)	0.9500	C(350)–C(351)	1.50(3)
C(2b2)–H(2bH)	0.9500	C(350)–H(35d)	0.9900
C(2b3)–C(2b4)	1.357(5)	C(350)–H(35e)	0.9900
C(2b3)–H(2bC)	0.9500	C(351)–H(35F)	0.9900
C(2b4)–H(2ba)	0.9500	C(351)–H(35g)	0.9900
C(2b5)–C(2b6)	1.350(5)	C(352)–C(353)	1.43(3)
C(2b5)–H(2bb)	0.9500	C(352)–H(35H)	0.9900
C(2b6)–H(2be)	0.9500	C(352)–H(35i)	0.9900
C(2b7)–C(2b8)	1.356(5)	C(353)–H(35j)	0.9900
C(2b7)–H(2bF)	0.9500	C(353)–H(35K)	0.9900
C(2b8)–H(2bg)	0.9500	C(354)–C(355)	1.47(3)
C(2m1)–C(23)	1.500(4)	C(354)–H(35L)	0.9900
C(2m2)–C(212)	1.507(5)	C(354)–H(35m)	0.9900
C(2m3)–C(221)	1.504(5)	C(355)–H(35N)	0.9900
C(2m4)–C(230)	1.499(4)	C(355)–H(35O)	0.9900
C(23)–C(24)	1.395(6)	C(356)–C(357)	1.55(3)
C(23)–C(210)	1.417(5)	C(356)–H(35P)	0.9900
C(24)–C(26)	1.395(5)	C(356)–H(35Q)	0.9900
C(24)–C(25)	1.514(5)	C(357)–H(35R)	0.9900

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(25)–H(25a)	0.9800	C(357)–H(35S)	0.9900
C(25)–H(25b)	0.9800	C(358)–C(359)	1.55(3)
C(25)–H(25C)	0.9800	C(358)–H(35T)	0.9524
C(26)–C(27)	1.384(7)	C(358)–H(35U)	0.9524
C(26)–H(26a)	0.9500	C(359)–H(35V)	0.9900
C(27)–C(29)	1.385(8)	C(359)–H(35W)	0.9900
C(27)–C(28)	1.516(6)	C(360)–C(361)	1.54(4)
C(28)–H(28a)	0.9800	C(360)–H(36b)	0.9900
C(28)–H(28b)	0.9800	C(360)–H(36C)	0.9900
C(28)–H(28C)	0.9800	C(361)–H(36d)	0.9900
C(29)–C(210)	1.403(6)	C(361)–H(36e)	0.9900
C(29)–H(29a)	0.9500	O(26)–C(45)	1.4348
C(210)–C(211)	1.495(7)	O(26)–C(48)	1.4391
C(211)–H(21i)	0.9800	C(45)–C(46)	1.5160
C(211)–H(21j)	0.9800	C(45)–H(42C)	0.9900
C(211)–H(21K)	0.9800	C(45)–H(42d)	0.9900
C(212)–C(219)	1.399(5)	C(46)–C(47)	1.5260
C(212)–C(213)	1.402(5)	C(46)–H(42K)	0.9900
C(213)–C(215)	1.399(5)	C(46)–H(42L)	0.9900
C(213)–C(214)	1.504(5)	C(47)–C(48)	1.5206
C(214)–H(21a)	0.9800	C(47)–H(42m)	0.9900
C(214)–H(21b)	0.9800	C(47)–H(42N)	0.9900
C(214)–H(21C)	0.9800	C(48)–H(43j)	0.9900
C(215)–C(216)	1.382(6)	C(48)–H(43K)	0.9900
C(215)–H(21d)	0.9500	O(27)–C(49)	1.418(6)
C(216)–C(218)	1.393(6)	O(27)–C(52)	1.442(6)
C(216)–C(217)	1.508(5)	C(49)–C(50)	1.524(7)
C(217)–H(21F)	0.9800	C(49)–H(42a)	0.9900
C(217)–H(21g)	0.9800	C(49)–H(42b)	0.9900
C(217)–H(21H)	0.9800	C(50)–C(51)	1.513(7)
C(218)–C(219)	1.395(5)	C(50)–H(42e)	0.9900
C(218)–H(21e)	0.9500	C(50)–H(42F)	0.9900
C(219)–C(220)	1.517(5)	C(51)–C(52)	1.524(6)
C(220)–H(22a)	0.9800	C(51)–H(42g)	0.9900

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(220)–H(22b)	0.9800	C(51)–H(42H)	0.9900
C(220)–H(22C)	0.9800	C(52)–H(42i)	0.9900
C(221)–C(222)	1.396(7)	C(52)–H(42j)	0.9900
C(221)–C(228)	1.411(6)	O(28)–C(56)	1.494(10)
C(222)–C(224)	1.402(5)	O(28)–C(53)	1.564(10)
C(222)–C(223)	1.505(6)	C(53)–C(54)	1.475(10)
C(223)–H(22F)	0.9800	C(53)–H(43m)	0.9900
C(223)–H(22g)	0.9800	C(53)–H(43g)	0.9900
C(223)–H(22H)	0.9800	C(54)–C(55)	1.386(11)
C(224)–C(225)	1.390(7)	C(54)–H(43e)	0.9900
C(224)–H(22d)	0.9500	C(54)–H(43F)	0.9900
C(225)–C(227)	1.376(7)	C(55)–C(56)	1.369(10)
C(225)–C(226)	1.524(6)	C(55)–H(55a)	0.9900
C(226)–H(22L)	0.9800	C(55)–H(55b)	0.9900
C(226)–H(22m)	0.9800	C(56)–H(43H)	0.9900
C(226)–H(22N)	0.9800	C(56)–H(43i)	0.9900
C(227)–C(228)	1.404(5)	O(30)–C(64)	1.394(7)
C(227)–H(22e)	0.9500	O(30)–C(61)	1.487(8)
C(228)–C(229)	1.486(7)	C(61)–C(62)	1.547(8)
C(229)–H(22i)	0.9800	C(61)–H(61a)	0.9900
C(229)–H(22j)	0.9800	C(61)–H(61b)	0.9900
C(229)–H(22K)	0.9800	C(62)–C(63)	1.496(9)
C(230)–C(231)	1.400(5)	C(62)–H(62a)	0.9900
C(230)–C(237)	1.401(5)	C(62)–H(62b)	0.9900
C(231)–C(233)	1.397(5)	C(63)–C(64)	1.442(8)
C(231)–C(232)	1.510(5)	C(63)–H(63a)	0.9900
C(232)–H(23C)	0.9800	C(63)–H(63b)	0.9900
C(232)–H(23d)	0.9800	C(64)–H(64a)	0.9900
C(232)–H(23e)	0.9800	C(64)–H(64b)	0.9900
C(233)–C(234)	1.390(5)	O(25)–C(41)	1.442(4)
C(233)–H(23b)	0.9500	O(25)–C(44)	1.443(5)
C(234)–C(236)	1.385(6)	C(41)–C(42)	1.513(6)
C(234)–C(235)	1.511(5)	C(41)–H(24m)	0.9900
C(235)–H(23i)	0.9800	C(41)–H(24N)	0.9900

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(235)–H(23j)	0.9800	C(42)–C(43)	1.537(6)
C(235)–H(23K)	0.9800	C(42)–H(24i)	0.9900
C(236)–C(237)	1.402(5)	C(42)–H(24j)	0.9900
C(236)–H(23a)	0.9500	C(43)–C(44)	1.526(6)
C(237)–C(238)	1.507(6)	C(43)–H(24C)	0.9900
C(238)–H(23F)	0.9800	C(43)–H(24d)	0.9900
C(238)–H(23g)	0.9800	C(44)–H(24a)	0.9900
C(238)–H(23H)	0.9800	C(44)–H(24b)	0.9900
C(239)–O(7)	1.418(5)	O(29a)–C(60a)	1.3771
C(239)–C(240)	1.514(6)	O(29a)–C(57a)	1.4319
C(239)–H(16C)	0.9900	C(57a)–C(58a)	1.6065
C(239)–H(16d)	0.9900	C(57a)–H(57a)	0.9900
C(240)–O(8)	1.419(5)	C(57a)–H(57b)	0.9900
C(240)–H(15a)	0.9900	C(58a)–C(59a)	1.5311
C(240)–H(15b)	0.9900	C(58a)–H(58a)	0.9900
C(241)–O(8)	1.426(4)	C(58a)–H(58b)	0.9900
C(241)–C(242)	1.497(6)	C(59a)–C(60a)	1.6842
C(241)–H(41a)	0.9900	C(59a)–H(59a)	0.9900
C(241)–H(41b)	0.9900	C(59a)–H(59b)	0.9900
C(242)–O(9)	1.431(5)	C(60a)–H(60a)	0.9900
C(242)–H(24O)	0.9900	C(60a)–H(60b)	0.9900
C(242)–H(24P)	0.9900	O(29b)–C(60b)	1.4345
C(243)–O(9)	1.415(5)	O(29b)–C(57b)	1.4419
C(243)–C(244)	1.492(6)	C(57b)–C(58b)	1.5151
C(243)–H(24Q)	0.9900	C(57b)–H(57C)	0.9900
C(243)–H(24R)	0.9900	C(57b)–H(57d)	0.9900
C(244)–O(10)	1.397(5)	C(58b)–C(59b)	1.5310
C(244)–H(18F)	0.9900	C(58b)–H(58C)	0.9900
C(244)–H(18g)	0.9900	C(58b)–H(58d)	0.9900
C(245)–C(26b)	1.407(19)	C(59b)–C(60b)	1.5176
C(245)–O(10)	1.408(5)	C(59b)–H(59C)	0.9900
C(245)–C(26a)	1.507(10)	C(59b)–H(59d)	0.9900
C(245)–H(18i)	0.9900	C(60b)–H(60C)	0.9900
C(245)–H(18j)	0.9900	C(60b)–H(60d)	0.9900

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(248)–O(12b)	1.36(3)	O(31)–H(311)	0.671(4)
C(248)–O(12a)	1.447(13)	O(31)–H(312)	0.663(5)
C(248)–C(249)	1.487(6)		
C(248)–H(24K)	0.9411		

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

Table S23. Bond Angles for 3[K(18-crown-6)][Fe(TMP)$(CN)_2$]·5.1(THF)·0.9H_2O[a]

angle	degree	angle	degree
C(11)–Fe(1)–N(13)	91.76(13)	O(11a)–C(26a)–H(26b)	109.9
C(11)–Fe(1)–N(14)	87.92(13)	C(245)–C(26a)–H(26b)	109.9
N(13)–Fe(1)–N(14)	89.44(11)	O(11a)–C(26a)–H(26C)	109.9
C(11)–Fe(1)–N(11)	89.33(13)	C(245)–C(26a)–H(26C)	109.9
N(13)–Fe(1)–N(11)	178.91(13)	H(26b)–C(26a)–H(26C)	108.3
N(14)–Fe(1)–N(11)	90.48(11)	C(26a)–O(11a)–C(27a)	113.9(6)
C(11)–Fe(1)–N(12)	90.23(13)	C(26a)–O(11a)–K(2)	110.2(4)
N(13)–Fe(1)–N(12)	89.72(11)	C(27a)–O(11a)–K(2)	111.0(5)
N(14)–Fe(1)–N(12)	177.95(12)	C(1a)–O(12a)–C(248)	113.1(9)
N(11)–Fe(1)–N(12)	90.39(11)	C(1a)–O(12a)–K(2)	114.4(6)
C(11)–Fe(1)–C(12)	173.06(13)	C(248)–O(12a)–K(2)	111.5(5)
N(13)–Fe(1)–C(12)	95.13(13)	C(27b)–C(1b)–O(12b)	108.1(17)
N(14)–Fe(1)–C(12)	91.32(13)	C(27b)–C(1b)–H(1b1)	110.1
N(11)–Fe(1)–C(12)	83.78(12)	O(12b)–C(1b)–H(1b1)	110.1
N(12)–Fe(1)–C(12)	90.62(13)	C(27b)–C(1b)–H(1b2)	110.1
O(4)–K(1)–O(1)	167.55(10)	O(12b)–C(1b)–H(1b2)	110.1
O(4)–K(1)–O(2)	115.89(8)	H(1b1)–C(1b)–H(1b2)	108.4
O(1)–K(1)–O(2)	60.57(8)	O(11b)–C(27b)–C(1b)	106.9(18)
O(4)–K(1)–O(6)	113.70(8)	O(11b)–C(27b)–H(27C)	110.3
O(1)–K(1)–O(6)	62.48(7)	C(1b)–C(27b)–H(27C)	110.3
O(2)–K(1)–O(6)	116.96(8)	O(11b)–C(27b)–H(27d)	110.3
O(4)–K(1)–N(16)	98.36(9)	C(1b)–C(27b)–H(27d)	110.3
O(1)–K(1)–N(16)	92.10(9)	H(27C)–C(27b)–H(27d)	108.6
O(2)–K(1)–N(16)	130.07(9)	C(245)–C(26b)–O(11b)	122.9(14)
O(6)–K(1)–N(16)	75.35(9)	C(245)–C(26b)–H(26d)	106.6
O(4)–K(1)–O(3)	57.87(8)	O(11b)–C(26b)–H(26d)	106.6
O(1)–K(1)–O(3)	120.05(8)	C(245)–C(26b)–H(26e)	106.6
O(2)–K(1)–O(3)	59.48(7)	O(11b)–C(26b)–H(26e)	106.6
O(6)–K(1)–O(3)	155.20(8)	H(26d)–C(26b)–H(26e)	106.6
N(16)–K(1)–O(3)	127.11(9)	C(27b)–O(11b)–C(26b)	111.6(13)
O(4)–K(1)–O(5)	54.74(8)	C(27b)–O(11b)–K(2)	107.2(11)
O(1)–K(1)–O(5)	119.84(8)	C(26b)–O(11b)–K(2)	107.6(9)
O(2)–K(1)–O(5)	143.23(8)	C(248)–O(12b)–C(1b)	103.5(17)
O(6)–K(1)–O(5)	58.97(7)	C(248)–O(12b)–K(2)	124.8(12)

Table S23. Continued

angle	degree	angle	degree
N(16)–K(1)–O(5)	85.99(8)	C(1b)–O(12b)–K(2)	118.1(12)
O(3)–K(1)–O(5)	107.70(8)	N(34)–Fe(3)–N(33)	90.18(11)
C(1a1)–N(11)–C(1a2)	106.7(3)	N(34)–Fe(3)–C(31)	93.03(14)
C(1a1)–N(11)–Fe(1)	126.2(2)	N(33)–Fe(3)–C(31)	94.20(13)
C(1a2)–N(11)–Fe(1)	126.6(2)	N(34)–Fe(3)–N(32)	178.72(13)
C(1a4)–N(12)–C(1a3)	106.1(3)	N(33)–Fe(3)–N(32)	89.08(11)
C(1a4)–N(12)–Fe(1)	127.6(2)	C(31)–Fe(3)–N(32)	85.99(13)
C(1a3)–N(12)–Fe(1)	126.2(2)	N(34)–Fe(3)–N(31)	89.62(12)
C(1a5)–N(13)–C(1a6)	106.3(3)	N(33)–Fe(3)–N(31)	178.61(13)
C(1a5)–N(13)–Fe(1)	126.9(2)	C(31)–Fe(3)–N(31)	87.18(13)
C(1a6)–N(13)–Fe(1)	126.8(2)	N(32)–Fe(3)–N(31)	91.15(12)
C(1a7)–N(14)–C(1a8)	106.2(3)	N(34)–Fe(3)–C(32)	90.89(13)
C(1a7)–N(14)–Fe(1)	127.1(2)	N(33)–Fe(3)–C(32)	92.13(13)
C(1a8)–N(14)–Fe(1)	126.5(2)	C(31)–Fe(3)–C(32)	172.54(14)
C(12)–N(16)–K(1)	172.2(3)	N(32)–Fe(3)–C(32)	90.17(13)
N(11)–C(1a1)–C(1m4)	125.2(3)	N(31)–Fe(3)–C(32)	86.50(13)
N(11)–C(1a1)–C(1b1)	109.7(3)	O(23)–K(3)–O(24)	66.6(5)
C(1m4)–C(1a1)–C(1b1)	124.8(3)	O(23)–K(3)–O(15)	134.0(4)
N(11)–C(1a2)–C(1m1)	125.8(3)	O(24)–K(3)–O(15)	138.0(4)
N(11)–C(1a2)–C(1b2)	109.6(3)	O(23)–K(3)–O(22)	63.5(5)
C(1m1)–C(1a2)–C(1b2)	124.5(3)	O(24)–K(3)–O(22)	110.0(5)
N(12)–C(1a3)–C(1m1)	125.6(3)	O(15)–K(3)–O(22)	70.7(3)
N(12)–C(1a3)–C(1b3)	110.0(3)	O(23)–K(3)–O(13)	96.7(4)
C(1m1)–C(1a3)–C(1b3)	124.0(3)	O(24)–K(3)–O(13)	30.4(3)
N(12)–C(1a4)–C(1m2)	125.3(3)	O(15)–K(3)–O(13)	117.33(13)
N(12)–C(1a4)–C(1b4)	110.2(3)	O(22)–K(3)–O(13)	131.5(4)
C(1m2)–C(1a4)–C(1b4)	124.4(3)	O(23)–K(3)–N(36)	105.0(4)
N(13)–C(1a5)–C(1m2)	126.1(3)	O(24)–K(3)–N(36)	97.3(4)
N(13)–C(1a5)–C(1b5)	109.6(3)	O(15)–K(3)–N(36)	107.34(13)
C(1m2)–C(1a5)–C(1b5)	123.5(3)	O(22)–K(3)–N(36)	140.4(4)
N(13)–C(1a6)–C(1m3)	126.4(3)	O(13)–K(3)–N(36)	85.71(10)
N(13)–C(1a6)–C(1b6)	109.6(3)	O(23)–K(3)–O(18)	41.5(4)
C(1m3)–C(1a6)–C(1b6)	123.9(3)	O(24)–K(3)–O(18)	30.0(3)
N(14)–C(1a7)–C(1m3)	125.6(3)	O(15)–K(3)–O(18)	135.70(14)

Table S23. Continued

angle	degree	angle	degree
N(14)–C(1a7)–C(1b7)	110.2(3)	O(22)–K(3)–O(18)	81.5(4)
C(1m3)–C(1a7)–C(1b7)	124.1(3)	O(13)–K(3)–O(18)	59.42(10)
N(14)–C(1a8)–C(1m4)	125.8(3)	N(36)–K(3)–O(18)	115.92(10)
N(14)–C(1a8)–C(1b8)	109.9(3)	O(23)–K(3)–O(14)	155.2(4)
C(1m4)–C(1a8)–C(1b8)	124.1(3)	O(24)–K(3)–O(14)	89.8(3)
C(1b2)–C(1b1)–C(1a1)	107.1(3)	O(15)–K(3)–O(14)	60.24(12)
C(1b2)–C(1b1)–H(1ba)	126.5	O(22)–K(3)–O(14)	122.5(3)
C(1a1)–C(1b1)–H(1ba)	126.5	O(13)–K(3)–O(14)	60.61(10)
C(1b1)–C(1b2)–C(1a2)	106.9(3)	N(36)–K(3)–O(14)	84.54(11)
C(1b1)–C(1b2)–H(1bF)	126.6	O(18)–K(3)–O(14)	113.68(11)
C(1a2)–C(1b2)–H(1bF)	126.6	O(23)–K(3)–O(19)	127.2(5)
C(1b4)–C(1b3)–C(1a3)	107.4(3)	O(24)–K(3)–O(19)	62.2(4)
C(1b4)–C(1b3)–H(1be)	126.3	O(15)–K(3)–O(19)	82.3(3)
C(1a3)–C(1b3)–H(1be)	126.3	O(22)–K(3)–O(19)	124.1(5)
C(1b3)–C(1b4)–C(1a4)	106.3(3)	O(13)–K(3)–O(19)	35.1(3)
C(1b3)–C(1b4)–H(1bd)	126.8	N(36)–K(3)–O(19)	93.7(3)
C(1a4)–C(1b4)–H(1bd)	126.8	O(18)–K(3)–O(19)	85.8(3)
C(1b6)–C(1b5)–C(1a5)	107.3(3)	O(14)–K(3)–O(19)	28.1(3)
C(1b6)–C(1b5)–H(1bg)	126.3	O(23)–K(3)–O(17)	22.5(4)
C(1a5)–C(1b5)–H(1bg)	126.3	O(24)–K(3)–O(17)	88.2(3)
C(1b5)–C(1b6)–C(1a6)	107.1(3)	O(15)–K(3)–O(17)	113.63(14)
C(1b5)–C(1b6)–H(1bH)	126.5	O(22)–K(3)–O(17)	46.0(3)
C(1a6)–C(1b6)–H(1bH)	126.5	O(13)–K(3)–O(17)	118.63(11)
C(1b8)–C(1b7)–C(1a7)	106.8(3)	N(36)–K(3)–O(17)	109.51(11)
C(1b8)–C(1b7)–H(1bC)	126.6	O(18)–K(3)–O(17)	60.63(11)
C(1a7)–C(1b7)–H(1bC)	126.6	O(14)–K(3)–O(17)	165.95(12)
C(1b7)–C(1b8)–C(1a8)	106.9(3)	O(19)–K(3)–O(17)	144.9(3)
C(1b7)–C(1b8)–H(1bb)	126.6	O(23)–K(3)–O(20)	174.0(7)
C(1a8)–C(1b8)–H(1bb)	126.6	O(24)–K(3)–O(20)	119.3(6)
C(1a3)–C(1m1)–C(1a2)	123.1(3)	O(15)–K(3)–O(20)	42.6(7)
C(1a3)–C(1m1)–C(13)	119.3(3)	O(22)–K(3)–O(20)	113.3(7)
C(1a2)–C(1m1)–C(13)	117.6(3)	O(13)–K(3)–O(20)	89.1(6)
C(1a5)–C(1m2)–C(1a4)	122.4(3)	N(36)–K(3)–O(20)	74.1(7)
C(1a5)–C(1m2)–C(112)	118.5(3)	O(18)–K(3)–O(20)	144.3(6)

Table S23. Continued

angle	degree	angle	degree
C(1a4)–C(1m2)–C(112)	118.8(3)	O(14)–K(3)–O(20)	30.7(6)
C(1a6)–C(1m3)–C(1a7)	121.6(3)	O(19)–K(3)–O(20)	58.7(6)
C(1a6)–C(1m3)–C(121)	118.1(3)	O(17)–K(3)–O(20)	152.0(6)
C(1a7)–C(1m3)–C(121)	120.3(3)	O(23)–K(3)–O(16a)	78.4(4)
C(1a8)–C(1m4)–C(1a1)	123.2(3)	O(24)–K(3)–O(16a)	132.5(4)
C(1a8)–C(1m4)–C(130)	118.3(3)	O(15)–K(3)–O(16a)	56.74(13)
C(1a1)–C(1m4)–C(130)	118.4(3)	O(22)–K(3)–O(16a)	22.6(4)
N(15)–C(11)–Fe(1)	176.4(3)	O(13)–K(3)–O(16a)	151.34(13)
N(16)–C(12)–Fe(1)	172.2(3)	N(36)–K(3)–O(16a)	122.91(12)
C(14)–C(13)–C(110)	120.4(3)	O(18)–K(3)–O(16a)	103.54(12)
C(14)–C(13)–C(1m1)	121.2(3)	O(14)–K(3)–O(16a)	116.06(11)
C(110)–C(13)–C(1m1)	118.5(3)	O(19)–K(3)–O(16a)	130.2(3)
C(13)–C(14)–C(16)	119.0(4)	O(17)–K(3)–O(16a)	56.95(12)
C(13)–C(14)–C(15)	121.8(3)	O(20)–K(3)–O(16a)	97.1(6)
C(16)–C(14)–C(15)	119.1(4)	C(3a1)–N(31)–C(3a2)	106.9(3)
C(14)–C(15)–H(15i)	109.5	C(3a1)–N(31)–Fe(3)	127.3(2)
C(14)–C(15)–H(15j)	109.5	C(3a2)–N(31)–Fe(3)	125.8(2)
H(15i)–C(15)–H(15j)	109.5	C(3a3)–N(32)–C(3a4)	106.7(3)
C(14)–C(15)–H(15K)	109.5	C(3a3)–N(32)–Fe(3)	126.1(2)
H(15i)–C(15)–H(15K)	109.5	C(3a4)–N(32)–Fe(3)	127.0(2)
H(15j)–C(15)–H(15K)	109.5	C(3a5)–N(33)–C(3a6)	106.4(3)
C(17)–C(16)–C(14)	121.7(4)	C(3a5)–N(33)–Fe(3)	127.8(2)
C(17)–C(16)–H(16a)	119.1	C(3a6)–N(33)–Fe(3)	125.8(2)
C(14)–C(16)–H(16a)	119.1	C(3a7)–N(34)–C(3a8)	106.4(3)
C(16)–C(17)–C(19)	118.4(3)	C(3a7)–N(34)–Fe(3)	126.6(2)
C(16)–C(17)–C(18)	120.7(4)	C(3a8)–N(34)–Fe(3)	126.9(2)
C(19)–C(17)–C(18)	120.9(4)	C(32)–N(36)–K(3)	164.0(3)
C(17)–C(18)–H(18a)	109.5	N(31)–C(3a1)–C(3m4)	125.6(3)
C(17)–C(18)–H(18b)	109.5	N(31)–C(3a1)–C(3b1)	109.6(3)
H(18a)–C(18)–H(18b)	109.5	C(3m4)–C(3a1)–C(3b1)	124.6(3)
C(17)–C(18)–H(18C)	109.5	N(31)–C(3a2)–C(3m1)	125.3(3)
H(18a)–C(18)–H(18C)	109.5	N(31)–C(3a2)–C(3b2)	109.3(3)
H(18b)–C(18)–H(18C)	109.5	C(3m1)–C(3a2)–C(3b2)	125.1(3)
C(17)–C(19)–C(110)	122.1(4)	N(32)–C(3a3)–C(3m1)	126.0(3)

Table S23. Continued

angle	degree	angle	degree
C(17)–C(19)–H(19a)	119.0	N(32)–C(3a3)–C(3b3)	109.5(3)
C(110)–C(19)–H(19a)	119.0	C(3m1)–C(3a3)–C(3b3)	124.3(3)
C(19)–C(110)–C(13)	118.4(4)	N(32)–C(3a4)–C(3m2)	125.5(3)
C(19)–C(110)–C(111)	120.9(3)	N(32)–C(3a4)–C(3b4)	109.7(3)
C(13)–C(110)–C(111)	120.7(3)	C(3m2)–C(3a4)–C(3b4)	124.6(3)
C(110)–C(111)–H(11C)	109.5	N(33)–C(3a5)–C(3m2)	125.1(3)
C(110)–C(111)–H(11d)	109.5	N(33)–C(3a5)–C(3b5)	109.7(3)
H(11C)–C(111)–H(11d)	109.5	C(3m2)–C(3a5)–C(3b5)	124.7(3)
C(110)–C(111)–H(11e)	109.5	N(33)–C(3a6)–C(3m3)	125.6(3)
H(11C)–C(111)–H(11e)	109.5	N(33)–C(3a6)–C(3b6)	109.4(3)
H(11d)–C(111)–H(11e)	109.5	C(3m3)–C(3a6)–C(3b6)	124.3(3)
C(113)–C(112)–C(119)	120.0(3)	N(34)–C(3a7)–C(3m3)	125.8(3)
C(113)–C(112)–C(1m2)	119.5(3)	N(34)–C(3a7)–C(3b7)	109.9(3)
C(119)–C(112)–C(1m2)	120.4(3)	C(3m3)–C(3a7)–C(3b7)	124.2(3)
C(112)–C(113)–C(115)	118.9(3)	N(34)–C(3a8)–C(3m4)	125.9(3)
C(112)–C(113)–C(114)	121.3(3)	N(34)–C(3a8)–C(3b8)	109.5(3)
C(115)–C(113)–C(114)	119.8(3)	C(3m4)–C(3a8)–C(3b8)	123.9(3)
C(113)–C(114)–H(11F)	109.5	C(3b2)–C(3b1)–C(3a1)	107.1(3)
C(113)–C(114)–H(11g)	109.5	C(3b2)–C(3b1)–H(3bH)	126.4
H(11f)–C(114)–H(11g)	109.5	C(3a1)–C(3b1)–H(3bH)	126.4
C(113)–C(114)–H(11H)	109.5	C(3b1)–C(3b2)–C(3a2)	107.0(3)
H(11f)–C(114)–H(11H)	109.5	C(3b1)–C(3b2)–H(3bg)	126.5
H(11g)–C(114)–H(11H)	109.5	C(3a2)–C(3b2)–H(3bg)	126.5
C(116)–C(115)–C(113)	121.5(4)	C(3b4)–C(3b3)–C(3a3)	107.3(3)
C(116)–C(115)–H(11a)	119.3	C(3b4)–C(3b3)–H(3bC)	126.4
C(113)–C(115)–H(11a)	119.3	C(3a3)–C(3b3)–H(3bC)	126.4
C(118)–C(116)–C(115)	118.5(3)	C(3b3)–C(3b4)–C(3a4)	106.7(3)
C(118)–C(116)–C(117)	120.8(4)	C(3b3)–C(3b4)–H(3ba)	126.7
C(115)–C(116)–C(117)	120.7(4)	C(3a4)–C(3b4)–H(3ba)	126.7
C(116)–C(117)–H(11i)	109.5	C(3b6)–C(3b5)–C(3a5)	107.5(3)
C(116)–C(117)–H(11j)	109.5	C(3b6)–C(3b5)–H(3bd)	126.2
H(11i)–C(117)–H(11j)	109.5	C(3a5)–C(3b5)–H(3bd)	126.2
C(116)–C(117)–H(11K)	109.5	C(3b5)–C(3b6)–C(3a6)	106.9(3)
H(11i)–C(117)–H(11K)	109.5	C(3b5)–C(3b6)–H(3bF)	126.6

Table S23. Continued

angle	degree	angle	degree
H(11j)–C(117)–H(11K)	109.5	C(3a6)–C(3b6)–H(3bF)	126.6
C(116)–C(118)–C(119)	121.8(3)	C(3b8)–C(3b7)–C(3a7)	107.1(3)
C(116)–C(118)–H(11b)	119.1	C(3b8)–C(3b7)–H(3bb)	126.4
C(119)–C(118)–H(11b)	119.1	C(3a7)–C(3b7)–H(3bb)	126.4
C(118)–C(119)–C(112)	119.2(3)	C(3b7)–C(3b8)–C(3a8)	106.9(3)
C(118)–C(119)–C(120)	120.3(3)	C(3b7)–C(3b8)–H(3be)	126.6
C(112)–C(119)–C(120)	120.4(3)	C(3a8)–C(3b8)–H(3be)	126.6
C(119)–C(120)–H(12C)	109.5	C(3a3)–C(3m1)–C(3a2)	123.7(3)
C(119)–C(120)–H(12d)	109.5	C(3a3)–C(3m1)–C(33)	118.5(3)
H(12C)–C(120)–H(12d)	109.5	C(3a2)–C(3m1)–C(33)	117.6(3)
C(119)–C(120)–H(12e)	109.5	C(3a5)–C(3m2)–C(3a4)	122.0(3)
H(12C)–C(120)–H(12e)	109.5	C(3a5)–C(3m2)–C(312)	120.5(3)
H(12d)–C(120)–H(12e)	109.5	C(3a4)–C(3m2)–C(312)	117.4(3)
C(128)–C(121)–C(122)	119.3(3)	C(3a6)–C(3m3)–C(3a7)	121.8(3)
C(128)–C(121)–C(1m3)	117.8(3)	C(3a6)–C(3m3)–C(321)	120.8(3)
C(122)–C(121)–C(1m3)	122.9(3)	C(3a7)–C(3m3)–C(321)	117.4(3)
C(124)–C(122)–C(121)	119.0(3)	C(3a8)–C(3m4)–C(3a1)	122.1(3)
C(124)–C(122)–C(123)	119.8(3)	C(3a8)–C(3m4)–C(330)	118.9(3)
C(121)–C(122)–C(123)	121.1(3)	C(3a1)–C(3m4)–C(330)	118.8(3)
C(122)–C(123)–H(12i)	109.5	N(35)–C(31)–Fe(3)	175.6(3)
C(122)–C(123)–H(12j)	109.5	N(36)–C(32)–Fe(3)	174.4(3)
H(12i)–C(123)–H(12j)	109.5	C(34)–C(33)–C(310)	120.5(3)
C(122)–C(123)–H(12K)	109.5	C(34)–C(33)–C(3m1)	119.7(3)
H(12i)–C(123)–H(12K)	109.5	C(310)–C(33)–C(3m1)	119.8(3)
H(12j)–C(123)–H(12K)	109.5	C(33)–C(34)–C(36)	119.0(4)
C(125)–C(124)–C(122)	122.3(3)	C(33)–C(34)–C(35)	121.3(3)
C(125)–C(124)–H(12b)	118.8	C(36)–C(34)–C(35)	119.7(4)
C(122)–C(124)–H(12b)	118.8	C(34)–C(35)–H(35a)	109.5
C(124)–C(125)–C(127)	118.0(3)	C(34)–C(35)–H(35b)	109.5
C(124)–C(125)–C(126)	121.6(4)	H(35a)–C(35)–H(35b)	109.5
C(127)–C(125)–C(126)	120.4(4)	C(34)–C(35)–H(35C)	109.5
C(125)–C(126)–H(12L)	109.5	H(35a)–C(35)–H(35C)	109.5
C(125)–C(126)–H(12m)	109.5	H(35b)–C(35)–H(35C)	109.5
H(12L)–C(126)–H(12m)	109.5	C(34)–C(36)–C(37)	121.0(4)

Table S23. Continued

angle	degree	angle	degree
C(125)–C(126)–H(12N)	109.5	C(34)–C(36)–H(36a)	119.5
H(12L)–C(126)–H(12N)	109.5	C(37)–C(36)–H(36a)	119.5
H(12m)–C(126)–H(12N)	109.5	C(39)–C(37)–C(36)	118.7(4)
C(125)–C(127)–C(128)	122.1(4)	C(39)–C(37)–C(38)	120.7(5)
C(125)–C(127)–H(12a)	118.9	C(36)–C(37)–C(38)	120.6(5)
C(128)–C(127)–H(12a)	118.9	C(37)–C(38)–H(38a)	109.5
C(127)–C(128)–C(121)	119.3(3)	C(37)–C(38)–H(38b)	109.5
C(127)–C(128)–C(129)	119.9(3)	H(38a)–C(38)–H(38b)	109.5
C(121)–C(128)–C(129)	120.8(3)	C(37)–C(38)–H(38C)	109.5
C(128)–C(129)–H(12F)	109.5	H(38a)–C(38)–H(38C)	109.5
C(128)–C(129)–H(12g)	109.5	H(38b)–C(38)–H(38C)	109.5
H(12f)–C(129)–H(12g)	109.5	C(37)–C(39)–C(310)	122.5(4)
C(128)–C(129)–H(12H)	109.5	C(37)–C(39)–H(39a)	118.8
H(12f)–C(129)–H(12H)	109.5	C(310)–C(39)–H(39a)	118.8
H(12g)–C(129)–H(12H)	109.5	C(39)–C(310)–C(33)	118.2(4)
C(131)–C(130)–C(137)	120.3(3)	C(39)–C(310)–C(311)	121.0(4)
C(131)–C(130)–C(1m4)	119.2(3)	C(33)–C(310)–C(311)	120.8(4)
C(137)–C(130)–C(1m4)	120.5(3)	C(310)–C(311)–H(31i)	109.5
C(130)–C(131)–C(133)	119.4(3)	C(310)–C(311)–H(31j)	109.5
C(130)–C(131)–C(132)	120.9(3)	H(31i)–C(311)–H(31j)	109.5
C(133)–C(131)–C(132)	119.7(3)	C(310)–C(311)–H(31K)	109.5
C(131)–C(132)–H(13F)	109.5	H(31i)–C(311)–H(31K)	109.5
C(131)–C(132)–H(13g)	109.5	H(31j)–C(311)–H(31K)	109.5
H(13f)–C(132)–H(13g)	109.5	C(319)–C(312)–C(313)	119.4(3)
C(131)–C(132)–H(13H)	109.5	C(319)–C(312)–C(3m2)	118.6(3)
H(13f)–C(132)–H(13H)	109.5	C(313)–C(312)–C(3m2)	121.9(3)
H(13g)–C(132)–H(13H)	109.5	C(315)–C(313)–C(312)	119.5(3)
C(134)–C(133)–C(131)	121.1(3)	C(315)–C(313)–C(314)	118.1(3)
C(134)–C(133)–H(13a)	119.5	C(312)–C(313)–C(314)	122.4(3)
C(131)–C(133)–H(13a)	119.5	C(313)–C(314)–H(31F)	109.5
C(133)–C(134)–C(136)	118.6(3)	C(313)–C(314)–H(31g)	109.5
C(133)–C(134)–C(135)	120.7(4)	H(31f)–C(314)–H(31g)	109.5
C(136)–C(134)–C(135)	120.7(3)	C(313)–C(314)–H(31H)	109.5
C(134)–C(135)–H(13C)	109.5	H(31f)–C(314)–H(31H)	109.5

Table S23. Continued

angle	degree	angle	degree
C(134)–C(135)–H(13d)	109.5	H(31g)–C(314)–H(31H)	109.5
H(13C)–C(135)–H(13d)	109.5	C(316)–C(315)–C(313)	122.0(3)
C(134)–C(135)–H(13e)	109.5	C(316)–C(315)–H(31a)	119.0
H(13C)–C(135)–H(13e)	109.5	C(313)–C(315)–H(31a)	119.0
H(13d)–C(135)–H(13e)	109.5	C(315)–C(316)–C(318)	117.9(3)
C(137)–C(136)–C(134)	122.1(3)	C(315)–C(316)–C(317)	120.9(3)
C(137)–C(136)–H(13b)	119.0	C(318)–C(316)–C(317)	121.2(4)
C(134)–C(136)–H(13b)	119.0	C(316)–C(317)–H(31C)	109.5
C(136)–C(137)–C(130)	118.5(3)	C(316)–C(317)–H(31d)	109.5
C(136)–C(137)–C(138)	119.9(3)	H(31C)–C(317)–H(31d)	109.5
C(130)–C(137)–C(138)	121.6(3)	C(316)–C(317)–H(31e)	109.5
C(137)–C(138)–H(13i)	109.5	H(31C)–C(317)–H(31e)	109.5
C(137)–C(138)–H(13j)	109.5	H(31d)–C(317)–H(31e)	109.5
H(13i)–C(138)–H(13j)	109.5	C(319)–C(318)–C(316)	122.0(4)
C(137)–C(138)–H(13K)	109.5	C(319)–C(318)–H(31b)	119.0
H(13i)–C(138)–H(13K)	109.5	C(316)–C(318)–H(31b)	119.0
H(13j)–C(138)–H(13K)	109.5	C(318)–C(319)–C(312)	119.2(3)
O(5)–C(139)–C(140)	114.4(3)	C(318)–C(319)–C(320)	119.8(4)
O(5)–C(139)–H(13L)	108.7	C(312)–C(319)–C(320)	121.0(3)
C(140)–C(139)–H(13L)	108.7	C(319)–C(320)–H(32L)	109.5
O(5)–C(139)–H(13m)	108.7	C(319)–C(320)–H(32m)	109.5
C(140)–C(139)–H(13m)	108.7	H(32L)–C(320)–H(32m)	109.5
H(13L)–C(139)–H(13m)	107.6	C(319)–C(320)–H(32N)	109.5
O(6)–C(140)–C(139)	108.0(3)	H(32L)–C(320)–H(32N)	109.5
O(6)–C(140)–H(14a)	110.1	H(32m)–C(320)–H(32N)	109.5
C(139)–C(140)–H(14a)	110.1	C(322)–C(321)–C(328)	120.4(3)
O(6)–C(140)–H(14b)	110.1	C(322)–C(321)–C(3m3)	117.4(3)
C(139)–C(140)–H(14b)	110.1	C(328)–C(321)–C(3m3)	122.1(3)
H(14a)–C(140)–H(14b)	108.4	C(324)–C(322)–C(321)	119.2(3)
O(6)–C(141)–C(142)	108.3(3)	C(324)–C(322)–C(323)	119.2(4)
O(6)–C(141)–H(43C)	110.0	C(321)–C(322)–C(323)	121.6(3)
C(142)–C(141)–H(43C)	110.0	C(322)–C(323)–H(32e)	109.5
O(6)–C(141)–H(43d)	110.0	C(322)–C(323)–H(32F)	109.5
C(142)–C(141)–H(43d)	110.0	H(32e)–C(323)–H(32f)	109.5

Table S23. Continued

angle	degree	angle	degree
H(43C)–C(141)–H(43d)	108.4	C(322)–C(323)–H(32g)	109.5
O(1)–C(142)–C(141)	108.2(3)	H(32e)–C(323)–H(32g)	109.5
O(1)–C(142)–H(70a)	110.1	H(32f)–C(323)–H(32g)	109.5
C(141)–C(142)–H(70a)	110.1	C(325)–C(324)–C(322)	121.3(4)
O(1)–C(142)–H(70b)	110.1	C(325)–C(324)–H(32H)	119.4
C(141)–C(142)–H(70b)	110.1	C(322)–C(324)–H(32H)	119.4
H(70a)–C(142)–H(70b)	108.4	C(327)–C(325)–C(324)	118.4(3)
O(1)–C(143)–C(144)	108.8(3)	C(327)–C(325)–C(326)	121.0(4)
O(1)–C(143)–H(43a)	109.9	C(324)–C(325)–C(326)	120.6(4)
C(144)–C(143)–H(43a)	109.9	C(325)–C(326)–H(32i)	109.5
O(1)–C(143)–H(43b)	109.9	C(325)–C(326)–H(32j)	109.5
C(144)–C(143)–H(43b)	109.9	H(32i)–C(326)–H(32j)	109.5
H(43a)–C(143)–H(43b)	108.3	C(325)–C(326)–H(32K)	109.5
O(2)–C(144)–C(143)	107.9(3)	H(32i)–C(326)–H(32K)	109.5
O(2)–C(144)–H(93a)	110.1	H(32j)–C(326)–H(32K)	109.5
C(143)–C(144)–H(93a)	110.1	C(325)–C(327)–C(328)	122.3(4)
O(2)–C(144)–H(93b)	110.1	C(325)–C(327)–H(32a)	118.9
C(143)–C(144)–H(93b)	110.1	C(328)–C(327)–H(32a)	118.9
H(93a)–C(144)–H(93b)	108.4	C(327)–C(328)–C(321)	118.4(4)
O(2)–C(145)–C(146)	107.6(3)	C(327)–C(328)–C(329)	119.5(3)
O(2)–C(145)–H(15e)	110.2	C(321)–C(328)–C(329)	122.1(3)
C(146)–C(145)–H(15e)	110.2	C(328)–C(329)–H(32b)	109.5
O(2)–C(145)–H(15F)	110.2	C(328)–C(329)–H(32C)	109.5
C(146)–C(145)–H(15F)	110.2	H(32b)–C(329)–H(32C)	109.5
H(15e)–C(145)–H(15f)	108.5	C(328)–C(329)–H(32d)	109.5
O(3)–C(146)–C(145)	109.4(3)	H(32b)–C(329)–H(32d)	109.5
O(3)–C(146)–H(15C)	109.8	H(32C)–C(329)–H(32d)	109.5
C(145)–C(146)–H(15C)	109.8	C(337)–C(330)–C(331)	119.6(3)
O(3)–C(146)–H(15d)	109.8	C(337)–C(330)–C(3m4)	119.0(3)
C(145)–C(146)–H(15d)	109.8	C(331)–C(330)–C(3m4)	121.4(3)
H(15C)–C(146)–H(15d)	108.2	C(330)–C(331)–C(333)	118.9(4)
O(3)–C(147)–C(148)	109.5(3)	C(330)–C(331)–C(332)	121.3(4)
O(3)–C(147)–H(94a)	109.8	C(333)–C(331)–C(332)	119.8(4)
C(148)–C(147)–H(94a)	109.8	C(331)–C(332)–H(33i)	109.5

Table S23. Continued

angle	degree	angle	degree
O(3)–C(147)–H(94b)	109.8	C(331)–C(332)–H(33j)	109.5
C(148)–C(147)–H(94b)	109.8	H(33i)–C(332)–H(33j)	109.5
H(94a)–C(147)–H(94b)	108.2	C(331)–C(332)–H(33K)	109.5
O(4)–C(148)–C(147)	107.9(3)	H(33i)–C(332)–H(33K)	109.5
O(4)–C(148)–H(14m)	110.1	H(33j)–C(332)–H(33K)	109.5
C(147)–C(148)–H(14m)	110.1	C(334)–C(333)–C(331)	121.8(4)
O(4)–C(148)–H(14e)	110.1	C(334)–C(333)–H(33e)	119.1
C(147)–C(148)–H(14e)	110.1	C(331)–C(333)–H(33e)	119.1
H(14m)–C(148)–H(14e)	108.4	C(333)–C(334)–C(336)	118.8(3)
O(4)–C(149)–C(150)	107.5(3)	C(333)–C(334)–C(335)	120.5(4)
O(4)–C(149)–H(15g)	110.2	C(336)–C(334)–C(335)	120.7(4)
C(150)–C(149)–H(15g)	110.2	C(334)–C(335)–H(33F)	109.5
O(4)–C(149)–H(15H)	110.2	C(334)–C(335)–H(33g)	109.5
C(150)–C(149)–H(15H)	110.2	H(33f)–C(335)–H(33g)	109.5
H(15g)–C(149)–H(15H)	108.5	C(334)–C(335)–H(33H)	109.5
O(5)–C(150)–C(149)	107.3(3)	H(33f)–C(335)–H(33H)	109.5
O(5)–C(150)–H(14C)	110.2	H(33g)–C(335)–H(33H)	109.5
C(149)–C(150)–H(14C)	110.2	C(334)–C(336)–C(337)	121.4(4)
O(5)–C(150)–H(14d)	110.2	C(334)–C(336)–H(33a)	119.3
C(149)–C(150)–H(14d)	110.2	C(337)–C(336)–H(33a)	119.3
H(14C)–C(150)–H(14d)	108.5	C(336)–C(337)–C(330)	119.5(4)
C(143)–O(1)–C(142)	112.3(3)	C(336)–C(337)–C(338)	119.5(3)
C(143)–O(1)–K(1)	119.1(2)	C(330)–C(337)–C(338)	120.9(3)
C(142)–O(1)–K(1)	117.42(19)	C(337)–C(338)–H(33b)	109.5
C(145)–O(2)–C(144)	112.4(3)	C(337)–C(338)–H(33C)	109.5
C(145)–O(2)–K(1)	117.6(2)	H(33b)–C(338)–H(33C)	109.5
C(144)–O(2)–K(1)	115.5(2)	C(337)–C(338)–H(33d)	109.5
C(147)–O(3)–C(146)	110.7(3)	H(33b)–C(338)–H(33d)	109.5
C(147)–O(3)–K(1)	112.0(2)	H(33C)–C(338)–H(33d)	109.5
C(146)–O(3)–K(1)	114.5(2)	C(349)–O(13)–C(339)	113.1(5)
C(148)–O(4)–C(149)	114.1(3)	C(349)–O(13)–K(3)	118.7(4)
C(148)–O(4)–K(1)	126.6(2)	C(339)–O(13)–K(3)	118.2(3)
C(149)–O(4)–K(1)	117.8(2)	C(341)–O(14)–C(340)	112.2(6)
C(150)–O(5)–C(139)	114.6(3)	C(341)–O(14)–K(3)	98.2(4)

Table S23. Continued

angle	degree	angle	degree
C(150)–O(5)–K(1)	86.64(19)	C(340)–O(14)–K(3)	104.1(3)
C(139)–O(5)–K(1)	110.31(19)	C(343)–O(15)–C(342)	113.7(5)
C(140)–O(6)–C(141)	112.5(3)	C(343)–O(15)–K(3)	129.4(4)
C(140)–O(6)–K(1)	112.5(2)	C(342)–O(15)–K(3)	116.9(3)
C(141)–O(6)–K(1)	104.3(2)	C(345)–O(17)–C(346)	113.5(5)
N(23)–Fe(2)–N(24)	89.70(11)	C(345)–O(17)–K(3)	117.5(3)
N(23)–Fe(2)–N(22)	89.58(11)	C(346)–O(17)–K(3)	109.4(3)
N(24)–Fe(2)–N(22)	178.23(13)	C(347)–O(18)–C(348)	113.4(4)
N(23)–Fe(2)–C(21)	93.11(14)	C(347)–O(18)–K(3)	116.6(3)
N(24)–Fe(2)–C(21)	93.37(14)	C(348)–O(18)–K(3)	117.4(3)
N(22)–Fe(2)–C(21)	85.06(13)	O(13)–C(339)–C(340)	107.9(5)
N(23)–Fe(2)–C(22)	93.58(14)	O(13)–C(339)–H(33L)	110.1
N(24)–Fe(2)–C(22)	91.72(13)	C(340)–C(339)–H(33L)	110.1
N(22)–Fe(2)–C(22)	89.93(13)	O(13)–C(339)–H(33m)	110.1
C(21)–Fe(2)–C(22)	171.61(14)	C(340)–C(339)–H(33m)	110.1
N(23)–Fe(2)–N(21)	178.38(13)	H(33L)–C(339)–H(33m)	108.4
N(24)–Fe(2)–N(21)	89.93(11)	O(14)–C(340)–C(339)	108.2(4)
N(22)–Fe(2)–N(21)	90.83(11)	O(14)–C(340)–H(34a)	110.1
C(21)–Fe(2)–N(21)	88.49(13)	C(339)–C(340)–H(34a)	110.1
C(22)–Fe(2)–N(21)	84.85(13)	O(14)–C(340)–H(34b)	110.1
O(8)–K(2)–O(10)	119.75(9)	C(339)–C(340)–H(34b)	110.1
O(8)–K(2)–O(12b)	117.8(5)	H(34a)–C(340)–H(34b)	108.4
O(10)–K(2)–O(12b)	111.7(5)	O(14)–C(341)–C(342)	106.8(9)
O(8)–K(2)–O(7)	60.60(8)	O(14)–C(341)–H(34C)	110.4
O(10)–K(2)–O(7)	149.15(11)	C(342)–C(341)–H(34C)	110.4
O(12b)–K(2)–O(7)	57.3(5)	O(14)–C(341)–H(34d)	110.4
O(8)–K(2)–N(26)	82.48(9)	C(342)–C(341)–H(34d)	110.4
O(10)–K(2)–N(26)	93.50(10)	H(34C)–C(341)–H(34d)	108.6
O(12b)–K(2)–N(26)	127.5(4)	O(15)–C(342)–C(341)	109.5(5)
O(7)–K(2)–N(26)	116.22(9)	O(15)–C(342)–H(34e)	109.8
O(8)–K(2)–O(9)	60.89(8)	C(341)–C(342)–H(34e)	109.8
O(10)–K(2)–O(9)	59.70(9)	O(15)–C(342)–H(34F)	109.8
O(12b)–K(2)–O(9)	155.4(4)	C(341)–C(342)–H(34F)	109.8
O(7)–K(2)–O(9)	116.76(9)	H(34e)–C(342)–H(34f)	108.2

Table S23. Continued

angle	degree	angle	degree
N(26)–K(2)–O(9)	77.02(9)	O(15)–C(343)–C(344)	111.0(6)
O(8)–K(2)–O(11b)	127.2(2)	O(15)–C(343)–H(34g)	109.4
O(10)–K(2)–O(11b)	59.77(19)	C(344)–C(343)–H(34g)	109.4
O(12b)–K(2)–O(11b)	57.4(5)	O(15)–C(343)–H(34H)	109.4
O(7)–K(2)–O(11b)	94.39(19)	C(344)–C(343)–H(34H)	109.4
N(26)–K(2)–O(11b)	146.4(2)	H(34g)–C(343)–H(34H)	108.0
O(9)–K(2)–O(11b)	102.32(19)	O(16b)–C(344)–O(16a)	58.6(16)
O(8)–K(2)–O(12a)	120.4(2)	O(16b)–C(344)–C(343)	121.3(16)
O(10)–K(2)–O(12a)	114.5(2)	O(16a)–C(344)–C(343)	111.2(6)
O(12b)–K(2)–O(12a)	10.2(5)	O(16a)–C(2a)–C(345)	106.7(7)
O(7)–K(2)–O(12a)	60.3(2)	O(16a)–C(2a)–H(2a1)	110.4
N(26)–K(2)–O(12a)	117.42(19)	C(345)–C(2a)–H(2a1)	110.4
O(9)–K(2)–O(12a)	165.42(19)	O(16a)–C(2a)–H(2a2)	110.4
O(11b)–K(2)–O(12a)	64.8(3)	C(345)–C(2a)–H(2a2)	110.4
O(8)–K(2)–O(11a)	150.72(12)	H(2a1)–C(2a)–H(2a2)	108.6
O(10)–K(2)–O(11a)	56.64(11)	C(344)–O(16a)–C(2a)	115.5(6)
O(12b)–K(2)–O(11a)	55.1(5)	C(344)–O(16a)–K(3)	110.8(4)
O(7)–K(2)–O(11a)	106.57(11)	C(2a)–O(16a)–K(3)	117.3(4)
N(26)–K(2)–O(11a)	125.43(12)	C(345)–C(2b)–O(16b)	146(3)
O(9)–K(2)–O(11a)	112.51(11)	C(345)–C(2b)–H(2b1)	100.3
O(11b)–K(2)–O(11a)	23.5(2)	O(16b)–C(2b)–H(2b1)	100.3
O(12a)–K(2)–O(11a)	58.5(2)	C(345)–C(2b)–H(2b2)	100.3
C(2a1)–N(21)–C(2a2)	106.9(3)	O(16b)–C(2b)–H(2b2)	100.3
C(2a1)–N(21)–Fe(2)	127.0(2)	H(2b1)–C(2b)–H(2b2)	104.3
C(2a2)–N(21)–Fe(2)	125.6(2)	C(344)–O(16b)–C(2b)	106(3)
C(2a3)–N(22)–C(2a4)	106.5(3)	C(344)–O(16b)–K(3)	114.3(18)
C(2a3)–N(22)–Fe(2)	126.4(2)	C(2b)–O(16b)–K(3)	87.5(19)
C(2a4)–N(22)–Fe(2)	126.7(2)	O(17)–C(345)–C(2a)	111.2(6)
C(2a6)–N(23)–C(2a5)	106.6(3)	O(17)–C(345)–C(2b)	98(2)
C(2a6)–N(23)–Fe(2)	126.5(2)	O(17)–C(346)–C(347)	108.8(5)
C(2a5)–N(23)–Fe(2)	126.9(2)	O(17)–C(346)–H(34m)	109.9
C(2a7)–N(24)–C(2a8)	106.3(3)	C(347)–C(346)–H(34m)	109.9
C(2a7)–N(24)–Fe(2)	126.8(2)	O(17)–C(346)–H(34N)	109.9
C(2a8)–N(24)–Fe(2)	126.9(2)	C(347)–C(346)–H(34N)	109.9

Table S23. Continued

angle	degree	angle	degree
C(22)–N(26)–K(2)	169.1(3)	H(34m)–C(346)–H(34N)	108.3
N(21)–C(2a1)–C(2m4)	125.6(3)	O(18)–C(347)–C(346)	108.5(4)
N(21)–C(2a1)–C(2b1)	109.7(3)	O(18)–C(347)–H(34O)	110.0
C(2m4)–C(2a1)–C(2b1)	124.6(3)	C(346)–C(347)–H(34O)	110.0
N(21)–C(2a2)–C(2m1)	125.3(3)	O(18)–C(347)–H(34P)	110.0
N(21)–C(2a2)–C(2b2)	109.3(3)	C(346)–C(347)–H(34P)	110.0
C(2m1)–C(2a2)–C(2b2)	125.0(3)	H(34O)–C(347)–H(34P)	108.4
N(22)–C(2a3)–C(2m1)	125.7(3)	O(18)–C(348)–C(349)	108.4(4)
N(22)–C(2a3)–C(2b3)	109.7(3)	O(18)–C(348)–H(34Q)	110.0
C(2m1)–C(2a3)–C(2b3)	124.4(3)	C(349)–C(348)–H(34Q)	110.0
N(22)–C(2a4)–C(2m2)	125.2(3)	O(18)–C(348)–H(34R)	110.0
N(22)–C(2a4)–C(2b4)	109.8(3)	C(349)–C(348)–H(34R)	110.0
C(2m2)–C(2a4)–C(2b4)	124.7(3)	H(34Q)–C(348)–H(34R)	108.4
N(23)–C(2a5)–C(2m2)	125.9(3)	O(13)–C(349)–C(348)	109.0(6)
N(23)–C(2a5)–C(2b5)	109.5(3)	O(13)–C(349)–H(34S)	109.9
C(2m2)–C(2a5)–C(2b5)	124.3(3)	C(348)–C(349)–H(34S)	109.9
N(23)–C(2a6)–C(2m3)	125.5(3)	O(13)–C(349)–H(34T)	109.9
N(23)–C(2a6)–C(2b6)	109.3(3)	C(348)–C(349)–H(34T)	109.9
C(2m3)–C(2a6)–C(2b6)	124.2(3)	H(34S)–C(349)–H(34T)	108.3
N(24)–C(2a7)–C(2m3)	126.0(3)	C(361)–O(19)–C(350)	109.1(19)
N(24)–C(2a7)–C(2b7)	109.9(3)	C(361)–O(19)–K(3)	109.7(17)
C(2m3)–C(2a7)–C(2b7)	124.0(3)	C(350)–O(19)–K(3)	115.7(14)
N(24)–C(2a8)–C(2m4)	124.8(3)	C(352)–O(20)–C(351)	119(3)
N(24)–C(2a8)–C(2b8)	109.9(3)	C(352)–O(20)–K(3)	114.5(17)
C(2m4)–C(2a8)–C(2b8)	124.3(3)	C(351)–O(20)–K(3)	111.7(18)
C(2b2)–C(2b1)–C(2a1)	107.0(3)	C(353)–O(21)–C(354)	118(3)
C(2b2)–C(2b1)–H(2bd)	126.5	C(353)–O(21)–K(3)	118(2)
C(2a1)–C(2b1)–H(2bd)	126.5	C(354)–O(21)–K(3)	106.8(16)
C(2b1)–C(2b2)–C(2a2)	107.0(3)	C(356)–O(22)–C(355)	114.0(19)
C(2b1)–C(2b2)–H(2bH)	126.5	C(356)–O(22)–K(3)	111.0(15)
C(2a2)–C(2b2)–H(2bH)	126.5	C(355)–O(22)–K(3)	121.2(15)
C(2b4)–C(2b3)–C(2a3)	107.2(3)	C(358)–O(23)–C(357)	112(2)
C(2b4)–C(2b3)–H(2bC)	126.4	C(358)–O(23)–K(3)	115.1(13)
C(2a3)–C(2b3)–H(2bC)	126.4	C(357)–O(23)–K(3)	122.7(16)

Table S23. Continued

angle	degree	angle	degree
C(2b3)–C(2b4)–C(2a4)	106.7(3)	C(359)–O(24)–C(360)	114(2)
C(2b3)–C(2b4)–H(2ba)	126.6	C(359)–O(24)–K(3)	114.2(15)
C(2a4)–C(2b4)–H(2ba)	126.6	C(360)–O(24)–K(3)	120.5(16)
C(2b6)–C(2b5)–C(2a5)	107.3(3)	O(19)–C(350)–C(351)	105(2)
C(2b6)–C(2b5)–H(2bb)	126.4	O(19)–C(350)–H(35d)	110.7
C(2a5)–C(2b5)–H(2bb)	126.4	C(351)–C(350)–H(35d)	110.7
C(2b5)–C(2b6)–C(2a6)	107.2(3)	O(19)–C(350)–H(35e)	110.7
C(2b5)–C(2b6)–H(2be)	126.4	C(351)–C(350)–H(35e)	110.7
C(2a6)–C(2b6)–H(2be)	126.4	H(35d)–C(350)–H(35e)	108.8
C(2b8)–C(2b7)–C(2a7)	106.6(3)	O(20)–C(351)–C(350)	109(2)
C(2b8)–C(2b7)–H(2bF)	126.7	O(20)–C(351)–H(35F)	109.8
C(2a7)–C(2b7)–H(2bF)	126.7	C(350)–C(351)–H(35F)	109.8
C(2b7)–C(2b8)–C(2a8)	107.2(3)	O(20)–C(351)–H(35g)	109.8
C(2b7)–C(2b8)–H(2bg)	126.4	C(350)–C(351)–H(35g)	109.8
C(2a8)–C(2b8)–H(2bg)	126.4	H(35f)–C(351)–H(35g)	108.2
C(2a2)–C(2m1)–C(2a3)	123.3(3)	O(20)–C(352)–C(353)	109(3)
C(2a2)–C(2m1)–C(23)	118.2(3)	O(20)–C(352)–H(35H)	109.9
C(2a3)–C(2m1)–C(23)	118.4(3)	C(353)–C(352)–H(35H)	109.9
C(2a5)–C(2m2)–C(2a4)	121.6(3)	O(20)–C(352)–H(35i)	109.9
C(2a5)–C(2m2)–C(212)	117.9(3)	C(353)–C(352)–H(35i)	109.9
C(2a4)–C(2m2)–C(212)	120.5(3)	H(35H)–C(352)–H(35i)	108.3
C(2a6)–C(2m3)–C(2a7)	121.3(3)	O(21)–C(353)–C(352)	111(3)
C(2a6)–C(2m3)–C(221)	121.6(3)	O(21)–C(353)–H(35j)	109.4
C(2a7)–C(2m3)–C(221)	117.1(3)	C(352)–C(353)–H(35j)	109.4
C(2a8)–C(2m4)–C(2a1)	122.8(3)	O(21)–C(353)–H(35K)	109.4
C(2a8)–C(2m4)–C(230)	118.5(3)	C(352)–C(353)–H(35K)	109.4
C(2a1)–C(2m4)–C(230)	118.6(3)	H(35j)–C(353)–H(35K)	108.0
N(25)–C(21)–Fe(2)	174.0(3)	O(21)–C(354)–C(355)	110(2)
N(26)–C(22)–Fe(2)	171.9(3)	O(21)–C(354)–H(35L)	109.7
C(24)–C(23)–C(210)	120.2(3)	C(355)–C(354)–H(35L)	109.7
C(24)–C(23)–C(2m1)	119.6(3)	O(21)–C(354)–H(35m)	109.7
C(210)–C(23)–C(2m1)	120.3(3)	C(355)–C(354)–H(35m)	109.7
C(26)–C(24)–C(23)	119.5(4)	H(35L)–C(354)–H(35m)	108.2
C(26)–C(24)–C(25)	119.6(4)	O(22)–C(355)–C(354)	110(2)

Table S23. Continued

angle	degree	angle	degree
C(23)–C(24)–C(25)	121.0(3)	O(22)–C(355)–H(35N)	109.8
C(24)–C(25)–H(25a)	109.5	C(354)–C(355)–H(35N)	109.8
C(24)–C(25)–H(25b)	109.5	O(22)–C(355)–H(35O)	109.8
H(25a)–C(25)–H(25b)	109.5	C(354)–C(355)–H(35O)	109.8
C(24)–C(25)–H(25C)	109.5	H(35N)–C(355)–H(35O)	108.2
H(25a)–C(25)–H(25C)	109.5	O(22)–C(356)–C(357)	112(2)
H(25b)–C(25)–H(25C)	109.5	O(22)–C(356)–H(35P)	109.2
C(27)–C(26)–C(24)	121.7(4)	C(357)–C(356)–H(35P)	109.2
C(27)–C(26)–H(26a)	119.1	O(22)–C(356)–H(35Q)	109.2
C(24)–C(26)–H(26a)	119.1	C(357)–C(356)–H(35Q)	109.2
C(26)–C(27)–C(29)	118.3(4)	H(35P)–C(356)–H(35Q)	107.9
C(26)–C(27)–C(28)	120.7(5)	O(23)–C(357)–C(356)	109(2)
C(29)–C(27)–C(28)	121.0(5)	O(23)–C(357)–H(35R)	109.9
C(27)–C(28)–H(28a)	109.5	C(356)–C(357)–H(35R)	109.9
C(27)–C(28)–H(28b)	109.5	O(23)–C(357)–H(35S)	109.9
H(28a)–C(28)–H(28b)	109.5	C(356)–C(357)–H(35S)	109.9
C(27)–C(28)–H(28C)	109.5	H(35R)–C(357)–H(35S)	108.3
H(28a)–C(28)–H(28C)	109.5	O(23)–C(358)–C(359)	111.5(19)
H(28b)–C(28)–H(28C)	109.5	O(23)–C(358)–H(35T)	109.3
C(27)–C(29)–C(210)	122.5(4)	C(359)–C(358)–H(35T)	109.3
C(27)–C(29)–H(29a)	118.8	O(23)–C(358)–H(35U)	109.3
C(210)–C(29)–H(29a)	118.8	C(359)–C(358)–H(35U)	109.3
C(29)–C(210)–C(23)	117.8(4)	H(35T)–C(358)–H(35U)	108.0
C(29)–C(210)–C(211)	120.2(4)	O(24)–C(359)–C(358)	112(2)
C(23)–C(210)–C(211)	122.0(4)	O(24)–C(359)–H(35V)	109.3
C(210)–C(211)–H(21i)	109.5	C(358)–C(359)–H(35V)	109.3
C(210)–C(211)–H(21j)	109.5	O(24)–C(359)–H(35W)	109.3
H(21i)–C(211)–H(21j)	109.5	C(358)–C(359)–H(35W)	109.3
C(210)–C(211)–H(21K)	109.5	H(35V)–C(359)–H(35W)	107.9
H(21i)–C(211)–H(21K)	109.5	O(24)–C(360)–C(361)	106(3)
H(21j)–C(211)–H(21K)	109.5	C(361)–C(360)–K(3)	78(2)
C(219)–C(212)–C(213)	119.9(3)	O(24)–C(360)–H(36b)	110.5
C(219)–C(212)–C(2m2)	118.5(3)	C(361)–C(360)–H(36b)	110.5
C(213)–C(212)–C(2m2)	121.4(3)	K(3)–C(360)–H(36b)	95.9

Table S23. Continued

angle	degree	angle	degree
C(215)–C(213)–C(212)	119.2(3)	O(24)–C(360)–H(36C)	110.5
C(215)–C(213)–C(214)	119.2(3)	C(361)–C(360)–H(36C)	110.5
C(212)–C(213)–C(214)	121.6(3)	K(3)–C(360)–H(36C)	147.7
C(213)–C(214)–H(21a)	109.5	H(36b)–C(360)–H(36C)	108.7
C(213)–C(214)–H(21b)	109.5	O(19)–C(361)–C(360)	109(2)
H(21a)–C(214)–H(21b)	109.5	O(19)–C(361)–H(36d)	109.8
C(213)–C(214)–H(21C)	109.5	C(360)–C(361)–H(36d)	109.8
H(21a)–C(214)–H(21C)	109.5	O(19)–C(361)–H(36e)	109.8
H(21b)–C(214)–H(21C)	109.5	C(360)–C(361)–H(36e)	109.8
C(216)–C(215)–C(213)	121.8(3)	H(36d)–C(361)–H(36e)	108.2
C(216)–C(215)–H(21d)	119.1	C(45)–O(26)–C(48)	104.4
C(213)–C(215)–H(21d)	119.1	O(26)–C(45)–C(46)	104.2
C(215)–C(216)–C(218)	117.9(4)	O(26)–C(45)–H(42C)	110.9
C(215)–C(216)–C(217)	121.6(4)	C(46)–C(45)–H(42C)	110.9
C(218)–C(216)–C(217)	120.4(4)	O(26)–C(45)–H(42d)	110.9
C(216)–C(217)–H(21F)	109.5	C(46)–C(45)–H(42d)	110.9
C(216)–C(217)–H(21g)	109.5	H(42C)–C(45)–H(42d)	108.9
H(21f)–C(217)–H(21g)	109.5	C(45)–C(46)–C(47)	103.7
C(216)–C(217)–H(21H)	109.5	C(45)–C(46)–H(42K)	111.0
H(21f)–C(217)–H(21H)	109.5	C(47)–C(46)–H(42K)	111.0
H(21g)–C(217)–H(21H)	109.5	C(45)–C(46)–H(42L)	111.0
C(216)–C(218)–C(219)	122.1(4)	C(47)–C(46)–H(42L)	111.0
C(216)–C(218)–H(21e)	118.9	H(42K)–C(46)–H(42L)	109.0
C(219)–C(218)–H(21e)	118.9	C(48)–C(47)–C(46)	104.4
C(218)–C(219)–C(212)	118.9(3)	C(48)–C(47)–H(42m)	110.9
C(218)–C(219)–C(220)	119.1(4)	C(46)–C(47)–H(42m)	110.9
C(212)–C(219)–C(220)	121.9(4)	C(48)–C(47)–H(42N)	110.9
C(219)–C(220)–H(22a)	109.5	C(46)–C(47)–H(42N)	110.9
C(219)–C(220)–H(22b)	109.5	H(42m)–C(47)–H(42N)	108.9
H(22a)–C(220)–H(22b)	109.5	O(26)–C(48)–C(47)	105.4
C(219)–C(220)–H(22C)	109.5	O(26)–C(48)–H(43j)	110.7
H(22a)–C(220)–H(22C)	109.5	C(47)–C(48)–H(43j)	110.7
H(22b)–C(220)–H(22C)	109.5	O(26)–C(48)–H(43K)	110.7
C(222)–C(221)–C(228)	120.7(4)	C(47)–C(48)–H(43K)	110.7

Table S23. Continued

angle	degree	angle	degree
C(222)–C(221)–C(2m3)	118.0(4)	H(43j)–C(48)–H(43K)	108.8
C(228)–C(221)–C(2m3)	121.2(4)	C(49)–O(27)–C(52)	109.0(4)
C(221)–C(222)–C(224)	118.9(4)	O(27)–C(49)–C(50)	106.7(4)
C(221)–C(222)–C(223)	121.7(4)	O(27)–C(49)–H(42a)	110.4
C(224)–C(222)–C(223)	119.3(4)	C(50)–C(49)–H(42a)	110.4
C(222)–C(223)–H(22F)	109.5	O(27)–C(49)–H(42b)	110.4
C(222)–C(223)–H(22g)	109.5	C(50)–C(49)–H(42b)	110.4
H(22f)–C(223)–H(22g)	109.5	H(42a)–C(49)–H(42b)	108.6
C(222)–C(223)–H(22H)	109.5	C(51)–C(50)–C(49)	102.4(4)
H(22f)–C(223)–H(22H)	109.5	C(51)–C(50)–H(42e)	111.3
H(22g)–C(223)–H(22H)	109.5	C(49)–C(50)–H(42e)	111.3
C(225)–C(224)–C(222)	121.4(5)	C(51)–C(50)–H(42F)	111.3
C(225)–C(224)–H(22d)	119.3	C(49)–C(50)–H(42F)	111.3
C(222)–C(224)–H(22d)	119.3	H(42e)–C(50)–H(42f)	109.2
C(227)–C(225)–C(224)	118.6(4)	C(50)–C(51)–C(52)	101.5(4)
C(227)–C(225)–C(226)	119.5(5)	C(50)–C(51)–H(42g)	111.5
C(224)–C(225)–C(226)	121.8(5)	C(52)–C(51)–H(42g)	111.5
C(225)–C(226)–H(22L)	109.5	C(50)–C(51)–H(42H)	111.5
C(225)–C(226)–H(22m)	109.5	C(52)–C(51)–H(42H)	111.5
H(22L)–C(226)–H(22m)	109.5	H(42g)–C(51)–H(42H)	109.3
C(225)–C(226)–H(22N)	109.5	O(27)–C(52)–C(51)	107.1(4)
H(22L)–C(226)–H(22N)	109.5	O(27)–C(52)–H(42i)	110.3
H(22m)–C(226)–H(22N)	109.5	C(51)–C(52)–H(42i)	110.3
C(225)–C(227)–C(228)	122.4(4)	O(27)–C(52)–H(42j)	110.3
C(225)–C(227)–H(22e)	118.8	C(51)–C(52)–H(42j)	110.3
C(228)–C(227)–H(22e)	118.8	H(42i)–C(52)–H(42j)	108.6
C(227)–C(228)–C(221)	117.8(4)	C(56)–O(28)–C(53)	100.5(6)
C(227)–C(228)–C(229)	120.1(4)	C(54)–C(53)–O(28)	102.7(6)
C(221)–C(228)–C(229)	122.1(4)	C(54)–C(53)–H(43m)	111.2
C(228)–C(229)–H(22i)	109.5	O(28)–C(53)–H(43m)	111.2
C(228)–C(229)–H(22j)	109.5	C(54)–C(53)–H(43g)	111.2
H(22i)–C(229)–H(22j)	109.5	O(28)–C(53)–H(43g)	111.2
C(228)–C(229)–H(22K)	109.5	H(43m)–C(53)–H(43g)	109.1
H(22i)–C(229)–H(22K)	109.5	C(55)–C(54)–C(53)	108.5(7)

Table S23. Continued

angle	degree	angle	degree
H(22j)–C(229)–H(22K)	109.5	C(55)–C(54)–H(43e)	110.0
C(231)–C(230)–C(237)	120.1(3)	C(53)–C(54)–H(43e)	110.0
C(231)–C(230)–C(2m4)	121.3(3)	C(55)–C(54)–H(43F)	110.0
C(237)–C(230)–C(2m4)	118.6(3)	C(53)–C(54)–H(43F)	110.0
C(233)–C(231)–C(230)	118.9(3)	H(43e)–C(54)–H(43f)	108.4
C(233)–C(231)–C(232)	119.1(3)	C(56)–C(55)–C(54)	109.2(6)
C(230)–C(231)–C(232)	122.0(3)	C(56)–C(55)–H(55a)	109.8
C(231)–C(232)–H(23C)	109.5	C(54)–C(55)–H(55a)	109.8
C(231)–C(232)–H(23d)	109.5	C(56)–C(55)–H(55b)	109.8
H(23C)–C(232)–H(23d)	109.5	C(54)–C(55)–H(55b)	109.8
C(231)–C(232)–H(23e)	109.5	H(55a)–C(55)–H(55b)	108.3
H(23C)–C(232)–H(23e)	109.5	C(55)–C(56)–O(28)	104.9(6)
H(23d)–C(232)–H(23e)	109.5	C(55)–C(56)–H(43H)	110.8
C(234)–C(233)–C(231)	121.8(3)	O(28)–C(56)–H(43H)	110.8
C(234)–C(233)–H(23b)	119.1	C(55)–C(56)–H(43i)	110.8
C(231)–C(233)–H(23b)	119.1	O(28)–C(56)–H(43i)	110.8
C(236)–C(234)–C(233)	118.7(3)	H(43H)–C(56)–H(43i)	108.8
C(236)–C(234)–C(235)	121.1(4)	C(64)–O(30)–C(61)	103.5(5)
C(233)–C(234)–C(235)	120.3(4)	O(30)–C(61)–C(62)	103.6(5)
C(234)–C(235)–H(23i)	109.5	O(30)–C(61)–H(61a)	111.1
C(234)–C(235)–H(23j)	109.5	C(62)–C(61)–H(61a)	111.1
H(23i)–C(235)–H(23j)	109.5	O(30)–C(61)–H(61b)	111.1
C(234)–C(235)–H(23K)	109.5	C(62)–C(61)–H(61b)	111.1
H(23i)–C(235)–H(23K)	109.5	H(61a)–C(61)–H(61b)	109.0
H(23j)–C(235)–H(23K)	109.5	C(63)–C(62)–C(61)	102.3(5)
C(234)–C(236)–C(237)	121.2(3)	C(63)–C(62)–H(62a)	111.3
C(234)–C(236)–H(23a)	119.4	C(61)–C(62)–H(62a)	111.3
C(237)–C(236)–H(23a)	119.4	C(63)–C(62)–H(62b)	111.3
C(230)–C(237)–C(236)	119.3(3)	C(61)–C(62)–H(62b)	111.3
C(230)–C(237)–C(238)	121.0(3)	H(62a)–C(62)–H(62b)	109.2
C(236)–C(237)–C(238)	119.7(3)	C(64)–C(63)–C(62)	107.4(5)
C(237)–C(238)–H(23F)	109.5	C(64)–C(63)–H(63a)	110.2
C(237)–C(238)–H(23g)	109.5	C(62)–C(63)–H(63a)	110.2
H(23f)–C(238)–H(23g)	109.5	C(64)–C(63)–H(63b)	110.2

Table S23. Continued

angle	degree	angle	degree
C(237)–C(238)–H(23H)	109.5	C(62)–C(63)–H(63b)	110.2
H(23f)–C(238)–H(23H)	109.5	H(63a)–C(63)–H(63b)	108.5
H(23g)–C(238)–H(23H)	109.5	O(30)–C(64)–C(63)	108.5(5)
O(7)–C(239)–C(240)	109.3(3)	O(30)–C(64)–H(64a)	110.0
O(7)–C(239)–H(16C)	109.8	C(63)–C(64)–H(64a)	110.0
C(240)–C(239)–H(16C)	109.8	O(30)–C(64)–H(64b)	110.0
O(7)–C(239)–H(16d)	109.8	C(63)–C(64)–H(64b)	110.0
C(240)–C(239)–H(16d)	109.8	H(64a)–C(64)–H(64b)	108.4
H(16C)–C(239)–H(16d)	108.3	C(41)–O(25)–C(44)	104.2(3)
O(8)–C(240)–C(239)	108.4(3)	O(25)–C(41)–C(42)	104.4(3)
O(8)–C(240)–H(15a)	110.0	O(25)–C(41)–H(24m)	110.9
C(239)–C(240)–H(15a)	110.0	C(42)–C(41)–H(24m)	110.9
O(8)–C(240)–H(15b)	110.0	O(25)–C(41)–H(24N)	110.9
C(239)–C(240)–H(15b)	110.0	C(42)–C(41)–H(24N)	110.9
H(15a)–C(240)–H(15b)	108.4	H(24m)–C(41)–H(24N)	108.9
O(8)–C(241)–C(242)	109.2(3)	C(41)–C(42)–C(43)	103.9(3)
O(8)–C(241)–H(41a)	109.8	C(41)–C(42)–H(24i)	111.0
C(242)–C(241)–H(41a)	109.8	C(43)–C(42)–H(24i)	111.0
O(8)–C(241)–H(41b)	109.8	C(41)–C(42)–H(24j)	111.0
C(242)–C(241)–H(41b)	109.8	C(43)–C(42)–H(24j)	111.0
H(41a)–C(241)–H(41b)	108.3	H(24i)–C(42)–H(24j)	109.0
O(9)–C(242)–C(241)	108.5(3)	C(44)–C(43)–C(42)	104.0(3)
O(9)–C(242)–H(24O)	110.0	C(44)–C(43)–H(24C)	111.0
C(241)–C(242)–H(24O)	110.0	C(42)–C(43)–H(24C)	111.0
O(9)–C(242)–H(24P)	110.0	C(44)–C(43)–H(24d)	111.0
C(241)–C(242)–H(24P)	110.0	C(42)–C(43)–H(24d)	111.0
H(24O)–C(242)–H(24P)	108.4	H(24C)–C(43)–H(24d)	109.0
O(9)–C(243)–C(244)	109.4(4)	O(25)–C(44)–C(43)	105.7(3)
O(9)–C(243)–H(24Q)	109.8	O(25)–C(44)–H(24a)	110.6
C(244)–C(243)–H(24Q)	109.8	C(43)–C(44)–H(24a)	110.6
O(9)–C(243)–H(24R)	109.8	O(25)–C(44)–H(24b)	110.6
C(244)–C(243)–H(24R)	109.8	C(43)–C(44)–H(24b)	110.6
H(24Q)–C(243)–H(24R)	108.2	H(24a)–C(44)–H(24b)	108.7
O(10)–C(244)–C(243)	109.8(3)	C(60a)–O(29a)–C(57a)	113.5

Table S23. Continued

angle	degree	angle	degree
O(10)–C(244)–H(18F)	109.7	O(29a)–C(57a)–C(58a)	100.1
C(243)–C(244)–H(18F)	109.7	O(29a)–C(57a)–H(57a)	111.8
O(10)–C(244)–H(18g)	109.7	C(58a)–C(57a)–H(57a)	111.8
C(243)–C(244)–H(18g)	109.7	O(29a)–C(57a)–H(57b)	111.8
H(18f)–C(244)–H(18g)	108.2	C(58a)–C(57a)–H(57b)	111.8
C(26b)–C(245)–O(10)	103.4(8)	H(57a)–C(57a)–H(57b)	109.5
O(10)–C(245)–C(26a)	111.9(5)	C(59a)–C(58a)–C(57a)	106.7
C(26b)–C(245)–H(18i)	90.8	C(59a)–C(58a)–H(58a)	110.4
O(10)–C(245)–H(18i)	109.2	C(57a)–C(58a)–H(58a)	110.4
C(26a)–C(245)–H(18i)	109.2	C(59a)–C(58a)–H(58b)	110.4
C(26b)–C(245)–H(18j)	133.7	C(57a)–C(58a)–H(58b)	110.4
O(10)–C(245)–H(18j)	109.2	H(58a)–C(58a)–H(58b)	108.6
C(26a)–C(245)–H(18j)	109.2	C(58a)–C(59a)–C(60a)	102.2
H(18i)–C(245)–H(18j)	107.9	C(58a)–C(59a)–H(59a)	111.3
O(12b)–C(248)–C(249)	111.0(10)	C(60a)–C(59a)–H(59a)	111.3
O(12a)–C(248)–C(249)	109.1(6)	C(58a)–C(59a)–H(59b)	111.3
O(12b)–C(248)–H(24K)	89.7	C(60a)–C(59a)–H(59b)	111.3
C(249)–C(248)–H(24K)	109.9	H(59a)–C(59a)–H(59b)	109.2
O(12b)–C(248)–H(24L)	125.5	O(29a)–C(60a)–C(59a)	100.5
C(249)–C(248)–H(24L)	109.9	O(29a)–C(60a)–H(60a)	111.7
O(7)–C(249)–C(248)	110.5(4)	C(59a)–C(60a)–H(60a)	111.7
O(7)–C(249)–H(18d)	109.5	O(29a)–C(60a)–H(60b)	111.7
C(248)–C(249)–H(18d)	109.5	C(59a)–C(60a)–H(60b)	111.7
O(7)–C(249)–H(18e)	109.5	H(60a)–C(60a)–H(60b)	109.4
C(248)–C(249)–H(18e)	109.5	C(60b)–O(29b)–C(57b)	104.6
H(18d)–C(249)–H(18e)	108.1	O(29b)–C(57b)–C(58b)	113.4
C(249)–O(7)–C(239)	111.8(3)	O(29b)–C(57b)–H(57C)	108.9
C(249)–O(7)–K(2)	114.7(2)	C(58b)–C(57b)–H(57C)	108.9
C(239)–O(7)–K(2)	113.8(2)	O(29b)–C(57b)–H(57d)	108.9
C(240)–O(8)–C(241)	112.8(3)	C(58b)–C(57b)–H(57d)	108.9
C(240)–O(8)–K(2)	118.8(2)	H(57C)–C(57b)–H(57d)	107.7
C(241)–O(8)–K(2)	118.8(2)	C(57b)–C(58b)–C(59b)	103.8
C(243)–O(9)–C(242)	112.3(3)	C(57b)–C(58b)–H(58C)	111.0
C(243)–O(9)–K(2)	103.0(2)	C(59b)–C(58b)–H(58C)	111.0

Table S23. Continued

angle	degree	angle	degree
C(242)–O(9)–K(2)	105.5(2)	C(57b)–C(58b)–H(58d)	111.0
C(244)–O(10)–C(245)	114.0(3)	C(59b)–C(58b)–H(58d)	111.0
C(244)–O(10)–K(2)	119.5(2)	H(58C)–C(58b)–H(58d)	109.0
C(245)–O(10)–K(2)	124.1(3)	C(60b)–C(59b)–C(58b)	104.3
O(12a)–C(1a)–C(27a)	114.7(7)	C(60b)–C(59b)–H(59C)	110.9
O(12a)–C(1a)–H(1a1)	108.6	C(58b)–C(59b)–H(59C)	110.9
C(27a)–C(1a)–H(1a1)	108.6	C(60b)–C(59b)–H(59d)	110.9
O(12a)–C(1a)–H(1a2)	108.6	C(58b)–C(59b)–H(59d)	110.9
C(27a)–C(1a)–H(1a2)	108.6	H(59C)–C(59b)–H(59d)	108.9
H(1a1)–C(1a)–H(1a2)	107.6	O(29b)–C(60b)–C(59b)	112.9
C(1a)–C(27a)–O(11a)	104.3(7)	O(29b)–C(60b)–H(60C)	109.0
C(1a)–C(27a)–H(27a)	110.9	C(59b)–C(60b)–H(60C)	109.0
O(11a)–C(27a)–H(27a)	110.9	O(29b)–C(60b)–H(60d)	109.0
C(1a)–C(27a)–H(27b)	110.9	C(59b)–C(60b)–H(60d)	109.0
O(11a)–C(27a)–H(27b)	110.9	H(60C)–C(60b)–H(60d)	107.8
H(27a)–C(27a)–H(27b)	108.9	H(311)–O(31)–H(312)	140.1(8)
O(11a)–C(26a)–C(245)	108.8(7)		

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

Table S24. Anisotropic Displacement Parameters (Å^2) for 3[K(18-crown-6)][Fe(TMP)(CN)$_2$]·5.1(THF)·0.9H$_2$O[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0129(2)	0.0193(3)	0.0141(2)	−0.0002(2)	0.0026(2)	0.0006(2)
K(1)	0.0250(4)	0.0276(5)	0.0230(3)	−0.0010(3)	0.0050(3)	−0.0056(3)
N(11)	0.0140(12)	0.0201(16)	0.0175(12)	0.0008(11)	0.0033(10)	−0.0019(10)
N(12)	0.0151(12)	0.0233(16)	0.0171(13)	−0.0016(11)	0.0028(10)	−0.0003(11)
N(13)	0.0173(13)	0.0229(17)	0.0162(12)	−0.0005(11)	0.0027(10)	0.0020(11)
N(14)	0.0160(12)	0.0190(16)	0.0156(12)	−0.0011(10)	0.0020(10)	0.0016(11)
N(15)	0.0295(16)	0.029(2)	0.0327(17)	0.0056(14)	0.0065(13)	−0.0015(14)
N(16)	0.0197(14)	0.0252(19)	0.0385(17)	0.0049(14)	0.0037(12)	0.0010(12)
C(1A1)	0.0133(14)	0.0216(19)	0.0188(15)	−0.0002(12)	0.0025(11)	−0.0009(12)
C(1A2)	0.0153(14)	0.0204(19)	0.0199(15)	−0.0012(13)	0.0022(12)	−0.0012(12)
C(1A3)	0.0152(14)	0.0233(19)	0.0196(15)	−0.0013(13)	0.0034(12)	−0.0009(12)
C(1A4)	0.0194(15)	0.0212(19)	0.0173(15)	−0.0016(13)	0.0019(12)	0.0006(13)
C(1A5)	0.0177(15)	0.026(2)	0.0184(15)	−0.0009(13)	0.0018(12)	0.0005(13)
C(1A6)	0.0191(15)	0.024(2)	0.0178(15)	0.0004(13)	0.0030(12)	0.0032(13)
C(1A7)	0.0167(14)	0.0196(19)	0.0195(15)	0.0007(13)	0.0034(12)	0.0016(12)
C(1A8)	0.0185(15)	0.0182(18)	0.0175(14)	0.0007(12)	0.0041(12)	−0.0011(12)
C(1B1)	0.0155(15)	0.029(2)	0.0197(15)	−0.0002(13)	0.0000(12)	0.0021(13)
C(1B2)	0.0145(15)	0.031(2)	0.0215(16)	0.0012(14)	0.0018(12)	0.0031(13)
C(1B3)	0.0179(15)	0.026(2)	0.0201(15)	−0.0030(13)	0.0060(12)	−0.0008(13)
C(1B4)	0.0199(16)	0.027(2)	0.0187(15)	−0.0035(13)	0.0028(12)	0.0038(13)
C(1B5)	0.0189(16)	0.037(2)	0.0181(15)	−0.0040(14)	−0.0020(12)	0.0053(14)
C(1B6)	0.0188(16)	0.035(2)	0.0197(16)	−0.0007(14)	0.0008(13)	0.0079(14)
C(1B7)	0.0214(16)	0.024(2)	0.0206(15)	−0.0002(13)	0.0054(12)	0.0054(13)
C(1B8)	0.0196(15)	0.0236(19)	0.0164(14)	−0.0010(13)	0.0037(12)	0.0019(13)
C(1M1)	0.0161(15)	0.0233(19)	0.0201(15)	−0.0018(13)	0.0047(12)	0.0000(13)
C(1M2)	0.0179(15)	0.026(2)	0.0142(14)	−0.0027(13)	0.0010(11)	0.0023(13)
C(1M3)	0.0170(15)	0.0224(19)	0.0192(15)	0.0012(13)	0.0051(12)	0.0049(13)
C(1M4)	0.0164(14)	0.0225(19)	0.0155(14)	−0.0009(12)	0.0023(11)	−0.0013(12)
C(11)	0.0191(15)	0.027(2)	0.0156(14)	0.0015(13)	0.0054(12)	0.0011(13)
C(12)	0.0120(14)	0.024(2)	0.0228(16)	−0.0043(14)	0.0014(12)	0.0016(12)
C(13)	0.0157(15)	0.029(2)	0.0185(15)	−0.0034(13)	0.0037(12)	0.0004(13)
C(14)	0.0193(16)	0.031(2)	0.0233(16)	−0.0028(14)	0.0034(13)	0.0008(14)
C(15)	0.0266(19)	0.029(2)	0.053(3)	−0.0026(19)	0.0119(17)	0.0004(16)
C(16)	0.0217(17)	0.035(2)	0.0300(18)	−0.0042(16)	0.0016(14)	0.0071(15)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(17)	0.0172(16)	0.046(3)	0.0262(17)	−0.0046(16)	0.0036(13)	0.0037(16)
C(18)	0.0171(18)	0.061(3)	0.061(3)	−0.004(2)	0.0079(18)	0.0060(19)
C(19)	0.0182(16)	0.043(2)	0.0212(16)	−0.0030(15)	0.0049(13)	−0.0055(15)
C(110)	0.0195(16)	0.033(2)	0.0174(15)	−0.0017(14)	0.0040(12)	−0.0015(14)
C(111)	0.0257(19)	0.032(2)	0.045(2)	0.0012(18)	0.0102(17)	−0.0005(16)
C(112)	0.0160(14)	0.028(2)	0.0160(14)	−0.0048(13)	0.0007(11)	0.0051(13)
C(113)	0.0185(15)	0.027(2)	0.0198(15)	−0.0014(14)	0.0016(12)	0.0048(13)
C(114)	0.0307(19)	0.032(2)	0.0240(17)	0.0034(15)	0.0010(14)	−0.0004(16)
C(115)	0.0233(17)	0.026(2)	0.0246(17)	−0.0042(14)	0.0022(13)	0.0019(14)
C(116)	0.0232(17)	0.034(2)	0.0208(16)	−0.0063(15)	0.0035(13)	0.0035(15)
C(117)	0.046(2)	0.046(3)	0.0208(18)	−0.0075(17)	−0.0002(16)	0.000(2)
C(118)	0.0258(17)	0.032(2)	0.0184(16)	0.0008(14)	0.0046(13)	0.0053(15)
C(119)	0.0174(15)	0.029(2)	0.0217(16)	−0.0016(14)	0.0037(12)	0.0045(13)
C(120)	0.037(2)	0.027(2)	0.0309(19)	−0.0008(16)	0.0081(16)	−0.0028(16)
C(121)	0.0185(15)	0.0239(19)	0.0160(14)	0.0013(13)	0.0033(12)	0.0084(13)
C(122)	0.0204(16)	0.029(2)	0.0201(15)	0.0018(14)	0.0056(12)	0.0047(14)
C(123)	0.0263(19)	0.032(3)	0.059(3)	0.012(2)	0.0166(18)	0.0034(16)
C(124)	0.0188(16)	0.032(2)	0.0224(16)	0.0000(14)	0.0027(13)	0.0060(14)
C(125)	0.0280(18)	0.028(2)	0.0186(15)	−0.0017(14)	−0.0005(13)	0.0106(15)
C(126)	0.035(2)	0.034(3)	0.035(2)	0.0020(17)	0.0015(16)	0.0162(18)
C(127)	0.0320(19)	0.020(2)	0.0258(17)	0.0039(14)	0.0028(14)	0.0042(15)
C(128)	0.0201(16)	0.028(2)	0.0197(15)	0.0009(13)	0.0047(12)	0.0028(14)
C(129)	0.0272(19)	0.031(2)	0.037(2)	0.0059(17)	0.0119(16)	0.0023(16)
C(130)	0.0143(14)	0.0249(19)	0.0165(14)	−0.0022(13)	0.0020(11)	0.0030(13)
C(131)	0.0154(14)	0.025(2)	0.0195(15)	0.0011(13)	0.0030(12)	0.0035(13)
C(132)	0.0206(16)	0.030(2)	0.0255(17)	0.0027(15)	0.0016(13)	−0.0036(14)
C(133)	0.0187(15)	0.028(2)	0.0196(15)	0.0043(13)	0.0046(12)	0.0050(13)
C(134)	0.0219(16)	0.033(2)	0.0177(15)	−0.0028(14)	−0.0001(12)	0.0105(15)
C(135)	0.0293(19)	0.042(3)	0.0208(17)	−0.0034(16)	−0.0023(14)	0.0097(17)
C(136)	0.0208(16)	0.030(2)	0.0242(17)	−0.0079(15)	−0.0036(13)	0.0052(14)
C(137)	0.0184(15)	0.023(2)	0.0242(16)	−0.0032(14)	0.0018(12)	0.0020(13)
C(138)	0.0306(19)	0.034(2)	0.034(2)	−0.0046(17)	0.0059(16)	−0.0089(17)
C(139)	0.0202(17)	0.033(2)	0.0340(19)	0.0010(16)	0.0019(14)	0.0016(15)
C(140)	0.0213(17)	0.037(2)	0.0276(18)	0.0002(16)	0.0069(14)	−0.0007(15)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(141)	0.0243(17)	0.039(2)	0.0200(16)	0.0029(15)	0.0040(13)	0.0043(15)
C(142)	0.0218(17)	0.045(3)	0.0203(16)	−0.0026(16)	0.0007(13)	0.0028(16)
C(143)	0.0203(17)	0.044(3)	0.0292(18)	−0.0032(17)	0.0037(14)	−0.0006(16)
C(144)	0.0195(16)	0.039(2)	0.0315(19)	0.0004(16)	0.0055(14)	0.0014(15)
C(145)	0.032(2)	0.041(3)	0.033(2)	−0.0057(18)	0.0146(16)	−0.0047(18)
C(146)	0.041(2)	0.034(2)	0.0247(18)	−0.0025(16)	0.0119(16)	−0.0100(18)
C(147)	0.043(2)	0.029(2)	0.0266(18)	0.0027(16)	0.0051(16)	0.0041(17)
C(148)	0.035(2)	0.034(2)	0.0255(18)	−0.0009(16)	0.0017(15)	0.0023(17)
C(149)	0.0225(17)	0.034(2)	0.0324(19)	0.0001(16)	−0.0045(14)	−0.0014(15)
C(150)	0.0201(16)	0.027(2)	0.0328(19)	0.0017(15)	−0.0006(14)	−0.0006(14)
O(1)	0.0187(12)	0.0423(17)	0.0238(12)	−0.0020(11)	0.0048(9)	0.0004(11)
O(2)	0.0230(12)	0.0317(16)	0.0252(12)	−0.0016(11)	0.0061(10)	−0.0016(10)
O(3)	0.0320(14)	0.0262(15)	0.0260(13)	0.0016(11)	0.0063(10)	−0.0037(11)
O(4)	0.0250(13)	0.0408(18)	0.0252(13)	−0.0014(11)	0.0011(10)	−0.0057(11)
O(5)	0.0249(13)	0.0283(16)	0.0319(13)	0.0021(11)	0.0019(10)	−0.0012(11)
O(6)	0.0189(12)	0.0337(16)	0.0249(12)	0.0024(11)	0.0022(9)	0.0014(10)
Fe(2)	0.0118(2)	0.0252(3)	0.0163(2)	−0.0018(2)	0.0025(2)	0.0004(2)
K(2)	0.0206(4)	0.0374(5)	0.0269(4)	0.0038(3)	0.0049(3)	−0.0012(3)
N(21)	0.0140(12)	0.0254(17)	0.0188(13)	−0.0003(11)	0.0014(10)	0.0009(11)
N(22)	0.0152(12)	0.0196(16)	0.0176(13)	−0.0019(11)	0.0022(10)	−0.0003(10)
N(23)	0.0143(13)	0.0345(19)	0.0182(13)	−0.0020(12)	0.0030(10)	0.0026(12)
N(24)	0.0138(12)	0.0285(18)	0.0200(13)	−0.0012(12)	0.0022(10)	0.0032(11)
N(25)	0.0297(17)	0.035(2)	0.0393(19)	0.0064(15)	0.0079(14)	−0.0026(15)
N(26)	0.0240(15)	0.030(2)	0.0332(17)	−0.0036(14)	0.0056(13)	−0.0022(13)
C(2A1)	0.0156(14)	0.024(2)	0.0208(15)	0.0006(13)	0.0022(12)	0.0008(13)
C(2A2)	0.0167(15)	0.0220(19)	0.0207(15)	−0.0012(13)	0.0006(12)	0.0010(13)
C(2A3)	0.0170(15)	0.0220(19)	0.0185(15)	−0.0015(13)	0.0023(12)	−0.0004(13)
C(2A4)	0.0186(15)	0.0214(19)	0.0199(15)	−0.0003(13)	0.0046(12)	−0.0017(13)
C(2A5)	0.0162(15)	0.031(2)	0.0226(16)	0.0010(14)	0.0034(12)	0.0040(14)
C(2A6)	0.0177(16)	0.043(2)	0.0202(16)	−0.0065(15)	0.0015(13)	0.0036(15)
C(2A7)	0.0184(16)	0.034(2)	0.0204(16)	−0.0043(14)	0.0028(13)	0.0026(14)
C(2A8)	0.0159(15)	0.026(2)	0.0234(16)	0.0003(14)	0.0048(12)	0.0010(13)
C(2B1)	0.0145(14)	0.027(2)	0.0239(16)	−0.0012(14)	0.0006(12)	0.0025(13)
C(2B2)	0.0181(15)	0.029(2)	0.0231(16)	0.0000(14)	−0.0003(13)	0.0027(14)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(2B3)	0.0207(16)	0.027(2)	0.0193(15)	−0.0040(13)	0.0033(12)	0.0016(14)
C(2B4)	0.0216(16)	0.023(2)	0.0236(16)	−0.0034(14)	0.0053(13)	0.0034(13)
C(2B5)	0.0175(16)	0.049(3)	0.0236(17)	−0.0030(16)	0.0010(13)	0.0094(16)
C(2B6)	0.0183(17)	0.060(3)	0.0238(18)	−0.0085(18)	−0.0010(14)	0.0110(17)
C(2B7)	0.0205(16)	0.035(2)	0.0213(16)	−0.0013(15)	0.0045(13)	0.0053(15)
C(2B8)	0.0185(16)	0.033(2)	0.0201(16)	0.0015(14)	0.0055(12)	0.0044(14)
C(2M1)	0.0170(15)	0.0222(19)	0.0191(15)	−0.0029(13)	0.0007(12)	−0.0024(13)
C(2M2)	0.0162(15)	0.024(2)	0.0216(15)	0.0014(13)	0.0061(12)	0.0013(13)
C(2M3)	0.0185(16)	0.040(2)	0.0209(16)	−0.0067(15)	0.0022(13)	0.0038(15)
C(2M4)	0.0115(14)	0.0233(19)	0.0234(16)	−0.0015(13)	0.0036(12)	0.0006(12)
C(21)	0.0169(15)	0.031(2)	0.0214(16)	0.0038(14)	0.0037(12)	0.0030(14)
C(22)	0.0157(15)	0.029(2)	0.0220(16)	−0.0078(14)	0.0049(12)	0.0003(14)
C(23)	0.0191(15)	0.030(2)	0.0190(15)	−0.0063(13)	−0.0018(12)	0.0059(13)
C(24)	0.0260(17)	0.031(2)	0.0199(16)	−0.0007(14)	0.0011(13)	0.0112(14)
C(25)	0.034(2)	0.036(2)	0.0302(19)	0.0048(17)	0.0049(16)	−0.0036(17)
C(26)	0.036(2)	0.046(3)	0.0253(17)	0.0036(16)	0.0046(15)	0.0216(18)
C(27)	0.043(2)	0.062(3)	0.0194(17)	−0.0076(17)	−0.0042(16)	0.032(2)
C(28)	0.069(3)	0.102(5)	0.021(2)	−0.010(2)	−0.010(2)	0.051(3)
C(29)	0.031(2)	0.062(3)	0.035(2)	−0.023(2)	−0.0134(16)	0.0172(19)
C(210)	0.0216(17)	0.040(2)	0.0306(18)	−0.0152(16)	−0.0053(14)	0.0085(15)
C(211)	0.035(2)	0.050(3)	0.055(3)	−0.022(2)	0.001(2)	−0.012(2)
C(212)	0.0200(16)	0.024(2)	0.0186(15)	0.0000(13)	0.0019(12)	0.0030(13)
C(213)	0.0220(16)	0.025(2)	0.0200(15)	−0.0014(13)	0.0030(13)	0.0013(14)
C(214)	0.0228(17)	0.028(2)	0.046(2)	0.0020(17)	0.0105(16)	−0.0006(15)
C(215)	0.0180(15)	0.031(2)	0.0242(16)	−0.0007(14)	0.0033(13)	0.0028(14)
C(216)	0.0270(18)	0.032(2)	0.0277(18)	0.0038(15)	0.0010(14)	0.0066(16)
C(217)	0.033(2)	0.033(3)	0.053(3)	0.007(2)	0.0044(19)	0.0122(18)
C(218)	0.0301(19)	0.027(2)	0.041(2)	0.0098(17)	0.0050(16)	0.0024(16)
C(219)	0.0209(17)	0.033(2)	0.035(2)	0.0100(16)	0.0039(14)	0.0031(15)
C(220)	0.027(2)	0.040(3)	0.057(3)	0.016(2)	0.0147(19)	0.0000(18)
C(221)	0.0144(15)	0.056(3)	0.0205(16)	−0.0104(17)	−0.0003(13)	0.0064(16)
C(222)	0.0178(16)	0.052(3)	0.0313(19)	−0.0136(18)	0.0000(14)	0.0102(17)
C(223)	0.033(2)	0.048(3)	0.042(2)	−0.008(2)	0.0018(18)	0.0053(19)
C(224)	0.0252(19)	0.056(3)	0.040(2)	−0.019(2)	−0.0028(17)	0.0063(19)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(225)	0.0243(19)	0.078(4)	0.029(2)	−0.025(2)	0.0000(16)	0.006(2)
C(226)	0.049(3)	0.099(5)	0.037(3)	−0.034(3)	−0.004(2)	−0.002(3)
C(227)	0.0230(18)	0.074(4)	0.0221(18)	−0.010(2)	0.0027(14)	0.007(2)
C(228)	0.0205(17)	0.058(3)	0.0216(17)	−0.0062(17)	0.0027(14)	0.0082(17)
C(229)	0.039(2)	0.066(4)	0.027(2)	0.000(2)	0.0035(17)	0.002(2)
C(230)	0.0110(14)	0.026(2)	0.0199(15)	0.0016(13)	0.0032(11)	0.0018(12)
C(231)	0.0202(16)	0.024(2)	0.0182(15)	0.0026(13)	0.0015(12)	0.0015(13)
C(232)	0.0306(19)	0.029(2)	0.034(2)	−0.0014(16)	0.0089(15)	−0.0052(16)
C(233)	0.0257(17)	0.024(2)	0.0231(16)	0.0020(14)	0.0054(13)	0.0073(14)
C(234)	0.0149(15)	0.037(2)	0.0250(17)	0.0035(15)	0.0048(13)	0.0071(14)
C(235)	0.0192(18)	0.051(3)	0.059(3)	−0.001(2)	0.0111(18)	0.0089(18)
C(236)	0.0147(15)	0.031(2)	0.0251(16)	0.0054(14)	0.0041(12)	−0.0017(13)
C(237)	0.0146(15)	0.024(2)	0.0234(16)	0.0030(13)	0.0023(12)	0.0003(13)
C(238)	0.0231(18)	0.026(2)	0.059(3)	−0.0035(19)	0.0085(17)	−0.0030(15)
C(239)	0.0284(19)	0.042(3)	0.037(2)	−0.0066(18)	0.0044(16)	−0.0006(17)
C(240)	0.0307(19)	0.035(2)	0.033(2)	−0.0066(17)	0.0086(16)	−0.0029(17)
C(241)	0.0307(19)	0.034(2)	0.0310(19)	0.0001(16)	0.0127(15)	0.0026(16)
C(242)	0.0311(19)	0.038(2)	0.0300(19)	0.0035(17)	0.0127(15)	0.0046(17)
C(243)	0.0229(19)	0.055(3)	0.046(2)	0.010(2)	0.0011(17)	−0.0073(19)
C(244)	0.0248(19)	0.051(3)	0.042(2)	0.008(2)	−0.0009(17)	0.0012(18)
C(245)	0.041(3)	0.072(4)	0.036(2)	0.005(2)	−0.0025(19)	0.010(2)
C(248)	0.0268(19)	0.044(3)	0.049(2)	−0.010(2)	0.0183(18)	−0.0061(18)
C(249)	0.0235(19)	0.061(3)	0.048(2)	−0.012(2)	0.0083(17)	−0.0014(19)
O(7)	0.0256(13)	0.0333(17)	0.0344(14)	−0.0006(12)	0.0118(11)	0.0001(11)
O(8)	0.0261(13)	0.0311(16)	0.0356(14)	−0.0057(12)	0.0103(11)	−0.0026(11)
O(9)	0.0274(13)	0.0378(18)	0.0344(14)	0.0061(12)	0.0059(11)	0.0020(12)
O(10)	0.0251(14)	0.079(3)	0.0327(15)	0.0051(16)	−0.0051(12)	0.0080(15)
C(1A)	0.029(3)	0.037(4)	0.033(3)	0.001(3)	0.008(2)	−0.003(3)
C(27A)	0.045(5)	0.054(4)	0.045(3)	0.016(3)	0.017(4)	0.001(4)
C(26A)	0.055(4)	0.046(5)	0.032(4)	0.004(3)	−0.011(3)	−0.010(3)
O(11A)	0.037(2)	0.043(3)	0.039(2)	0.0069(18)	0.0026(17)	−0.0008(19)
O(12A)	0.025(3)	0.027(4)	0.045(3)	−0.005(3)	0.006(2)	0.002(2)
C(1B)	0.043(7)	0.065(9)	0.047(7)	−0.003(6)	0.013(6)	−0.009(6)
C(27B)	0.045(5)	0.054(4)	0.045(3)	0.016(3)	0.017(4)	0.001(4)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(26B)	0.055(4)	0.046(5)	0.032(4)	0.004(3)	−0.011(3)	−0.010(3)
O(11B)	0.037(2)	0.043(3)	0.039(2)	0.0069(18)	0.0026(17)	−0.0008(19)
O(12B)	0.035(10)	0.076(17)	0.032(6)	−0.006(10)	0.012(6)	−0.017(9)
Fe(3)	0.0130(2)	0.0239(3)	0.0156(2)	−0.0002(2)	0.0033(2)	−0.0018(2)
K(3)	0.0272(4)	0.0304(5)	0.0308(4)	0.0018(3)	0.0068(3)	0.0031(3)
N(31)	0.0149(13)	0.0266(17)	0.0189(13)	0.0004(11)	0.0031(10)	−0.0026(11)
N(32)	0.0166(13)	0.0237(17)	0.0167(13)	−0.0003(11)	0.0039(10)	−0.0014(11)
N(33)	0.0161(12)	0.0229(16)	0.0174(13)	0.0010(11)	0.0050(10)	−0.0013(11)
N(34)	0.0141(12)	0.0257(17)	0.0188(13)	−0.0010(11)	0.0038(10)	−0.0019(11)
N(35)	0.0328(18)	0.037(2)	0.0389(19)	0.0014(15)	0.0072(14)	−0.0100(16)
N(36)	0.0258(16)	0.031(2)	0.0340(17)	0.0002(14)	0.0087(13)	−0.0036(14)
C(3A1)	0.0142(15)	0.031(2)	0.0235(16)	0.0014(14)	0.0027(12)	−0.0033(13)
C(3A2)	0.0163(15)	0.029(2)	0.0200(15)	−0.0003(14)	0.0020(12)	−0.0017(13)
C(3A3)	0.0210(16)	0.024(2)	0.0186(15)	−0.0025(13)	0.0031(12)	−0.0036(13)
C(3A4)	0.0193(15)	0.0216(19)	0.0201(15)	−0.0001(13)	0.0042(12)	−0.0019(13)
C(3A5)	0.0149(14)	0.028(2)	0.0186(15)	0.0037(13)	0.0046(12)	0.0005(13)
C(3A6)	0.0173(15)	0.025(2)	0.0175(15)	0.0009(13)	0.0020(12)	−0.0016(13)
C(3A7)	0.0165(15)	0.025(2)	0.0194(15)	−0.0013(13)	0.0038(12)	0.0000(13)
C(3A8)	0.0130(14)	0.028(2)	0.0210(15)	0.0002(13)	0.0049(12)	−0.0035(13)
C(3B1)	0.0165(16)	0.044(3)	0.0240(17)	0.0008(16)	0.0009(13)	0.0008(15)
C(3B2)	0.0206(17)	0.044(3)	0.0201(16)	0.0017(15)	0.0013(13)	0.0007(16)
C(3B3)	0.0256(17)	0.027(2)	0.0178(15)	−0.0035(14)	0.0040(13)	−0.0019(14)
C(3B4)	0.0245(17)	0.028(2)	0.0200(16)	−0.0051(14)	0.0045(13)	−0.0001(14)
C(3B5)	0.0178(15)	0.031(2)	0.0184(15)	0.0024(14)	0.0028(12)	0.0004(14)
C(3B6)	0.0158(15)	0.034(2)	0.0198(15)	0.0013(14)	0.0029(12)	−0.0001(14)
C(3B7)	0.0208(16)	0.029(2)	0.0197(15)	−0.0027(14)	0.0065(13)	−0.0009(14)
C(3B8)	0.0160(15)	0.032(2)	0.0237(16)	−0.0028(14)	0.0053(13)	−0.0014(14)
C(3M1)	0.0185(15)	0.027(2)	0.0172(15)	−0.0015(13)	0.0017(12)	−0.0049(13)
C(3M2)	0.0172(15)	0.024(2)	0.0213(15)	0.0015(13)	0.0053(12)	0.0003(13)
C(3M3)	0.0170(15)	0.026(2)	0.0170(15)	−0.0007(13)	0.0017(12)	−0.0033(13)
C(3M4)	0.0137(14)	0.025(2)	0.0240(16)	0.0002(13)	0.0052(12)	−0.0037(13)
C(31)	0.0196(16)	0.031(2)	0.0207(16)	0.0015(14)	0.0041(13)	−0.0002(14)
C(32)	0.0154(15)	0.029(2)	0.0198(15)	−0.0027(14)	0.0046(12)	0.0014(13)
C(33)	0.0232(10)	0.0255(11)	0.0229(10)	−0.0009(8)	0.0022(8)	0.0015(8)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(34)	0.0285(11)	0.0301(11)	0.0279(10)	0.0015(9)	0.0049(8)	0.0024(8)
C(35)	0.0372(16)	0.0394(18)	0.0394(16)	0.0051(14)	0.0082(13)	−0.0034(14)
C(36)	0.0369(12)	0.0393(12)	0.0349(11)	0.0018(9)	0.0065(9)	0.0049(9)
C(37)	0.0389(12)	0.0427(13)	0.0377(12)	−0.0019(9)	0.0037(9)	0.0069(9)
C(38)	0.058(2)	0.070(2)	0.0499(18)	−0.0009(16)	0.0033(16)	0.0151(17)
C(39)	0.0383(12)	0.0422(13)	0.0389(12)	−0.0054(9)	0.0022(9)	0.0034(9)
C(310)	0.0303(11)	0.0341(12)	0.0330(11)	−0.0038(9)	0.0016(9)	0.0009(9)
C(311)	0.039(2)	0.053(3)	0.067(3)	−0.023(3)	0.002(2)	−0.020(2)
C(312)	0.0206(16)	0.024(2)	0.0173(14)	0.0009(13)	0.0051(12)	0.0036(13)
C(313)	0.0216(16)	0.024(2)	0.0219(16)	0.0005(13)	0.0058(13)	0.0005(14)
C(314)	0.0259(19)	0.028(2)	0.051(2)	−0.0029(18)	0.0117(17)	0.0000(16)
C(315)	0.0200(16)	0.032(2)	0.0228(16)	0.0002(14)	0.0048(13)	0.0048(14)
C(316)	0.0269(17)	0.029(2)	0.0184(15)	0.0022(14)	0.0011(13)	0.0068(15)
C(317)	0.036(2)	0.031(2)	0.035(2)	−0.0030(17)	0.0013(16)	0.0114(17)
C(318)	0.0301(18)	0.026(2)	0.0232(17)	0.0011(14)	0.0045(14)	0.0001(15)
C(319)	0.0239(17)	0.029(2)	0.0195(15)	0.0010(14)	0.0053(13)	−0.0001(14)
C(320)	0.0265(19)	0.030(2)	0.045(2)	−0.0042(18)	0.0111(16)	−0.0037(16)
C(321)	0.0135(14)	0.033(2)	0.0204(16)	−0.0055(14)	0.0015(12)	0.0022(13)
C(322)	0.0156(15)	0.033(2)	0.0249(17)	−0.0024(15)	0.0016(13)	0.0033(14)
C(323)	0.0228(17)	0.031(2)	0.0293(18)	−0.0034(15)	0.0012(14)	−0.0004(15)
C(324)	0.0204(17)	0.034(2)	0.0316(19)	−0.0078(16)	−0.0004(14)	0.0020(15)
C(325)	0.0184(16)	0.043(3)	0.0238(17)	−0.0089(16)	−0.0006(13)	0.0063(15)
C(326)	0.035(2)	0.059(3)	0.0268(19)	−0.0158(19)	−0.0057(16)	0.005(2)
C(327)	0.0230(17)	0.040(2)	0.0196(16)	−0.0003(15)	0.0028(13)	0.0097(16)
C(328)	0.0156(15)	0.038(2)	0.0212(16)	−0.0046(15)	0.0025(12)	0.0055(14)
C(329)	0.0312(19)	0.040(3)	0.0247(18)	0.0028(16)	0.0073(15)	0.0056(17)
C(330)	0.0132(14)	0.032(2)	0.0196(15)	0.0007(14)	0.0026(12)	0.0008(13)
C(331)	0.0248(18)	0.030(2)	0.0336(19)	0.0020(16)	0.0051(15)	−0.0003(15)
C(332)	0.036(2)	0.034(3)	0.080(4)	0.005(2)	0.011(2)	−0.0067(19)
C(333)	0.0286(19)	0.032(2)	0.041(2)	0.0008(18)	0.0043(16)	0.0083(16)
C(334)	0.0162(16)	0.045(3)	0.0287(18)	0.0016(17)	0.0020(13)	0.0065(15)
C(335)	0.0206(19)	0.060(3)	0.064(3)	0.002(2)	0.0067(19)	0.012(2)
C(336)	0.0152(15)	0.038(2)	0.0229(16)	0.0024(15)	0.0009(12)	−0.0018(14)
C(337)	0.0156(15)	0.031(2)	0.0197(15)	0.0003(14)	0.0027(12)	−0.0007(13)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(338)	0.0253(18)	0.034(2)	0.045(2)	0.0006(18)	0.0097(16)	−0.0021(16)
O(13)	0.0202(15)	0.033(2)	0.0324(17)	−0.0024(14)	0.0080(13)	−0.0003(14)
O(14)	0.0256(17)	0.044(2)	0.0273(17)	0.0007(15)	0.0030(13)	0.0037(15)
O(15)	0.030(2)	0.070(3)	0.031(2)	0.008(2)	0.0018(18)	0.018(2)
O(17)	0.046(2)	0.032(2)	0.048(2)	−0.0098(17)	0.0261(18)	−0.0095(17)
O(18)	0.0165(15)	0.038(2)	0.0245(17)	0.0065(15)	0.0014(13)	−0.0013(13)
C(339)	0.024(3)	0.042(4)	0.028(3)	0.001(2)	0.008(2)	0.002(2)
C(340)	0.024(2)	0.048(4)	0.026(2)	0.001(2)	0.0089(19)	0.001(2)
C(341)	0.014(4)	0.073(7)	0.035(4)	−0.003(4)	0.005(3)	−0.005(4)
C(342)	0.021(2)	0.074(5)	0.040(3)	−0.004(3)	−0.002(2)	0.010(3)
C(343)	0.054(5)	0.076(6)	0.034(4)	0.011(3)	−0.005(3)	0.005(4)
C(344)	0.058(5)	0.061(5)	0.045(3)	0.019(3)	0.024(4)	0.019(4)
C(2A)	0.043(4)	0.067(5)	0.036(4)	−0.015(4)	0.029(4)	−0.014(3)
O(16A)	0.035(3)	0.038(3)	0.042(3)	0.010(2)	0.016(2)	0.003(2)
C(2B)	0.043(4)	0.067(5)	0.036(4)	−0.015(4)	0.029(4)	−0.014(3)
O(16B)	0.050(12)	0.053(13)	0.038(11)	0.000(8)	0.001(8)	−0.009(8)
C(345)	0.043(3)	0.067(5)	0.046(3)	−0.015(3)	0.012(3)	0.000(3)
C(346)	0.021(2)	0.036(5)	0.038(4)	0.001(2)	0.010(2)	−0.006(2)
C(347)	0.014(2)	0.056(4)	0.039(3)	0.007(3)	0.0062(19)	0.002(2)
C(348)	0.023(2)	0.042(4)	0.026(3)	0.001(2)	−0.003(2)	−0.003(2)
C(349)	0.027(4)	0.041(3)	0.029(3)	0.000(2)	0.002(3)	−0.003(3)
O(19)	0.027(7)	0.040(9)	0.039(8)	−0.011(6)	0.008(6)	−0.003(6)
O(20)	0.016(12)	0.041(13)	0.068(17)	0.003(10)	0.017(9)	0.001(9)
O(21)	0.067(14)	0.043(13)	0.061(16)	−0.006(12)	0.004(13)	0.002(10)
O(22)	0.036(6)	0.044(8)	0.052(7)	0.001(6)	0.010(6)	0.006(6)
O(23)	0.042(9)	0.051(11)	0.043(9)	0.000(8)	0.013(7)	0.006(7)
O(24)	0.023(7)	0.061(11)	0.045(9)	−0.002(8)	0.008(6)	−0.004(7)
C(350)	0.044(9)	0.053(10)	0.054(10)	−0.001(8)	0.012(8)	−0.004(8)
C(351)	0.042(9)	0.037(9)	0.053(9)	0.003(8)	0.004(7)	0.000(8)
C(352)	0.052(10)	0.062(11)	0.070(11)	−0.003(9)	0.002(8)	−0.005(8)
C(353)	0.054(10)	0.056(10)	0.059(10)	−0.013(8)	0.004(8)	0.002(8)
C(354)	0.040(9)	0.040(9)	0.033(9)	0.015(7)	−0.007(8)	0.002(8)
C(355)	0.058(5)	0.061(5)	0.045(3)	0.019(3)	0.024(4)	0.019(4)
C(356)	0.043(3)	0.067(5)	0.046(3)	−0.015(3)	0.012(3)	0.000(3)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(357)	0.021(2)	0.036(5)	0.038(4)	0.001(2)	0.010(2)	−0.006(2)
C(358)	0.034(11)	0.019(12)	0.067(16)	−0.007(10)	0.004(10)	0.002(8)
C(359)	0.047(15)	0.038(15)	0.040(16)	−0.006(12)	−0.004(13)	0.012(11)
C(360)	0.027(4)	0.041(3)	0.029(3)	0.000(2)	0.002(3)	−0.003(3)
C(361)	0.052(11)	0.064(12)	0.039(10)	0.005(8)	0.009(9)	−0.006(9)
O(26)	0.070(4)	0.073(4)	0.070(4)	0.002(3)	−0.016(3)	−0.019(3)
C(45)	0.016(2)	0.017(2)	0.021(2)	−0.0005(17)	−0.0040(16)	0.0011(17)
C(46)	0.076(5)	0.045(4)	0.044(3)	−0.008(3)	−0.013(3)	−0.008(3)
C(47)	0.042(3)	0.041(4)	0.068(4)	−0.021(3)	0.019(3)	−0.005(3)
C(48)	0.033(3)	0.051(4)	0.044(3)	0.005(3)	0.003(3)	0.001(3)
O(27)	0.0450(18)	0.039(2)	0.0457(18)	0.0067(14)	0.0004(14)	−0.0037(14)
C(49)	0.073(4)	0.054(4)	0.043(3)	−0.007(2)	0.009(2)	−0.013(3)
C(50)	0.069(3)	0.035(3)	0.044(3)	−0.002(2)	0.006(2)	−0.007(2)
C(51)	0.042(2)	0.040(3)	0.042(2)	0.001(2)	−0.0038(19)	−0.002(2)
C(52)	0.041(2)	0.035(3)	0.033(2)	0.0013(18)	−0.0076(17)	−0.0012(18)
O(28)	0.101(5)	0.104(6)	0.056(4)	−0.003(4)	−0.012(3)	−0.039(4)
C(53)	0.109(6)	0.029(3)	0.029(3)	0.003(3)	−0.026(3)	−0.017(4)
C(54)	0.107(6)	0.038(4)	0.044(3)	0.016(3)	−0.010(4)	−0.022(4)
C(55)	0.109(5)	0.011(3)	0.051(4)	0.009(2)	−0.051(4)	−0.003(3)
C(56)	0.058(4)	0.038(4)	0.048(3)	−0.009(3)	−0.017(3)	0.007(3)
O(30)	0.084(4)	0.076(4)	0.081(4)	−0.004(3)	0.010(3)	−0.014(3)
C(61)	0.032(2)	0.045(3)	0.027(2)	−0.010(2)	0.0013(19)	0.005(2)
C(62)	0.050(3)	0.046(3)	0.041(3)	−0.008(2)	0.001(2)	−0.005(3)
C(63)	0.061(4)	0.055(4)	0.035(3)	−0.016(2)	0.008(3)	0.007(3)
C(64)	0.046(3)	0.023(3)	0.026(2)	−0.0107(18)	0.001(2)	−0.012(2)
O(25)	0.0311(14)	0.0387(18)	0.0348(15)	−0.0003(12)	0.0035(11)	0.0104(12)
C(41)	0.0241(18)	0.032(2)	0.034(2)	−0.0024(16)	0.0017(15)	0.0014(15)
C(42)	0.037(2)	0.033(2)	0.033(2)	−0.0005(17)	0.0016(16)	0.0085(17)
C(43)	0.056(3)	0.030(3)	0.032(2)	−0.0034(17)	0.0030(19)	0.006(2)
C(44)	0.037(2)	0.048(3)	0.031(2)	0.0022(18)	0.0039(17)	0.0101(19)
O(29A)	0.088(4)	0.059(4)	0.069(4)	−0.012(3)	0.018(3)	−0.011(3)
C(57A)	0.067(5)	0.051(4)	0.061(4)	−0.005(3)	0.003(4)	−0.007(4)
C(58A)	0.045(4)	0.056(4)	0.056(3)	−0.007(3)	0.007(3)	0.003(3)
C(59A)	0.048(4)	0.057(4)	0.072(4)	−0.006(4)	0.010(4)	−0.012(3)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(60A)	0.077(5)	0.052(5)	0.075(4)	−0.015(4)	0.006(4)	−0.007(4)
O(29B)	0.088(4)	0.059(4)	0.069(4)	−0.012(3)	0.018(3)	−0.011(3)
C(57B)	0.067(5)	0.051(4)	0.061(4)	−0.005(3)	0.003(4)	−0.007(4)
C(58B)	0.045(4)	0.056(4)	0.056(3)	−0.007(3)	0.007(3)	0.003(3)
C(59B)	0.048(4)	0.057(4)	0.072(4)	−0.006(4)	0.010(4)	−0.012(3)
C(60B)	0.077(5)	0.052(5)	0.075(4)	−0.015(4)	0.006(4)	−0.007(4)
O(31)	0.050(3)	0.031(3)	0.042(3)	−0.001(2)	0.003(2)	−0.005(2)
O(32)	0.093(10)	0.045(8)	0.045(7)	0.004(5)	−0.006(6)	−0.011(7)

[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 S25. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for 3[K(18-crown-6)][Fe(TMP)$(CN)_2$]·5.1(THF)·0.9H_2O[a]

atom	x	y	z	U(eq)
H(1BA)	0.6708	0.6202	0.3907	0.026
H(1BF)	0.7286	0.6004	0.3502	0.027
H(1BE)	0.6751	0.5953	0.2345	0.025
H(1BD)	0.5793	0.5876	0.2017	0.026
H(1BG)	0.3655	0.6754	0.2110	0.030
H(1BH)	0.3304	0.7540	0.2458	0.030
H(1BC)	0.3990	0.8079	0.3581	0.026
H(1BB)	0.4745	0.7570	0.3959	0.024
H(15I)	0.6790	0.5003	0.3076	0.053
H(15J)	0.7353	0.4529	0.3121	0.053
H(15K)	0.6994	0.4638	0.2800	0.053
H(16A)	0.8269	0.4888	0.2961	0.035
H(18A)	0.9235	0.5259	0.2949	0.069
H(18B)	0.9373	0.6029	0.3005	0.069
H(18C)	0.9217	0.5756	0.2678	0.069
H(19A)	0.8511	0.6827	0.2813	0.033
H(11C)	0.7752	0.7611	0.2812	0.051
H(11D)	0.7210	0.7414	0.2975	0.051
H(11E)	0.7160	0.7325	0.2628	0.051
H(11F)	0.4697	0.4999	0.2300	0.044
H(11G)	0.4283	0.4525	0.2081	0.044
H(11H)	0.3998	0.5089	0.2259	0.044
H(11A)	0.4000	0.4837	0.1586	0.030
H(11I)	0.4186	0.5572	0.0951	0.057
H(11J)	0.3549	0.5787	0.1018	0.057
H(11K)	0.3775	0.5044	0.1081	0.057
H(11B)	0.4406	0.6632	0.1292	0.030
H(12C)	0.4791	0.7482	0.1611	0.047
H(12D)	0.5322	0.7167	0.1831	0.047
H(12E)	0.4743	0.7416	0.1951	0.047
H(12I)	0.2416	0.7415	0.3191	0.057
H(12J)	0.3088	0.7240	0.3308	0.057
H(12K)	0.2814	0.7073	0.2977	0.057
H(12B)	0.2198	0.8500	0.3048	0.029

Table S25. Continued

atom	x	y	z	U(eq)
H(12L)	0.1907	0.9606	0.2941	0.053
H(12M)	0.2183	0.9868	0.2664	0.053
H(12N)	0.2425	1.0143	0.2984	0.053
H(12A)	0.3394	0.9737	0.2799	0.031
H(12F)	0.4343	0.9398	0.2751	0.047
H(12G)	0.4474	0.8623	0.2726	0.047
H(12H)	0.4593	0.8984	0.3038	0.047
H(13F)	0.4781	0.5608	0.4189	0.038
H(13G)	0.5081	0.5666	0.3899	0.038
H(13H)	0.4595	0.6193	0.3960	0.038
H(13A)	0.5302	0.6030	0.4622	0.026
H(13C)	0.5787	0.6403	0.5078	0.047
H(13D)	0.6052	0.7137	0.5087	0.047
H(13E)	0.6471	0.6513	0.5064	0.047
H(13B)	0.6536	0.7452	0.4625	0.031
H(13I)	0.6657	0.8040	0.4195	0.049
H(13J)	0.6226	0.7901	0.3896	0.049
H(13K)	0.6807	0.7464	0.3980	0.049
H(13L)	0.6132	0.3162	0.3205	0.035
H(13M)	0.6532	0.3811	0.3214	0.035
H(14A)	0.5702	0.4436	0.2998	0.034
H(14B)	0.5827	0.3831	0.2790	0.034
H(43C)	0.4854	0.3803	0.2569	0.033
H(43D)	0.4636	0.4375	0.2769	0.033
H(70A)	0.3858	0.3607	0.2593	0.035
H(70B)	0.4227	0.3031	0.2777	0.035
H(43A)	0.3553	0.2859	0.3122	0.037
H(43B)	0.3123	0.3319	0.2902	0.037
H(93A)	0.3035	0.4065	0.3287	0.036
H(93B)	0.2836	0.3338	0.3373	0.036
H(15E)	0.3011(13)	0.3514(8)	0.38658(11)	0.041
H(15F)	0.3312(4)	0.4320(17)	0.38431(9)	0.041
H(15C)	0.3744	0.3727	0.4285	0.039
H(15D)	0.3986	0.3153	0.4095	0.039

Table S25. Continued

atom	x	y	z	U(eq)
H(94A)	0.4987	0.3338	0.4233	0.039
H(94B)	0.4787	0.3812	0.4479	0.039
H(14M)	0.5330	0.4693	0.4328	0.038
H(14E)	0.5760	0.4065	0.4387	0.038
H(15G)	0.6386	0.4242	0.4038	0.037
H(15H)	0.6111	0.4974	0.3993	0.037
H(14C)	0.5817	0.4769	0.3493	0.032
H(14D)	0.6507	0.4609	0.3569	0.032
H(2BD)	0.6105	0.3797	−0.0075	0.026
H(2BH)	0.6648	0.3684	−0.0498	0.029
H(2BC)	0.8565	0.2294	−0.0642	0.027
H(2BA)	0.9306	0.1668	−0.0302	0.027
H(2BB)	1.0081	0.1974	0.0832	0.036
H(2BE)	0.9822	0.2776	0.1198	0.041
H(2BF)	0.7727	0.3649	0.1376	0.031
H(2BG)	0.6733	0.3583	0.1079	0.028
H(25A)	0.8223	0.4198	−0.0483	0.050
H(25B)	0.8480	0.4383	−0.0776	0.050
H(25C)	0.8724	0.3749	−0.0589	0.050
H(26A)	0.7983	0.4011	−0.1223	0.043
H(28A)	0.7117	0.3014	−0.1729	0.099
H(28B)	0.7532	0.3653	−0.1698	0.099
H(28C)	0.6852	0.3724	−0.1666	0.099
H(29A)	0.6756	0.2582	−0.1279	0.053
H(21I)	0.7112	0.1903	−0.0607	0.071
H(21J)	0.6593	0.1946	−0.0879	0.071
H(21K)	0.6580	0.2410	−0.0599	0.071
H(21A)	1.0141	0.2474	0.0015	0.048
H(21B)	1.0816	0.2262	0.0033	0.048
H(21C)	1.0579	0.2550	0.0316	0.048
H(21D)	1.1138	0.1203	0.0204	0.029
H(21F)	1.1458	0.0091	0.0273	0.060
H(21G)	1.0960	−0.0470	0.0240	0.060
H(21H)	1.1224	−0.0196	0.0557	0.060

Table S25. Continued

atom	x	y	z	U(eq)
H(21E)	0.9986	−0.0146	0.0417	0.039
H(22A)	0.8732	0.0755	0.0273	0.061
H(22B)	0.8974	0.0758	0.0616	0.061
H(22C)	0.9006	0.0095	0.0430	0.061
H(22F)	0.9257	0.4447	0.0952	0.061
H(22G)	0.9154	0.5104	0.1131	0.061
H(22H)	0.8605	0.4663	0.0992	0.061
H(22D)	0.9366	0.5019	0.1634	0.050
H(22L)	0.9245	0.4462	0.2324	0.094
H(22M)	0.9555	0.5029	0.2158	0.094
H(22N)	0.9911	0.4373	0.2268	0.094
H(22E)	0.9187	0.3322	0.2067	0.048
H(22I)	0.8816	0.2364	0.1835	0.066
H(22J)	0.9097	0.2248	0.1542	0.066
H(22K)	0.8417	0.2437	0.1522	0.066
H(23C)	0.6270	0.5193	0.0549	0.046
H(23D)	0.6788	0.4661	0.0556	0.046
H(23E)	0.6557	0.4870	0.0853	0.046
H(23B)	0.5316	0.4803	0.0698	0.029
H(23I)	0.4260	0.4490	0.0584	0.064
H(23J)	0.4342	0.4020	0.0866	0.064
H(23K)	0.4091	0.3722	0.0551	0.064
H(23A)	0.4841	0.2916	0.0499	0.028
H(23F)	0.5514	0.2121	0.0397	0.054
H(23G)	0.6187	0.2242	0.0531	0.054
H(23H)	0.5960	0.2413	0.0195	0.054
H(16C)	1.0204	0.6542	0.0491	0.043
H(16D)	0.9988	0.5789	0.0510	0.043
H(15A)	0.9432	0.6496	0.0778	0.039
H(15B)	0.9221	0.6917	0.0486	0.039
H(41A)	0.8242	0.6605	0.0585	0.037
H(41B)	0.8481	0.6081	0.0836	0.037
H(24O)	0.8030	0.5211	0.0530	0.039
H(24P)	0.7555	0.5730	0.0616	0.039

Table S25. Continued

atom	x	y	z	U(eq)
H(24Q)	0.6933	0.5375	0.0173	0.050
H(24R)	0.7442	0.4911	0.0082	0.050
H(18F)	0.6795	0.5245	−0.0337	0.048
H(18G)	0.6937	0.6007	−0.0256	0.048
H(18I)	0.7096	0.5945	−0.0726	0.061
H(18J)	0.7399	0.5269	−0.0806	0.061
H(24K)	0.9929(6)	0.6485(16)	−0.0388(2)	0.046
H(24L)	1.0422(13)	0.5995(3)	−0.0418(3)	0.046
H(18D)	1.0337	0.5564	0.0050	0.053
H(18E)	1.0559	0.6318	0.0060	0.053
H(1A1)	0.9330	0.5141	−0.0812	0.039
H(1A2)	0.9790	0.5721	−0.0840	0.039
H(27A)	0.8893	0.6102	−0.1046	0.056
H(27B)	0.9053	0.6492	−0.0740	0.056
H(26B)	0.7871	0.6134	−0.1009	0.055
H(26C)	0.7984	0.6514	−0.0700	0.055
H(1B1)	0.9403(11)	0.659(6)	−0.0703(4)	0.061
H(1B2)	0.957(3)	0.599(2)	−0.0859(19)	0.061
H(27C)	0.8619	0.6179	−0.1012	0.056
H(27D)	0.8684	0.5514	−0.0819	0.056
H(26D)	0.7623	0.6613	−0.0610	0.055
H(26E)	0.7735	0.6381	−0.0926	0.055
H(3BH)	−0.0551	0.3747	0.3192	0.034
H(3BG)	0.0029	0.3575	0.2785	0.034
H(3BC)	0.1947	0.2142	0.2705	0.028
H(3BA)	0.2641	0.1503	0.3065	0.029
H(3BD)	0.3268	0.1751	0.4217	0.027
H(3BF)	0.3013	0.2593	0.4568	0.028
H(3BB)	0.0974	0.3736	0.4661	0.027
H(3BE)	−0.0003	0.3707	0.4349	0.029
H(35A)	0.1880	0.4196	0.2517	0.058
H(35B)	0.2107	0.3585	0.2724	0.058
H(35C)	0.1607	0.4066	0.2811	0.058
H(36A)	0.1383	0.3783	0.2078	0.044

Table S25. Continued

atom	x	y	z	U(eq)
H(38A)	0.0582	0.2709	0.1597	0.090
H(38B)	0.0909	0.3411	0.1615	0.090
H(38C)	0.0221	0.3373	0.1636	0.090
H(39A)	0.0159	0.2354	0.2054	0.048
H(31I)	0.0059	0.1708	0.2474	0.081
H(31J)	−0.0072	0.2251	0.2708	0.081
H(31K)	0.0513	0.1813	0.2768	0.081
H(31F)	0.3557	0.2384	0.3649	0.052
H(31G)	0.4164	0.2115	0.3565	0.052
H(31H)	0.4056	0.2113	0.3899	0.052
H(31A)	0.4404	0.0927	0.3642	0.030
H(31C)	0.4564	−0.0203	0.3492	0.052
H(31D)	0.4026	−0.0713	0.3442	0.052
H(31E)	0.4343	−0.0553	0.3767	0.052
H(31B)	0.3049	−0.0359	0.3548	0.031
H(32L)	0.2099	−0.0042	0.3608	0.050
H(32M)	0.1934	0.0605	0.3413	0.050
H(32N)	0.2008	0.0652	0.3762	0.050
H(32E)	0.1818	0.4567	0.4302	0.042
H(32F)	0.2482	0.4395	0.4264	0.042
H(32G)	0.2341	0.5049	0.4437	0.042
H(32H)	0.2611	0.4978	0.4938	0.035
H(32I)	0.2609	0.4412	0.5644	0.062
H(32J)	0.2817	0.5013	0.5459	0.062
H(32K)	0.3247	0.4399	0.5547	0.062
H(32A)	0.2465	0.3291	0.5391	0.033
H(32B)	0.1987	0.2353	0.5169	0.047
H(32C)	0.2367	0.2186	0.4915	0.047
H(32D)	0.1687	0.2374	0.4834	0.047
H(33I)	0.0000	0.4691	0.3665	0.074
H(33J)	−0.0137	0.4967	0.3973	0.074
H(33K)	−0.0513	0.5222	0.3674	0.074
H(33E)	−0.1451	0.4886	0.3814	0.041
H(33F)	−0.2460	0.4569	0.3794	0.072

Table S25. Continued

atom	x	y	z	U(eq)
H(33G)	−0.2406	0.4113	0.4080	0.072
H(33H)	−0.2639	0.3804	0.3765	0.072
H(33A)	−0.1841	0.2950	0.3848	0.031
H(33B)	−0.1153	0.2119	0.3802	0.051
H(33C)	−0.0572	0.2310	0.4022	0.051
H(33D)	−0.0561	0.2302	0.3676	0.051
H(33L)	0.1567	0.6592	0.3876	0.037
H(33M)	0.1715	0.6059	0.4135	0.037
H(34A)	0.1334	0.5206	0.3802	0.039
H(34B)	0.0838	0.5743	0.3845	0.039
H(34C)	0.0357	0.5378	0.3365	0.048
H(34D)	0.0899	0.4920	0.3307	0.048
H(34E)	0.0395	0.5318	0.2852	0.054
H(34F)	0.0499	0.6067	0.2964	0.054
H(34G)	0.0943	0.6147	0.2529	0.067
H(34H)	0.1013	0.5374	0.2465	0.067
H(2A1)	0.2951	0.5903	0.2562	0.055
H(2A2)	0.2774	0.5290	0.2344	0.055
H(2B1)	0.2586	0.5293	0.2428	0.055
H(2B2)	0.3025	0.5852	0.2551	0.055
H(34M)	0.3357	0.6184	0.3002	0.037
H(34N)	0.3944	0.5747	0.3016	0.037
H(34O)	0.3866	0.5492	0.3517	0.043
H(34P)	0.3986	0.6264	0.3466	0.043
H(34Q)	0.3548	0.6527	0.3884	0.037
H(34R)	0.3346	0.5783	0.3942	0.037
H(34S)	0.2704	0.6531	0.4117	0.039
H(34T)	0.2567	0.6872	0.3801	0.039
H(35D)	0.0785	0.6266	0.3788	0.060
H(35E)	0.1018	0.5514	0.3785	0.060
H(35F)	0.0231	0.5774	0.3387	0.053
H(35G)	0.0688	0.6249	0.3257	0.053
H(35H)	0.0164	0.5062	0.2974	0.075
H(35I)	0.0722	0.4614	0.2934	0.075

Table S25. Continued

atom	x	y	z	U(eq)
H(35J)	0.0499	0.5370	0.2557	0.068
H(35K)	0.0609	0.5962	0.2789	0.068
H(35L)	0.1561	0.6414	0.2663	0.046
H(35M)	0.1275	0.6042	0.2370	0.046
H(35N)	0.2118	0.5361	0.2403	0.063
H(35O)	0.2272	0.6129	0.2365	0.063
H(35P)	0.3234	0.5753	0.2585	0.061
H(35Q)	0.3039	0.5050	0.2699	0.061
H(35R)	0.3889	0.5373	0.3015	0.037
H(35S)	0.3613	0.6087	0.3066	0.037
H(35T)	0.399(7)	0.556(2)	0.3501(7)	0.048
H(35U)	0.3617(10)	0.507(7)	0.365(2)	0.048
H(35V)	0.3594	0.6077	0.3898	0.052
H(35W)	0.3412	0.6464	0.3595	0.052
H(36B)	0.2503	0.6904	0.3741	0.039
H(36C)	0.2765	0.6602	0.4056	0.039
H(36D)	0.1929	0.5858	0.4023	0.062
H(36E)	0.1719	0.6617	0.4020	0.062
H(42C)	0.6566	0.9296	0.3574	0.022
H(42D)	0.7084	0.8990	0.3809	0.022
H(42K)	0.6688	0.8320	0.3344	0.069
H(42L)	0.7376	0.8276	0.3478	0.069
H(42M)	0.7581	0.8755	0.3068	0.059
H(42N)	0.6894	0.8886	0.2956	0.059
H(43J)	0.7633	0.9852	0.3146	0.052
H(43K)	0.6934	0.9915	0.3140	0.052
H(42A)	0.5221	0.6410	0.0769	0.068
H(42B)	0.4603	0.6706	0.0615	0.068
H(42E)	0.5013	0.7187	0.0245	0.059
H(42F)	0.5566	0.7236	0.0503	0.059
H(42G)	0.5995	0.6293	0.0348	0.051
H(42H)	0.5703	0.6599	0.0037	0.051
H(42I)	0.4923	0.5896	−0.0003	0.045
H(42J)	0.5395	0.5426	0.0190	0.045

Table S25. Continued

atom	x	y	z	U(eq)
H(43M)	0.2091	0.8635	0.2382	0.071
H(43G)	0.1396	0.8682	0.2263	0.071
H(43E)	0.1980	0.7647	0.2552	0.078
H(43F)	0.1283	0.7720	0.2459	0.078
H(55A)	0.2074	0.7061	0.2190	0.076
H(55B)	0.1382	0.6933	0.2177	0.076
H(43H)	0.1152	0.7644	0.1836	0.060
H(43I)	0.1749	0.7334	0.1750	0.060
H(61A)	0.8984	0.6539	0.3632	0.042
H(61B)	0.8381	0.6143	0.3526	0.042
H(62A)	0.8137	0.6109	0.3990	0.055
H(62B)	0.8837	0.6179	0.4087	0.055
H(63A)	0.8027	0.7109	0.4164	0.060
H(63B)	0.8728	0.7199	0.4237	0.060
H(64A)	0.8085	0.7864	0.3841	0.039
H(64B)	0.8773	0.7735	0.3839	0.039
H(24M)	0.3474	0.4768	0.4557	0.037
H(24N)	0.3905	0.4984	0.4329	0.037
H(24I)	0.3306	0.5877	0.4554	0.041
H(24J)	0.3957	0.6051	0.4488	0.041
H(24C)	0.4237	0.6171	0.4973	0.048
H(24D)	0.3612	0.5901	0.5040	0.048
H(24A)	0.4590	0.5188	0.5148	0.046
H(24B)	0.3946	0.4858	0.5107	0.046
H(57A)	0.8672	−0.0629	0.3458	0.073
H(57B)	0.9378	−0.0625	0.3551	0.073
H(58A)	0.9378	−0.0071	0.3104	0.063
H(58B)	0.8708	0.0167	0.3092	0.063
H(59A)	0.9018	0.1151	0.3277	0.070
H(59B)	0.9691	0.0912	0.3289	0.070
H(60A)	0.9757	0.0552	0.3796	0.082
H(60B)	0.9223	0.1066	0.3808	0.082
H(57C)	0.9528	−0.0321	0.3141	0.073
H(57D)	0.8862	−0.0076	0.3065	0.073

Table S25. Continued

atom	x	y	z	U(eq)
H(58C)	0.9446	−0.0312	0.3607	0.063
H(58D)	0.8787	−0.0026	0.3532	0.063
H(59C)	0.9129	0.0959	0.3705	0.070
H(59D)	0.9797	0.0698	0.3737	0.070
H(60C)	0.9200	0.1440	0.3284	0.082
H(60D)	0.9891	0.1300	0.3349	0.082
H(311)	0.7707	0.1067	−0.0385	0.050
H(312)	0.7454	0.1146	−0.0165	0.050

[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.

Supporting Information

Supporting Information Figure Captions

Figure S1. ORTEP diagram of the second unit in the cell of [K(18-C-6)][Fe(TMP)$(CN)_2$] displaying the atom labeling scheme. Thermal ellipsoids of all atoms are contoured at the 50% probability level. Hydrogen atoms have been omitted for clarity.

Figure S2. ORTEP diagram of the third unit in [K(18-C-6)][Fe(TMP)$(CN)_2$] displaying the atom labeling scheme. Thermal ellipsoids of all atoms are contoured at the 50% probability level. Hydrogen atoms have been omitted for clarity.

Figure S3. ORTEP diagram of the ordered 18-crown-6 ring in the first [K(18-C-6)][Fe-(TMP)$(CN)_2$] unit displaying the atom labeling scheme. 50% probablity countours are shown.

Figure S4. ORTEP diagram of the disordered 18-crown-6 ring in the second [K(18-C-6)]-[Fe(TMP)$(CN)_2$] unit displaying the atom labeling scheme. 50% probablity countours are shown.

Figure S5. ORTEP diagram of the disordered 18-crown-6 ring in the third [K(18-C-6)][Fe-(TMP)$(CN)_2$] unit displaying the atom labeling scheme. 50% probablity countours are shown.

Figure S6. Formal diagrams of the porphyrin cores for all entities (1, 2, 3) of [K(18-C-6)][Fe(TMP)$(CN)_2$]. Averaged values of the chemically unique bond distances (in 0.01 Å) and angles (in degrees) are shown. Positive values of displacements are toward the cyanide ligand that is not also coordinated to the [K(18-crown-6)] cation.

Figure S7. EPR spectra for [Fe(TPP)(CN)(Py)] in the solid state and in a frozen CH_2Cl_2 solution.

Figure S8. EPR spectra for [Fe(TPP)(CN)(1-MeIm)] in the solid state and in a frozen CH_2Cl_2 solution.

Figure S9. EPR spectra for [Fe(TMP)(CN)(1-MeIm)] in the solid state and in a frozen CH_2Cl_2 solution.

Figure S10. Mössbauer spectra for $[K((CH_3)_2CO)_2][Fe(TPP)(CN)_2]$ over the temperature range of 298 – 15 K.

Figure S11. Mössbauer spectra for $[K(18\text{-}C\text{-}6)][Fe(TMP)(CN)_2]$ over the temperature range of 298 – 15 K.

Figure S12. Mössbauer spectra for [Fe(TMP)(CN)(1-MeIm)] over the temperature range of 298 – 15 K.

Figure S13. Mössbauer spectra for [Fe(TPP)(CN)(1-MeIm)] over the temperature range of 298 – 15 K.

Figure S14. Mössbauer spectra for [Fe(TPP)(CN)(Py)] over the temperature range of 298 – 15 K.

Figure S15. ΔE_Q predictions.