Supporting Information for

Proton-Mediated Electron Configuration Change in High-Spin Iron(II) Porphyrinates.

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Synthetic Procedures

Synthesis of [K(222)][Fe(OEP)(2-MeIm$^-$)]. [Fe(OEP)]$_2$O (38 mg, 0.03 mmol) was dissolved in 10 mL of benzene, and 1 mL of ethanethiol was added by syringe. The mixture was stirred at room temperature for 3 days, then the solvent was removed under vacuum, and the solid was dried for another hour. A suspension of excess K(2-MeIm$^-$) (28 mg, 0.23 mmol) and Kryptofix 222 (70 mg, 0.19 mmol) in 15 mL of chlorobenzene was added to solid Fe(II)(OEP) by cannula. The reaction mixture was then stirred for 1/2 h. Then it was cannula filtered to another Schlenk flask. X-Ray quality crystals were obtained in 8 mm × 250 mm sealed glass tubes by liquid diffusion using hexanes as nonsolvent after three weeks.

Synthesis of [K(222)][Fe(TPP)(2-MeIm$^-$)]. [Fe(TPP)]$_2$O (40 mg, 0.03 mmol) was dissolved in 10 mL of benzene, and 1 mL of ethanethiol was added by syringe. The mixture was stirred at room temperature for 3 days, then the solvent was removed under vacuum, the solid was dried for another hour and dissolved in 10 mL of toluene. A suspension of excess K(2-MeIm$^-$) (24 mg, 0.20 mmol) and Kryptofix 222 (49 mg, 0.13 mmol) in 10 mL of toluene was added to the above solution, the resulting precipitates were cannula filtered, dried under vacuum for 1/2 h, then 10 mL of chlorobenzene was added to the precipitates. The resulting solution was cannula filtered to another Schlenk flask. X-Ray quality crystals were obtained in 8 mm × 250 mm sealed glass tubes by liquid diffusion using hexanes as nonsolvent after three weeks.

Microcrystalline solids for Mössbauer measurements were obtained by liquid diffusion in Schlenk tubes using hexanes as the nonsolvent. The solids were isolated in an inert-atmosphere box and immobilized in Apiezon M grease.

Captions for Supporting Information Figures

Figure S1. ORTEP diagram of K(222)[Fe(OEP)(2-MeIm$^-$)] showing the anion and cation. All atoms are contoured at the 50% level. For clarity, no hydrogen atoms have been shown.

Figure S2. ORTEP diagram of K(222)[Fe(TPP)(2-MeIm$^-$)] showing the anion and cation. All atoms are contoured at the 50% level. For clarity, no hydrogen atoms have been shown.

Figure S3. Comparison of the experimental and calculated high field spectra for K(222)[Fe-(OEP)(2-MeIm$^-$)]. Fits were obtained from the simultaneous fit to the 1, 5, and 9 T specta.

Figure S4. Comparison of the experimental and calculated high field spectra forr K(222)[Fe-(TPP)(2-MeIm$^-$).] Fits were obtained from the simultaneous fit to the 1, 5, and 9 T specta.
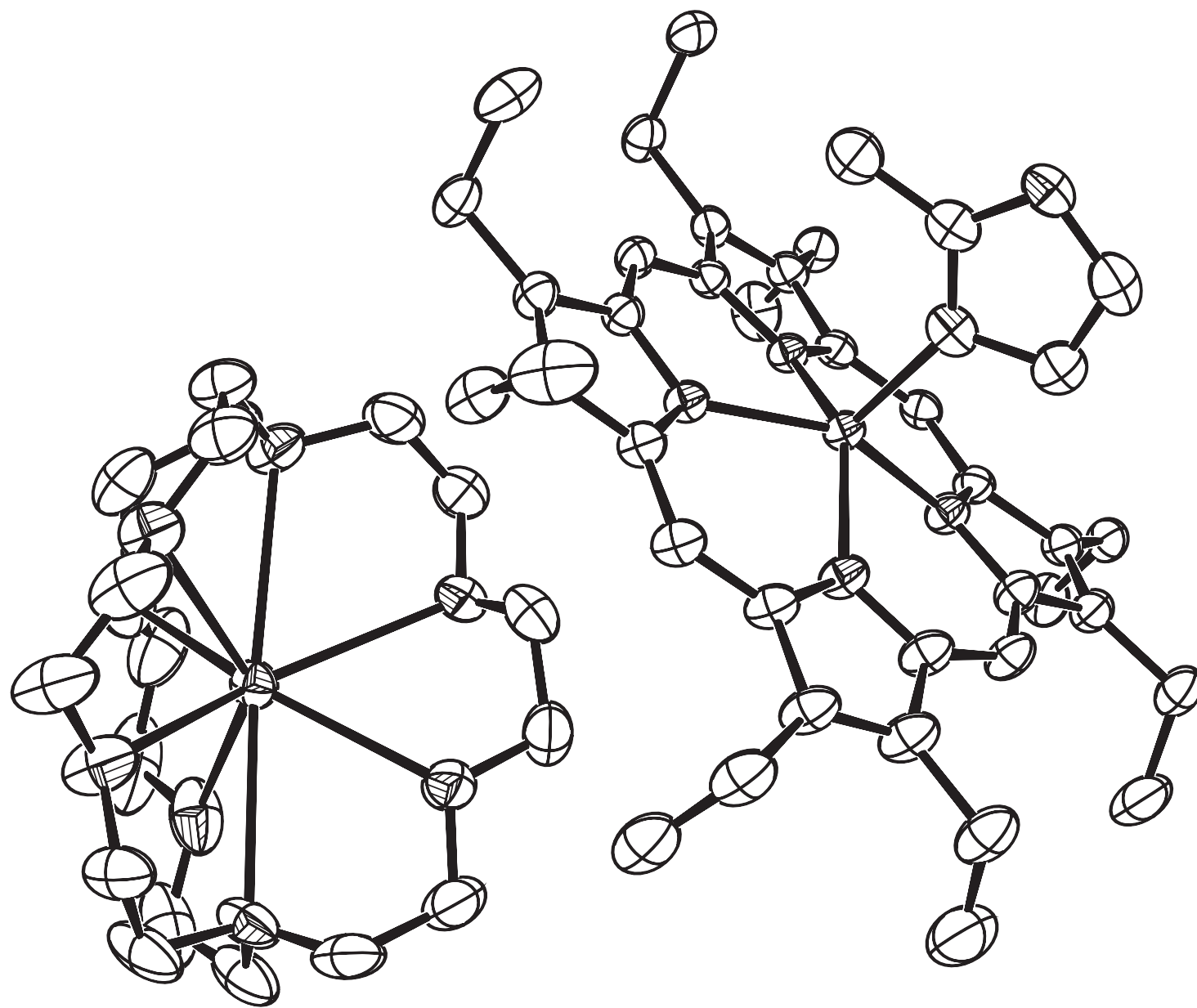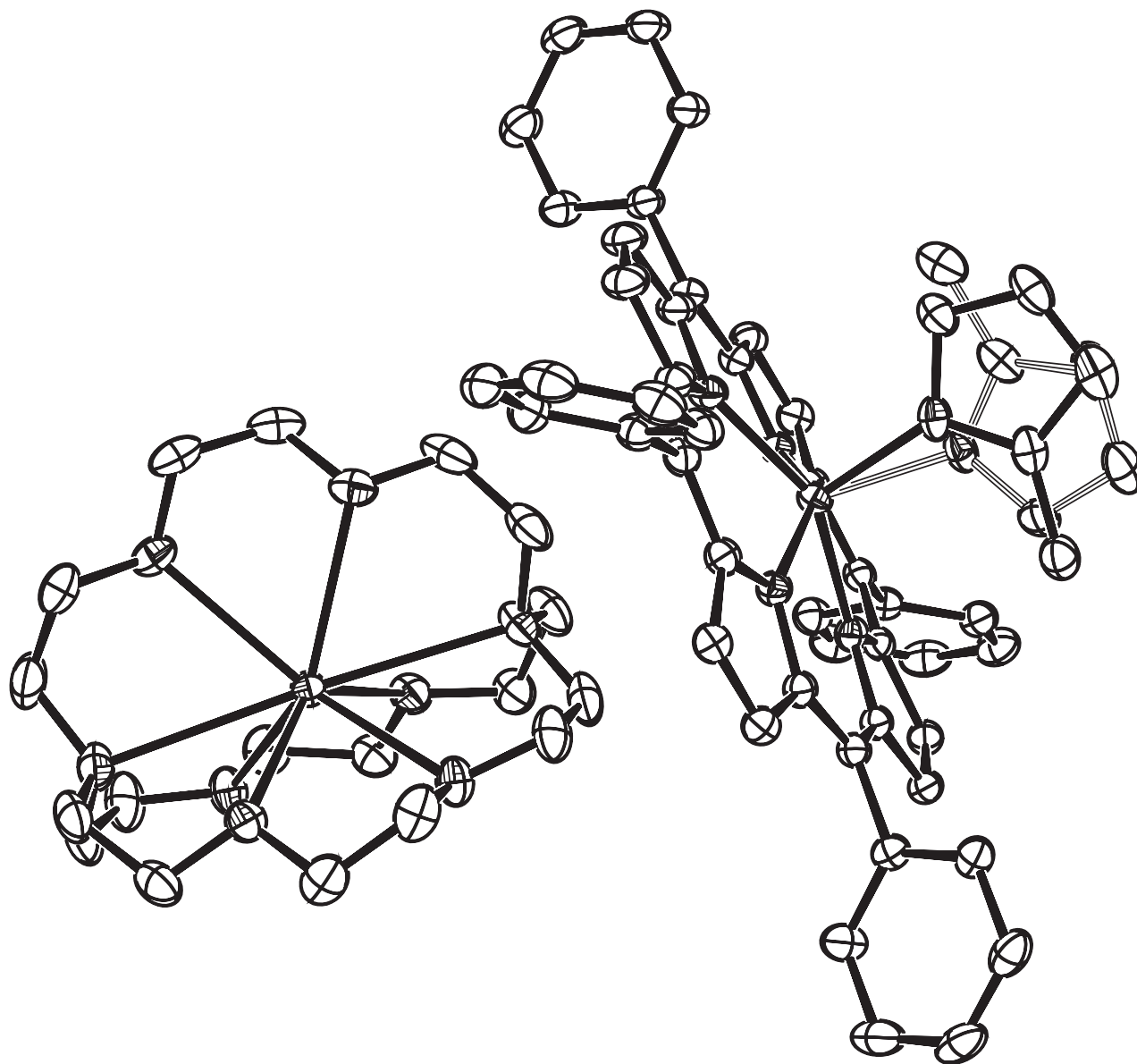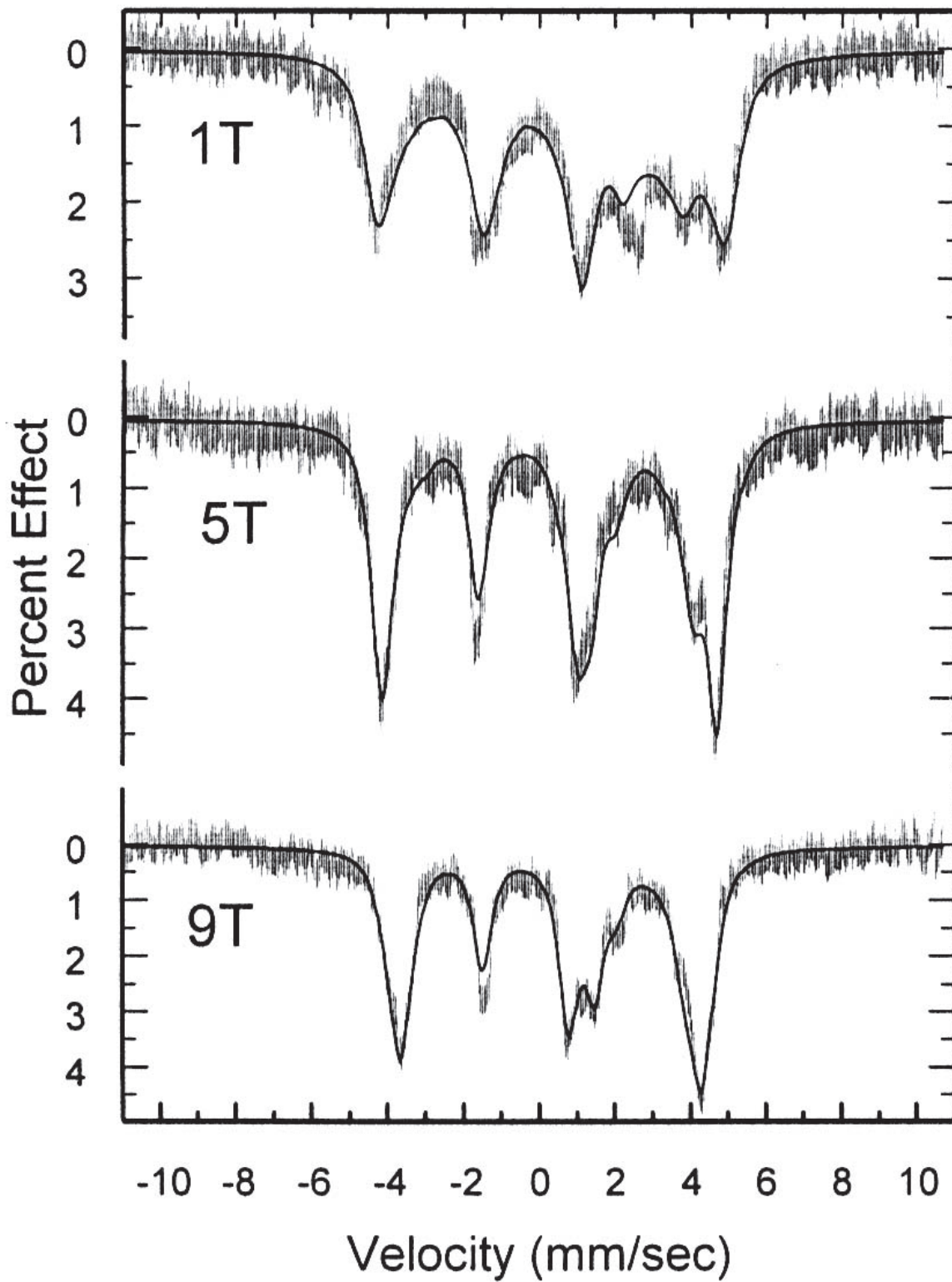
Figure S3
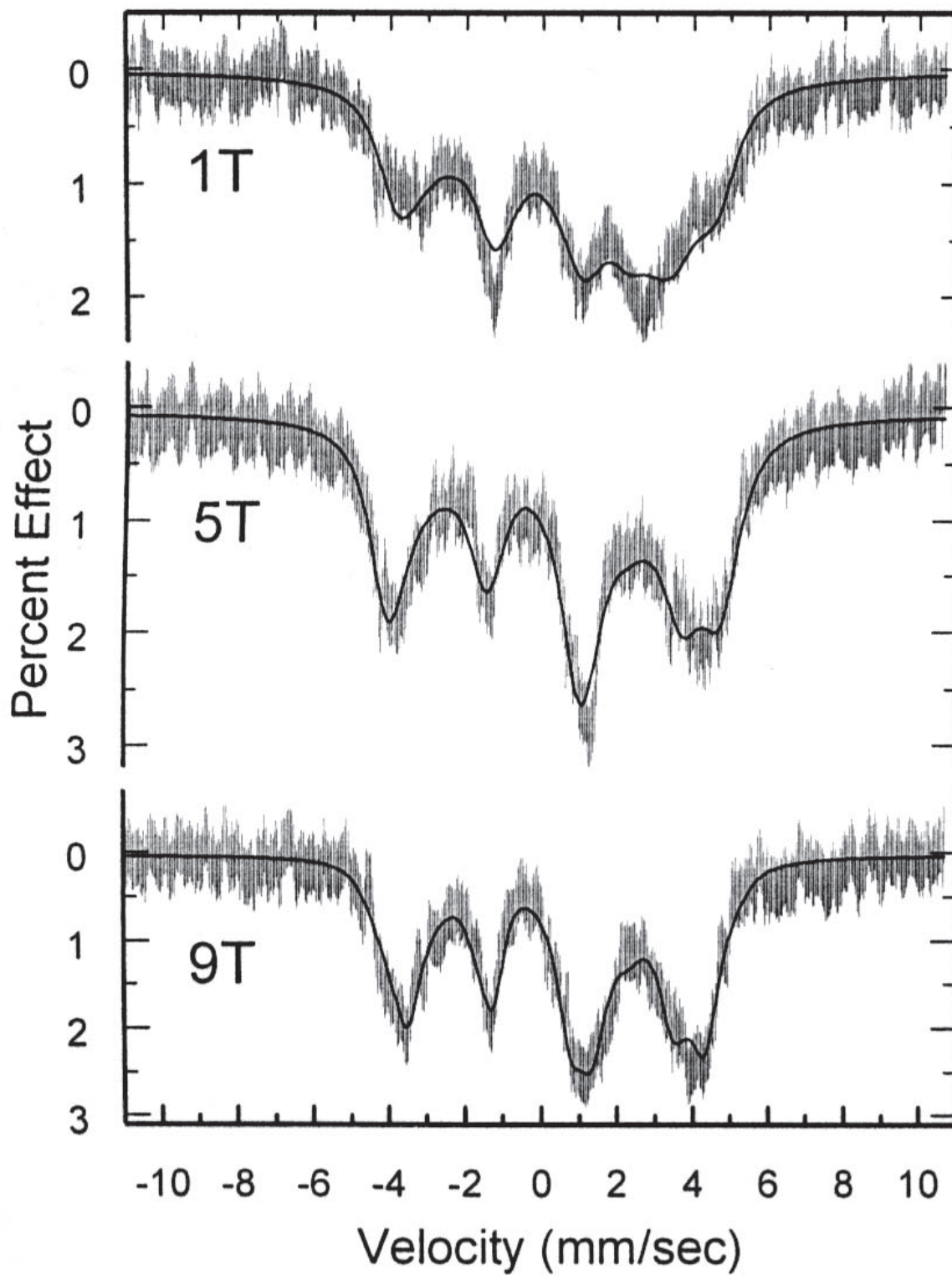
Table S1. Variable Temperature Mössbauer Parameters for Two Imidazolate-Ligated Iron(II) Porphyrinates.

Complex	ΔE_Q, mm/s	δ_{Fe}, mm/s	T,K
[K⊂222][Fe(OEP)(2-MeIm$^-$)]	3.23	0.86	298
	3.57	0.85	200
	3.75	0.99	100
	3.75	1.00	15
	3.71	1.00	4.2
[K⊂222][Fe(TPP)(2-MeIm$^-$)]	3.17	0.85	298
	3.32	0.90	250
	3.42	0.93	200
	3.53	0.96	150
	3.62	0.98	100
	3.66	0.99	50
	3.63	0.99	15
	3.60	1.00	4.2

Table S2. Mössbauer Fit Parameters for Two Imidazolate-Ligated Iron(II) Porphyrinates in 1, 5, and 9 T magnetic field and 4.2 K

Complex	[K⊂222][Fe(OEP)(2-MeIm$^-$)]	[K⊂222][Fe(TPP)(2-MeIm$^-$)]
ΔE_Q, mm/s[a]	3.71	3.60
δ_{Fe}, mm/s[a]	1.00	1.00
η	0.25	0.24
D, cm^{-1}	−4.09	4.42
E, cm^{-1}	−1.34	1.05
E/D	0.33	0.24
g [a]	2.0	2.0
$A^*_{xx}/g^*_N\beta_N$, T	−15.5	−7.6
$A^*_{yy}/g^*_N\beta_N$, T	−0.4	−14.8
$A^*_{zz}/g^*_N\beta_N$, T	−14.5	−25.9
α^b	80	−12
β^b	76	92
γ^b	−37	−71
χ^2	0.631	0.339
Γ(1T)	0.80	1.20
Γ(5T)	0.63	1.18
Γ(9T)	0.60	0.84

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

Table S3. Complete Crystallographic Details for [K⊂222][Fe(OEP)(2-MeIm$^-$)]

formula	$C_{58}H_{85}FeKN_8O_6$
FW, amu	1085.29
a, Å	12.9232(1)
b, Å	19.6316(2)
c, Å	22.5922(3)
β, deg	94.371(1)
V, Å^3	5715.04(11)
space group	P2(1)/n
Z	4
D_c, g/cm^3	1.261
F(000)	2328
μ, mm^{-1}	0.393
crystal dimensions, mm	$0.27 \times 0.20 \times 0.07$
radiation	MoKα, $\bar{\lambda} = 0.71073$ Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.38–27.50
index range	$-16 \le$ h ≤ 16
	$-25 \le$ k ≤ 25
	$-29 \le$ l ≤ 29
total data collected	102317
absorption correction	Semi-empirical from equivalents
relative transmission coefficients (I)	0.9723 and 0.9003
unique data	13121 ($R_{int} = 0.038$)
unique observed data [I $> 2\sigma$(I)]	10561
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	13121/0/676
goodness-of-fit (pased on F^2)	1.020
final R indices [I $> 2\sigma$(I)]	$R_1 = 0.0605$, $wR_2 = 0.1599$
final R indices (all data)	$R_1 = 0.0760$, $wR_2 = 0.1747$

Table S4. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $[\text{K}{\subset}222][\text{Fe(OEP)(2-MeIm}^-)]^a$

atom	x	y	z	$U(\text{eq})$
Fe(1)	0.37586(3)	0.25829(2)	0.27810(2)	0.0219(1)
N(1)	0.46128(16)	0.33995(11)	0.24593(9)	0.0244(4)
N(2)	0.24760(15)	0.32566(11)	0.27042(9)	0.0227(4)
N(3)	0.29918(16)	0.21052(11)	0.34625(10)	0.0257(4)
N(4)	0.51495(16)	0.22954(12)	0.32709(10)	0.0278(5)
C(a1)	0.56681(19)	0.34264(14)	0.24397(12)	0.0279(5)
C(a2)	0.42141(19)	0.38943(13)	0.20771(11)	0.0249(5)
C(a3)	0.23647(19)	0.37913(13)	0.23155(11)	0.0234(5)
C(a4)	0.15239(18)	0.31632(13)	0.29206(11)	0.0233(5)
C(a5)	0.19647(19)	0.21523(13)	0.35702(11)	0.0244(5)
C(a6)	0.3386(2)	0.15693(14)	0.37991(12)	0.0287(5)
C(a7)	0.5257(2)	0.17542(15)	0.36536(13)	0.0325(6)
C(a8)	0.6127(2)	0.25268(15)	0.31979(12)	0.0297(6)
C(b1)	0.5948(2)	0.39333(15)	0.20131(12)	0.0308(6)
C(b2)	0.5045(2)	0.42247(14)	0.17856(12)	0.0285(5)
C(b3)	0.13024(19)	0.40436(13)	0.22789(11)	0.0248(5)
C(b4)	0.07834(19)	0.36569(13)	0.26613(11)	0.0252(5)
C(b5)	0.16954(19)	0.16217(14)	0.39798(11)	0.0267(5)
C(b6)	0.2575(2)	0.12494(14)	0.41122(12)	0.0292(5)
C(b7)	0.6348(2)	0.16349(17)	0.38278(14)	0.0380(7)
C(b8)	0.6884(2)	0.21285(17)	0.35595(13)	0.0364(7)
C(m1)	0.31660(19)	0.40713(13)	0.20118(11)	0.0250(5)
C(m2)	0.12930(18)	0.26518(13)	0.33193(11)	0.0238(5)
C(m3)	0.4437(2)	0.13967(15)	0.38725(13)	0.0323(6)
C(m4)	0.6365(2)	0.30404(15)	0.28005(12)	0.0302(6)
C(11)	0.7035(2)	0.40709(19)	0.18467(15)	0.0435(8)
C(12)	0.7480(3)	0.3447(3)	0.15270(18)	0.0659(12)
C(21)	0.4889(2)	0.47458(15)	0.13024(13)	0.0339(6)
C(22)	0.4673(3)	0.44125(19)	0.06962(14)	0.0484(8)
C(31)	0.0865(2)	0.45903(14)	0.18680(13)	0.0313(6)
C(32)	0.0499(3)	0.42998(18)	0.12587(15)	0.0460(8)
C(41)	−0.03308(19)	0.37315(14)	0.28007(13)	0.0299(6)
C(42)	−0.0476(2)	0.42286(17)	0.33003(16)	0.0420(7)
C(51)	0.0657(2)	0.15378(14)	0.42328(12)	0.0295(5)

Table S4. Continued

atom	x	y	z	$U(\text{eq})$
C(52)	0.0496(2)	0.20257(16)	0.47405(14)	0.0391(7)
C(61)	0.2727(2)	0.06503(16)	0.45217(14)	0.0368(6)
C(62)	0.3118(4)	0.0850(2)	0.51402(17)	0.0621(11)
C(71)	0.6770(2)	0.10680(19)	0.42312(16)	0.0472(8)
C(72)	0.6821(4)	0.1250(2)	0.48672(19)	0.0662(11)
C(81)	0.8010(2)	0.22872(19)	0.36436(16)	0.0450(8)
C(82)	0.8224(2)	0.2880(2)	0.40519(18)	0.0557(10)
N(5)	0.36179(17)	0.18617(13)	0.21172(11)	0.0327(5)
C(1)	0.3442(2)	0.18608(16)	0.15243(13)	0.0358(6)
N(6)	0.33514(18)	0.12486(13)	0.12715(11)	0.0350(5)
C(2)	0.3503(2)	0.08088(17)	0.17530(16)	0.0437(7)
C(3)	0.3659(2)	0.11608(17)	0.22629(15)	0.0390(7)
C(4)	0.3376(3)	0.24972(18)	0.11788(16)	0.0479(8)
K(1)	0.64350(4)	0.59507(3)	0.40075(3)	0.0316(1)
O(1c)	0.47779(17)	0.49972(12)	0.38352(10)	0.0410(5)
O(2c)	0.67350(17)	0.45916(12)	0.43852(10)	0.0415(5)
O(3c)	0.71339(17)	0.62925(13)	0.28883(11)	0.0469(6)
O(4c)	0.84829(17)	0.63373(17)	0.39341(12)	0.0617(8)
O(5c)	0.5306(2)	0.71748(14)	0.39501(15)	0.0634(7)
O(6c)	0.6100(2)	0.65739(13)	0.50426(12)	0.0602(7)
N(1c)	0.4870(2)	0.61507(15)	0.29865(12)	0.0426(6)
N(2c)	0.7923(2)	0.56574(18)	0.50205(11)	0.0482(7)
C(1c)	0.4282(3)	0.5502(2)	0.28836(16)	0.0521(9)
C(2c)	0.3939(3)	0.5187(2)	0.34169(17)	0.0524(9)
C(3c)	0.5258(3)	0.43800(19)	0.37204(15)	0.0451(8)
C(4c)	0.5881(3)	0.41517(18)	0.42657(18)	0.0499(8)
C(5c)	0.7227(3)	0.4479(2)	0.49652(16)	0.0536(9)
C(6c)	0.8149(3)	0.4929(2)	0.50575(16)	0.0562(10)
C(7c)	0.5413(3)	0.6291(2)	0.24544(15)	0.0469(8)
C(8c)	0.6467(3)	0.5965(2)	0.24460(16)	0.0542(9)
C(9c)	0.8199(3)	0.6096(3)	0.2889(2)	0.0681(12)
C(10c)	0.8817(3)	0.6451(3)	0.33469(18)	0.0719(14)
C(11c)	0.9226(3)	0.6028(2)	0.43249(15)	0.0545(10)
C(12c)	0.8873(3)	0.6045(3)	0.49383(17)	0.0711(14)

Table S4. Continued

atom	x	y	z	U(eq)
C(13c)	0.4179(3)	0.6704(2)	0.31093(17)	0.0524(9)
C(14c)	0.4718(3)	0.7296(2)	0.3366(2)	0.0605(10)
C(15c)	0.4763(4)	0.7174(2)	0.4422(2)	0.0755(13)
C(16c)	0.5467(5)	0.7205(2)	0.4978(2)	0.093(2)
C(17c)	0.6916(4)	0.6576(2)	0.54984(19)	0.0768(15)
C(18c)	0.7432(3)	0.5891(3)	0.55545(15)	0.0647(13)

[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 S5. Bond Lengths for [K⊂222][Fe(OEP)(2-MeIm⁻)]^a

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	2.060(2)	C(81)–H(81a)	0.9900
Fe(1)–N(1)	2.107(2)	C(81)–H(81b)	0.9900
Fe(1)–N(3)	2.113(2)	C(82)–H(82a)	0.9800
Fe(1)–N(4)	2.115(2)	C(82)–H(82b)	0.9800
Fe(1)–N(2)	2.117(2)	C(82)–H(82c)	0.9800
N(1)–C(a1)	1.369(3)	N(5)–C(1)	1.342(4)
N(1)–C(a2)	1.374(3)	N(5)–C(3)	1.415(4)
N(2)–C(a3)	1.369(3)	C(1)–N(6)	1.332(4)
N(2)–C(a4)	1.370(3)	C(1)–C(4)	1.472(5)
N(3)–C(a5)	1.371(3)	N(6)–C(2)	1.391(4)
N(3)–C(a6)	1.373(3)	C(2)–C(3)	1.345(5)
N(4)–C(a8)	1.364(3)	C(2)–H(2)	0.9500
N(4)–C(a7)	1.370(4)	C(3)–H(3)	0.9500
C(a1)–C(m4)	1.392(4)	C(4)–H(4a)	0.9800
C(a1)–C(b1)	1.450(4)	C(4)–H(4b)	0.9800
C(a2)–C(m1)	1.395(3)	C(4)–H(4c)	0.9800
C(a2)–C(b2)	1.455(4)	K(1)–O(6c)	2.703(3)
C(a3)–C(m1)	1.398(4)	K(1)–O(4c)	2.770(2)
C(a3)–C(b3)	1.456(3)	K(1)–O(5c)	2.809(3)
C(a4)–C(m2)	1.396(4)	K(1)–O(2c)	2.819(2)
C(a4)–C(b4)	1.454(3)	K(1)–O(3c)	2.830(2)
C(a5)–C(m2)	1.401(3)	K(1)–O(1c)	2.848(2)
C(a5)–C(b5)	1.453(4)	K(1)–N(2c)	2.932(3)
C(a6)–C(m3)	1.397(4)	K(1)–N(1c)	2.976(3)
C(a6)–C(b6)	1.452(4)	O(1c)–C(3c)	1.394(4)
C(a7)–C(m3)	1.393(4)	O(1c)–C(2c)	1.432(4)
C(a7)–C(b7)	1.454(4)	O(2c)–C(4c)	1.412(4)
C(a8)–C(m4)	1.400(4)	O(2c)–C(5c)	1.429(4)
C(a8)–C(b8)	1.454(4)	O(3c)–C(8c)	1.422(5)
C(b1)–C(b2)	1.364(4)	O(3c)–C(9c)	1.429(4)
C(b1)–C(11)	1.507(4)	O(4c)–C(11c)	1.394(4)
C(b2)–C(21)	1.498(4)	O(4c)–C(10c)	1.443(4)
C(b3)–C(b4)	1.364(4)	O(5c)–C(15c)	1.321(5)
C(b3)–C(31)	1.501(4)	O(5c)–C(14c)	1.490(5)

bond	length (Å)	bond	length (Å)
C(b4)–C(41)	1.504(3)	O(6c)–C(17c)	1.416(6)
C(b5)–C(b6)	1.365(4)	O(6c)–C(16c)	1.486(6)
C(b5)–C(51)	1.507(3)	N(1c)–C(13c)	1.446(5)
C(b6)–C(61)	1.500(4)	N(1c)–C(7c)	1.464(4)
C(b7)–C(b8)	1.360(4)	N(1c)–C(1c)	1.493(5)
C(b7)–C(71)	1.513(4)	N(2c)–C(6c)	1.461(6)
C(b8)–C(81)	1.487(4)	N(2c)–C(12c)	1.468(4)
C(m1)–H(m1)	0.9500	N(2c)–C(18c)	1.478(5)
C(m2)–H(m2)	0.9500	C(1c)–C(2c)	1.452(5)
C(m3)–H(m3)	0.9500	C(1c)–H(1ca)	0.9900
C(m4)–H(m4)	0.9500	C(1c)–H(1cb)	0.9900
C(11)–C(12)	1.555(6)	C(2c)–H(2ca)	0.9900
C(11)–H(11a)	0.9900	C(2c)–H(2cb)	0.9900
C(11)–H(11b)	0.9900	C(3c)–C(4c)	1.489(5)
C(12)–H(12a)	0.9800	C(3c)–H(3ca)	0.9900
C(12)–H(12b)	0.9800	C(3c)–H(3cb)	0.9900
C(12)–H(12c)	0.9800	C(4c)–H(4ca)	0.9900
C(21)–C(22)	1.524(5)	C(4c)–H(4cb)	0.9900
C(21)–H(21a)	0.9900	C(5c)–C(6c)	1.485(5)
C(21)–H(21b)	0.9900	C(5c)–H(5ca)	0.9900
C(22)–H(22a)	0.9800	C(5c)–H(5cb)	0.9900
C(22)–H(22b)	0.9800	C(6c)–H(6ca)	0.9900
C(22)–H(22c)	0.9800	C(6c)–H(6cb)	0.9900
C(31)–C(32)	1.531(4)	C(7c)–C(8c)	1.507(5)
C(31)–H(31a)	0.9900	C(7c)–H(7ca)	0.9900
C(31)–H(31b)	0.9900	C(7c)–H(7cb)	0.9900
C(32)–H(32a)	0.9800	C(8c)–H(8ca)	0.9900
C(32)–H(32b)	0.9800	C(8c)–H(8cb)	0.9900
C(32)–H(32c)	0.9800	C(9c)–C(10c)	1.438(7)
C(41)–C(42)	1.515(4)	C(9c)–H(9ca)	0.9900
C(41)–H(41a)	0.9900	C(9c)–H(9cb)	0.9900
C(41)–H(41b)	0.9900	C(10c)–H(10a)	0.9900
C(42)–H(42a)	0.9800	C(10c)–H(10b)	0.9900
C(42)–H(42b)	0.9800	C(11c)–C(12c)	1.492(5)

Table S5. Continued

bond	length (Å)	bond	length (Å)
C(42)–H(42c)	0.9800	C(11c)–H(11c)	0.9900
C(51)–C(52)	1.521(4)	C(11c)–H(11d)	0.9900
C(51)–H(51a)	0.9900	C(12c)–H(12d)	0.9900
C(51)–H(51b)	0.9900	C(12c)–H(12e)	0.9900
C(52)–H(52a)	0.9800	C(13c)–C(14c)	1.453(6)
C(52)–H(52b)	0.9800	C(13c)–H(13a)	0.9900
C(52)–H(52c)	0.9800	C(13c)–H(13b)	0.9900
C(61)–C(62)	1.501(5)	C(14c)–H(14a)	0.9900
C(61)–H(61a)	0.9900	C(14c)–H(14b)	0.9900
C(61)–H(61b)	0.9900	C(15c)–C(16c)	1.494(8)
C(62)–H(62a)	0.9800	C(15c)–H(15a)	0.9900
C(62)–H(62b)	0.9800	C(15c)–H(15b)	0.9900
C(62)–H(62c)	0.9800	C(16c)–H(16a)	0.9900
C(71)–C(72)	1.477(6)	C(16c)–H(16b)	0.9900
C(71)–H(71a)	0.9900	C(17c)–C(18c)	1.503(7)
C(71)–H(71b)	0.9900	C(17c)–H(17a)	0.9900
C(72)–H(72a)	0.9800	C(17c)–H(17b)	0.9900
C(72)–H(72b)	0.9800	C(18c)–H(18a)	0.9900
C(72)–H(72c)	0.9800	C(18c)–H(18b)	0.9900
C(81)–C(82)	1.498(6)		

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

Table S6. Bond Angles for [K⊂222][Fe(OEP)(2-MeIm⁻)]^a

angle	degree	angle	degree
N(5)–Fe(1)–N(1)	106.93(9)	N(6)–C(1)–C(4)	122.6(3)
N(5)–Fe(1)–N(3)	101.84(9)	N(5)–C(1)–C(4)	121.8(3)
N(1)–Fe(1)–N(3)	151.19(9)	C(1)–N(6)–C(2)	102.8(2)
N(5)–Fe(1)–N(4)	102.82(9)	C(3)–C(2)–N(6)	110.7(3)
N(1)–Fe(1)–N(4)	86.38(8)	C(3)–C(2)–H(2)	124.6
N(3)–Fe(1)–N(4)	85.83(8)	N(6)–C(2)–H(2)	124.6
N(5)–Fe(1)–N(2)	110.15(9)	C(2)–C(3)–N(5)	107.5(3)
N(1)–Fe(1)–N(2)	85.63(8)	C(2)–C(3)–H(3)	126.3
N(3)–Fe(1)–N(2)	85.94(8)	N(5)–C(3)–H(3)	126.3
N(4)–Fe(1)–N(2)	146.99(9)	C(1)–C(4)–H(4a)	109.5
C(a1)–N(1)–C(a2)	106.2(2)	C(1)–C(4)–H(4b)	109.5
C(a1)–N(1)–Fe(1)	126.15(17)	H(4a)–C(4)–H(4b)	109.5
C(a2)–N(1)–Fe(1)	125.00(16)	C(1)–C(4)–H(4c)	109.5
C(a3)–N(2)–C(a4)	106.1(2)	H(4a)–C(4)–H(4c)	109.5
C(a3)–N(2)–Fe(1)	125.08(16)	H(4b)–C(4)–H(4c)	109.5
C(a4)–N(2)–Fe(1)	127.28(17)	O(6c)–K(1)–O(4c)	98.30(9)
C(a5)–N(3)–C(a6)	106.1(2)	O(6c)–K(1)–O(5c)	62.35(10)
C(a5)–N(3)–Fe(1)	127.86(17)	O(4c)–K(1)–O(5c)	104.94(9)
C(a6)–N(3)–Fe(1)	124.66(17)	O(6c)–K(1)–O(2c)	101.18(8)
C(a8)–N(4)–C(a7)	106.5(2)	O(4c)–K(1)–O(2c)	99.64(8)
C(a8)–N(4)–Fe(1)	127.28(18)	O(5c)–K(1)–O(2c)	151.97(8)
C(a7)–N(4)–Fe(1)	125.34(18)	O(6c)–K(1)–O(3c)	138.48(8)
N(1)–C(a1)–C(m4)	124.2(2)	O(4c)–K(1)–O(3c)	60.67(7)
N(1)–C(a1)–C(b1)	110.3(2)	O(5c)–K(1)–O(3c)	87.47(8)
C(m4)–C(a1)–C(b1)	125.4(2)	O(2c)–K(1)–O(3c)	116.68(7)
N(1)–C(a2)–C(m1)	123.9(2)	O(6c)–K(1)–O(1c)	104.33(8)
N(1)–C(a2)–C(b2)	110.2(2)	O(4c)–K(1)–O(1c)	152.07(9)
C(m1)–C(a2)–C(b2)	125.8(2)	O(5c)–K(1)–O(1c)	100.00(8)
N(2)–C(a3)–C(m1)	124.8(2)	O(2c)–K(1)–O(1c)	60.27(6)
N(2)–C(a3)–C(b3)	110.5(2)	O(3c)–K(1)–O(1c)	108.76(7)
C(m1)–C(a3)–C(b3)	124.7(2)	O(6c)–K(1)–N(2c)	63.40(9)
N(2)–C(a4)–C(m2)	124.6(2)	O(4c)–K(1)–N(2c)	61.82(7)
N(2)–C(a4)–C(b4)	110.4(2)	O(5c)–K(1)–N(2c)	120.76(10)
C(m2)–C(a4)–C(b4)	125.0(2)	O(2c)–K(1)–N(2c)	60.72(8)

angle	degree	angle	degree
N(3)–C(a5)–C(m2)	123.7(2)	O(3c)–K(1)–N(2c)	120.60(7)
N(3)–C(a5)–C(b5)	110.3(2)	O(1c)–K(1)–N(2c)	114.78(8)
C(m2)–C(a5)–C(b5)	126.0(2)	O(6c)–K(1)–N(1c)	117.83(9)
N(3)–C(a6)–C(m3)	124.6(2)	O(4c)–K(1)–N(1c)	120.90(7)
N(3)–C(a6)–C(b6)	110.5(2)	O(5c)–K(1)–N(1c)	62.06(9)
C(m3)–C(a6)–C(b6)	124.7(2)	O(2c)–K(1)–N(1c)	115.42(8)
N(4)–C(a7)–C(m3)	124.9(2)	O(3c)–K(1)–N(1c)	61.34(7)
N(4)–C(a7)–C(b7)	110.2(2)	O(1c)–K(1)–N(1c)	61.40(7)
C(m3)–C(a7)–C(b7)	124.8(3)	N(2c)–K(1)–N(1c)	176.04(9)
N(4)–C(a8)–C(m4)	124.7(2)	C(3c)–O(1c)–C(2c)	115.4(3)
N(4)–C(a8)–C(b8)	110.0(2)	C(3c)–O(1c)–K(1)	104.85(17)
C(m4)–C(a8)–C(b8)	125.2(2)	C(2c)–O(1c)–K(1)	116.24(19)
C(b2)–C(b1)–C(a1)	106.8(2)	C(4c)–O(2c)–C(5c)	111.6(3)
C(b2)–C(b1)–C(11)	128.2(3)	C(4c)–O(2c)–K(1)	115.70(19)
C(a1)–C(b1)–C(11)	125.0(2)	C(5c)–O(2c)–K(1)	117.7(2)
C(b1)–C(b2)–C(a2)	106.4(2)	C(8c)–O(3c)–C(9c)	114.2(3)
C(b1)–C(b2)–C(21)	128.7(2)	C(8c)–O(3c)–K(1)	107.64(19)
C(a2)–C(b2)–C(21)	124.8(2)	C(9c)–O(3c)–K(1)	107.9(2)
C(b4)–C(b3)–C(a3)	106.4(2)	C(11c)–O(4c)–C(10c)	114.2(3)
C(b4)–C(b3)–C(31)	127.6(2)	C(11c)–O(4c)–K(1)	117.3(2)
C(a3)–C(b3)–C(31)	126.0(2)	C(10c)–O(4c)–K(1)	116.8(2)
C(b3)–C(b4)–C(a4)	106.6(2)	C(15c)–O(5c)–C(14c)	116.6(4)
C(b3)–C(b4)–C(41)	127.1(2)	C(15c)–O(5c)–K(1)	105.6(3)
C(a4)–C(b4)–C(41)	126.3(2)	C(14c)–O(5c)–K(1)	113.9(2)
C(b6)–C(b5)–C(a5)	106.7(2)	C(17c)–O(6c)–C(16c)	116.3(4)
C(b6)–C(b5)–C(51)	127.5(2)	C(17c)–O(6c)–K(1)	118.1(2)
C(a5)–C(b5)–C(51)	125.7(2)	C(16c)–O(6c)–K(1)	114.5(3)
C(b5)–C(b6)–C(a6)	106.4(2)	C(13c)–N(1c)–C(7c)	111.0(3)
C(b5)–C(b6)–C(61)	128.5(2)	C(13c)–N(1c)–C(1c)	110.9(3)
C(a6)–C(b6)–C(61)	125.0(2)	C(7c)–N(1c)–C(1c)	107.6(3)
C(b8)–C(b7)–C(a7)	106.3(2)	C(13c)–N(1c)–K(1)	110.1(2)
C(b8)–C(b7)–C(71)	128.4(3)	C(7c)–N(1c)–K(1)	108.73(18)
C(a7)–C(b7)–C(71)	125.4(3)	C(1c)–N(1c)–K(1)	108.43(19)
C(b7)–C(b8)–C(a8)	106.9(2)	C(6c)–N(2c)–C(12c)	110.4(3)

angle	degree	angle	degree
C(b7)–C(b8)–C(81)	128.2(3)	C(6c)–N(2c)–C(18c)	110.7(3)
C(a8)–C(b8)–C(81)	124.7(3)	C(12c)–N(2c)–C(18c)	110.9(3)
C(a2)–C(m1)–C(a3)	126.8(2)	C(6c)–N(2c)–K(1)	110.70(19)
C(a2)–C(m1)–H(m1)	116.6	C(12c)–N(2c)–K(1)	107.7(2)
C(a3)–C(m1)–H(m1)	116.6	C(18c)–N(2c)–K(1)	106.2(2)
C(a4)–C(m2)–C(a5)	127.5(2)	C(2c)–C(1c)–N(1c)	114.7(3)
C(a4)–C(m2)–H(m2)	116.3	C(2c)–C(1c)–H(1ca)	108.6
C(a5)–C(m2)–H(m2)	116.3	N(1c)–C(1c)–H(1ca)	108.6
C(a7)–C(m3)–C(a6)	126.5(3)	C(2c)–C(1c)–H(1cb)	108.6
C(a7)–C(m3)–H(m3)	116.8	N(1c)–C(1c)–H(1cb)	108.6
C(a6)–C(m3)–H(m3)	116.8	H(1ca)–C(1c)–H(1cb)	107.6
C(a1)–C(m4)–C(a8)	127.1(2)	O(1c)–C(2c)–C(1c)	113.3(3)
C(a1)–C(m4)–H(m4)	116.5	O(1c)–C(2c)–H(2ca)	108.9
C(a8)–C(m4)–H(m4)	116.5	C(1c)–C(2c)–H(2ca)	108.9
C(b1)–C(11)–C(12)	111.1(3)	O(1c)–C(2c)–H(2cb)	108.9
C(b1)–C(11)–H(11a)	109.4	C(1c)–C(2c)–H(2cb)	108.9
C(12)–C(11)–H(11a)	109.4	H(2ca)–C(2c)–H(2cb)	107.7
C(b1)–C(11)–H(11b)	109.4	O(1c)–C(3c)–C(4c)	109.1(3)
C(12)–C(11)–H(11b)	109.4	O(1c)–C(3c)–H(3ca)	109.9
H(11a)–C(11)–H(11b)	108.0	C(4c)–C(3c)–H(3ca)	109.9
C(11)–C(12)–H(12a)	109.5	O(1c)–C(3c)–H(3cb)	109.9
C(11)–C(12)–H(12b)	109.5	C(4c)–C(3c)–H(3cb)	109.9
H(12a)–C(12)–H(12b)	109.5	H(3ca)–C(3c)–H(3cb)	108.3
C(11)–C(12)–H(12c)	109.5	O(2c)–C(4c)–C(3c)	109.9(3)
H(12a)–C(12)–H(12c)	109.5	O(2c)–C(4c)–H(4ca)	109.7
H(12b)–C(12)–H(12c)	109.5	C(3c)–C(4c)–H(4ca)	109.7
C(b2)–C(21)–C(22)	111.5(3)	O(2c)–C(4c)–H(4cb)	109.7
C(b2)–C(21)–H(21a)	109.3	C(3c)–C(4c)–H(4cb)	109.7
C(22)–C(21)–H(21a)	109.3	H(4ca)–C(4c)–H(4cb)	108.2
C(b2)–C(21)–H(21b)	109.3	O(2c)–C(5c)–C(6c)	109.5(3)
C(22)–C(21)–H(21b)	109.3	O(2c)–C(5c)–H(5ca)	109.8
H(21a)–C(21)–H(21b)	108.0	C(6c)–C(5c)–H(5ca)	109.8
C(21)–C(22)–H(22a)	109.5	O(2c)–C(5c)–H(5cb)	109.8
C(21)–C(22)–H(22b)	109.5	C(6c)–C(5c)–H(5cb)	109.8

Table S6. Continued

angle	degree	angle	degree
H(22a)–C(22)–H(22b)	109.5	H(5ca)–C(5c)–H(5cb)	108.2
C(21)–C(22)–H(22c)	109.5	N(2c)–C(6c)–C(5c)	114.7(3)
H(22a)–C(22)–H(22c)	109.5	N(2c)–C(6c)–H(6ca)	108.6
H(22b)–C(22)–H(22c)	109.5	C(5c)–C(6c)–H(6ca)	108.6
C(b3)–C(31)–C(32)	111.5(2)	N(2c)–C(6c)–H(6cb)	108.6
C(b3)–C(31)–H(31a)	109.3	C(5c)–C(6c)–H(6cb)	108.6
C(32)–C(31)–H(31a)	109.3	H(6ca)–C(6c)–H(6cb)	107.6
C(b3)–C(31)–H(31b)	109.3	N(1c)–C(7c)–C(8c)	114.9(3)
C(32)–C(31)–H(31b)	109.3	N(1c)–C(7c)–H(7ca)	108.5
H(31a)–C(31)–H(31b)	108.0	C(8c)–C(7c)–H(7ca)	108.5
C(31)–C(32)–H(32a)	109.5	N(1c)–C(7c)–H(7cb)	108.5
C(31)–C(32)–H(32b)	109.5	C(8c)–C(7c)–H(7cb)	108.5
H(32a)–C(32)–H(32b)	109.5	H(7ca)–C(7c)–H(7cb)	107.5
C(31)–C(32)–H(32c)	109.5	O(3c)–C(8c)–C(7c)	107.4(3)
H(32a)–C(32)–H(32c)	109.5	O(3c)–C(8c)–H(8ca)	110.2
H(32b)–C(32)–H(32c)	109.5	C(7c)–C(8c)–H(8ca)	110.2
C(b4)–C(41)–C(42)	113.2(2)	O(3c)–C(8c)–H(8cb)	110.2
C(b4)–C(41)–H(41a)	108.9	C(7c)–C(8c)–H(8cb)	110.2
C(42)–C(41)–H(41a)	108.9	H(8ca)–C(8c)–H(8cb)	108.5
C(b4)–C(41)–H(41b)	108.9	O(3c)–C(9c)–C(10c)	110.7(4)
C(42)–C(41)–H(41b)	108.9	O(3c)–C(9c)–H(9ca)	109.5
H(41a)–C(41)–H(41b)	107.8	C(10c)–C(9c)–H(9ca)	109.5
C(41)–C(42)–H(42a)	109.5	O(3c)–C(9c)–H(9cb)	109.5
C(41)–C(42)–H(42b)	109.5	C(10c)–C(9c)–H(9cb)	109.5
H(42a)–C(42)–H(42b)	109.5	H(9ca)–C(9c)–H(9cb)	108.1
C(41)–C(42)–H(42c)	109.5	C(9c)–C(10c)–O(4c)	113.4(3)
H(42a)–C(42)–H(42c)	109.5	C(9c)–C(10c)–H(10a)	108.9
H(42b)–C(42)–H(42c)	109.5	O(4c)–C(10c)–H(10a)	108.9
C(b5)–C(51)–C(52)	113.2(2)	C(9c)–C(10c)–H(10b)	108.9
C(b5)–C(51)–H(51a)	108.9	O(4c)–C(10c)–H(10b)	108.9
C(52)–C(51)–H(51a)	108.9	H(10a)–C(10c)–H(10b)	107.7
C(b5)–C(51)–H(51b)	108.9	O(4c)–C(11c)–C(12c)	109.5(3)
C(52)–C(51)–H(51b)	108.9	O(4c)–C(11c)–H(11c)	109.8
H(51a)–C(51)–H(51b)	107.7	C(12c)–C(11c)–H(11c)	109.8

Table S6. Continued

angle	degree	angle	degree
C(51)–C(52)–H(52a)	109.5	O(4c)–C(11c)–H(11d)	109.8
C(51)–C(52)–H(52b)	109.5	C(12c)–C(11c)–H(11d)	109.8
H(52a)–C(52)–H(52b)	109.5	H(11c)–C(11c)–H(11d)	108.2
C(51)–C(52)–H(52c)	109.5	N(2c)–C(12c)–C(11c)	115.1(3)
H(52a)–C(52)–H(52c)	109.5	N(2c)–C(12c)–H(12d)	108.5
H(52b)–C(52)–H(52c)	109.5	C(11c)–C(12c)–H(12d)	108.5
C(b6)–C(61)–C(62)	112.9(3)	N(2c)–C(12c)–H(12e)	108.5
C(b6)–C(61)–H(61a)	109.0	C(11c)–C(12c)–H(12e)	108.5
C(62)–C(61)–H(61a)	109.0	H(12d)–C(12c)–H(12e)	107.5
C(b6)–C(61)–H(61b)	109.0	N(1c)–C(13c)–C(14c)	113.2(3)
C(62)–C(61)–H(61b)	109.0	N(1c)–C(13c)–H(13a)	108.9
H(61a)–C(61)–H(61b)	107.8	C(14c)–C(13c)–H(13a)	108.9
C(61)–C(62)–H(62a)	109.5	N(1c)–C(13c)–H(13b)	108.9
C(61)–C(62)–H(62b)	109.5	C(14c)–C(13c)–H(13b)	108.9
H(62a)–C(62)–H(62b)	109.5	H(13a)–C(13c)–H(13b)	107.8
C(61)–C(62)–H(62c)	109.5	C(13c)–C(14c)–O(5c)	115.0(3)
H(62a)–C(62)–H(62c)	109.5	C(13c)–C(14c)–H(14a)	108.5
H(62b)–C(62)–H(62c)	109.5	O(5c)–C(14c)–H(14a)	108.5
C(72)–C(71)–C(b7)	113.3(3)	C(13c)–C(14c)–H(14b)	108.5
C(72)–C(71)–H(71a)	108.9	O(5c)–C(14c)–H(14b)	108.5
C(b7)–C(71)–H(71a)	108.9	H(14a)–C(14c)–H(14b)	107.5
C(72)–C(71)–H(71b)	108.9	O(5c)–C(15c)–C(16c)	110.5(4)
C(b7)–C(71)–H(71b)	108.9	O(5c)–C(15c)–H(15a)	109.5
H(71a)–C(71)–H(71b)	107.7	C(16c)–C(15c)–H(15a)	109.5
C(71)–C(72)–H(72a)	109.5	O(5c)–C(15c)–H(15b)	109.5
C(71)–C(72)–H(72b)	109.5	C(16c)–C(15c)–H(15b)	109.5
H(72a)–C(72)–H(72b)	109.5	H(15a)–C(15c)–H(15b)	108.1
C(71)–C(72)–H(72c)	109.5	O(6c)–C(16c)–C(15c)	110.2(3)
H(72a)–C(72)–H(72c)	109.5	O(6c)–C(16c)–H(16a)	109.6
H(72b)–C(72)–H(72c)	109.5	C(15c)–C(16c)–H(16a)	109.6
C(b8)–C(81)–C(82)	112.0(3)	O(6c)–C(16c)–H(16b)	109.6
C(b8)–C(81)–H(81a)	109.2	C(15c)–C(16c)–H(16b)	109.6
C(82)–C(81)–H(81a)	109.2	H(16a)–C(16c)–H(16b)	108.1
C(b8)–C(81)–H(81b)	109.2	O(6c)–C(17c)–C(18c)	111.1(3)

Table S6. Continued

angle	degree	angle	degree
C(82)–C(81)–H(81b)	109.2	O(6c)–C(17c)–H(17a)	109.4
H(81a)–C(81)–H(81b)	107.9	C(18c)–C(17c)–H(17a)	109.4
C(81)–C(82)–H(82a)	109.5	O(6c)–C(17c)–H(17b)	109.4
C(81)–C(82)–H(82b)	109.5	C(18c)–C(17c)–H(17b)	109.4
H(82a)–C(82)–H(82b)	109.5	H(17a)–C(17c)–H(17b)	108.0
C(81)–C(82)–H(82c)	109.5	N(2c)–C(18c)–C(17c)	115.1(3)
H(82a)–C(82)–H(82c)	109.5	N(2c)–C(18c)–H(18a)	108.5
H(82b)–C(82)–H(82c)	109.5	C(17c)–C(18c)–H(18a)	108.5
C(1)–N(5)–C(3)	103.4(2)	N(2c)–C(18c)–H(18b)	108.5
C(1)–N(5)–Fe(1)	136.6(2)	C(17c)–C(18c)–H(18b)	108.5
C(3)–N(5)–Fe(1)	120.0(2)	H(18a)–C(18c)–H(18b)	107.5
N(6)–C(1)–N(5)	115.6(3)		

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

Table S7. Anisotropic Displacement Parameters (Å^2) for [K⊂222][Fe(OEP)(2-MeIm$^-$)]^a

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0190(2)	0.0239(2)	0.0228(2)	0.0010(1)	0.0023(1)	0.0028(1)
N(1)	0.0198(9)	0.0276(11)	0.0257(10)	0.0012(8)	0.0021(8)	0.0023(8)
N(2)	0.0196(9)	0.0248(10)	0.0237(10)	0.0010(8)	0.0012(8)	0.0016(8)
N(3)	0.0210(10)	0.0286(11)	0.0274(10)	0.0039(9)	0.0018(8)	0.0029(8)
N(4)	0.0209(10)	0.0341(12)	0.0288(11)	0.0060(9)	0.0037(8)	0.0048(9)
C(a1)	0.0221(11)	0.0333(14)	0.0285(12)	0.0022(11)	0.0046(10)	0.0012(10)
C(a2)	0.0238(12)	0.0252(12)	0.0257(12)	0.0005(10)	0.0021(9)	−0.0003(10)
C(a3)	0.0218(11)	0.0224(12)	0.0255(11)	−0.0012(9)	−0.0011(9)	0.0015(9)
C(a4)	0.0185(10)	0.0264(12)	0.0247(11)	−0.0022(10)	−0.0006(9)	0.0006(9)
C(a5)	0.0211(11)	0.0279(12)	0.0238(11)	0.0015(10)	−0.0006(9)	−0.0009(10)
C(a6)	0.0265(12)	0.0297(13)	0.0302(13)	0.0047(11)	0.0031(10)	0.0032(10)
C(a7)	0.0242(12)	0.0393(15)	0.0341(14)	0.0084(12)	0.0026(11)	0.0092(11)
C(a8)	0.0198(11)	0.0404(15)	0.0292(13)	0.0059(11)	0.0040(10)	0.0061(11)
C(b1)	0.0235(12)	0.0369(15)	0.0325(13)	0.0064(11)	0.0056(10)	−0.0008(11)
C(b2)	0.0246(12)	0.0308(13)	0.0306(13)	0.0043(11)	0.0052(10)	−0.0014(10)
C(b3)	0.0203(11)	0.0217(12)	0.0318(13)	−0.0013(10)	−0.0019(10)	0.0017(9)
C(b4)	0.0203(11)	0.0257(12)	0.0292(12)	−0.0014(10)	−0.0007(9)	0.0021(9)
C(b5)	0.0235(12)	0.0296(13)	0.0268(12)	0.0026(10)	0.0013(10)	−0.0023(10)
C(b6)	0.0258(12)	0.0304(13)	0.0312(13)	0.0061(11)	0.0006(10)	−0.0012(10)
C(b7)	0.0245(13)	0.0492(18)	0.0405(15)	0.0136(14)	0.0046(11)	0.0091(12)
C(b8)	0.0227(12)	0.0497(18)	0.0371(15)	0.0129(13)	0.0031(11)	0.0078(12)
C(m1)	0.0245(12)	0.0225(12)	0.0276(12)	0.0021(10)	0.0003(10)	0.0018(10)
C(m2)	0.0174(10)	0.0280(12)	0.0257(12)	−0.0005(10)	0.0007(9)	−0.0007(9)
C(m3)	0.0275(13)	0.0336(14)	0.0359(14)	0.0111(12)	0.0033(11)	0.0078(11)
C(m4)	0.0193(11)	0.0411(15)	0.0309(13)	0.0041(11)	0.0053(10)	0.0041(11)
C(11)	0.0220(13)	0.063(2)	0.0464(17)	0.0184(16)	0.0072(12)	−0.0021(13)
C(12)	0.0394(18)	0.110(4)	0.050(2)	0.014(2)	0.0146(16)	0.006(2)
C(21)	0.0281(13)	0.0337(15)	0.0404(15)	0.0129(12)	0.0061(11)	0.0005(11)
C(22)	0.062(2)	0.0500(19)	0.0349(16)	0.0137(14)	0.0137(15)	0.0152(17)
C(31)	0.0241(12)	0.0272(13)	0.0422(15)	0.0074(11)	−0.0006(11)	0.0039(10)
C(32)	0.0466(18)	0.0428(18)	0.0456(18)	0.0148(14)	−0.0153(15)	−0.0075(14)
C(41)	0.0183(11)	0.0319(14)	0.0393(14)	0.0037(11)	−0.0003(10)	0.0024(10)
C(42)	0.0287(14)	0.0435(17)	0.0556(19)	−0.0055(15)	0.0143(13)	−0.0007(13)
C(51)	0.0235(12)	0.0317(14)	0.0333(13)	0.0051(11)	0.0025(10)	−0.0026(10)

Table S7. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(52)	0.0367(15)	0.0380(16)	0.0437(16)	0.0017(13)	0.0101(13)	0.0007(13)
C(61)	0.0296(13)	0.0370(15)	0.0439(16)	0.0141(13)	0.0040(12)	0.0000(12)
C(62)	0.089(3)	0.051(2)	0.0441(19)	0.0169(17)	−0.009(2)	0.010(2)
C(71)	0.0286(14)	0.055(2)	0.058(2)	0.0228(17)	0.0044(14)	0.0078(14)
C(72)	0.078(3)	0.062(3)	0.057(2)	0.013(2)	−0.004(2)	0.012(2)
C(81)	0.0220(13)	0.061(2)	0.0518(19)	0.0210(16)	0.0048(13)	0.0065(13)
C(82)	0.0267(14)	0.069(2)	0.070(2)	0.029(2)	−0.0020(15)	0.0013(16)
N(5)	0.0229(10)	0.0383(13)	0.0376(12)	−0.0069(10)	0.0066(9)	0.0015(9)
C(1)	0.0266(13)	0.0435(17)	0.0374(15)	−0.0063(13)	0.0041(11)	0.0004(12)
N(6)	0.0283(11)	0.0383(13)	0.0384(13)	−0.0109(11)	0.0029(10)	0.0020(10)
C(2)	0.0324(15)	0.0377(17)	0.061(2)	−0.0114(15)	0.0011(14)	0.0027(13)
C(3)	0.0318(14)	0.0423(17)	0.0430(16)	0.0020(13)	0.0031(12)	0.0052(13)
C(4)	0.057(2)	0.0448(19)	0.0423(17)	−0.0043(14)	0.0030(15)	−0.0009(16)
K(1)	0.0232(3)	0.0372(3)	0.0349(3)	0.0003(2)	0.0050(2)	−0.0031(2)
O(1c)	0.0365(11)	0.0449(12)	0.0399(11)	0.0004(9)	−0.0074(9)	−0.0070(9)
O(2c)	0.0363(11)	0.0448(12)	0.0425(12)	0.0057(10)	−0.0023(9)	−0.0022(9)
O(3c)	0.0300(11)	0.0617(15)	0.0497(13)	0.0064(11)	0.0084(9)	0.0054(10)
O(4c)	0.0276(11)	0.100(2)	0.0579(15)	0.0320(15)	0.0093(10)	−0.0016(12)
O(5c)	0.0565(16)	0.0478(15)	0.087(2)	−0.0088(14)	0.0130(15)	0.0037(13)
O(6c)	0.0744(18)	0.0486(15)	0.0616(16)	−0.0189(12)	0.0315(14)	−0.0159(13)
N(1c)	0.0312(12)	0.0551(17)	0.0418(14)	0.0166(12)	0.0046(11)	0.0032(12)
N(2c)	0.0366(14)	0.080(2)	0.0285(12)	−0.0048(13)	0.0031(10)	−0.0241(14)
C(1c)	0.0385(17)	0.066(2)	0.0496(19)	0.0038(17)	−0.0093(15)	−0.0091(16)
C(2c)	0.0431(18)	0.056(2)	0.055(2)	0.0062(17)	−0.0112(16)	−0.0117(16)
C(3c)	0.0379(16)	0.052(2)	0.0456(18)	−0.0130(15)	0.0058(14)	−0.0097(14)
C(4c)	0.0476(19)	0.0385(17)	0.064(2)	0.0037(16)	0.0041(17)	−0.0058(15)
C(5c)	0.057(2)	0.058(2)	0.0452(19)	0.0172(17)	−0.0017(16)	0.0024(18)
C(6c)	0.0403(18)	0.088(3)	0.0384(17)	0.0158(18)	−0.0085(14)	−0.0023(18)
C(7c)	0.0393(17)	0.064(2)	0.0383(16)	0.0097(15)	0.0050(13)	0.0058(16)
C(8c)	0.053(2)	0.069(2)	0.0424(18)	0.0089(17)	0.0124(16)	0.0028(18)
C(9c)	0.0414(19)	0.099(3)	0.066(2)	0.032(2)	0.0198(18)	0.012(2)
C(10c)	0.0271(16)	0.131(4)	0.059(2)	0.042(3)	0.0083(16)	−0.003(2)
C(11c)	0.0287(15)	0.092(3)	0.0426(18)	0.0110(18)	0.0031(13)	−0.0110(17)
C(12c)	0.046(2)	0.126(4)	0.0417(19)	−0.009(2)	0.0034(16)	−0.047(2)

Table S7. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(13c)	0.0412(17)	0.067(2)	0.0506(19)	0.0192(18)	0.0109(15)	0.0123(17)
C(14c)	0.056(2)	0.056(2)	0.072(3)	0.023(2)	0.016(2)	0.0136(19)
C(15c)	0.100(4)	0.046(2)	0.083(3)	0.009(2)	0.030(3)	0.009(2)
C(16c)	0.165(6)	0.043(2)	0.083(3)	−0.024(2)	0.080(4)	−0.016(3)
C(17c)	0.103(4)	0.074(3)	0.059(2)	−0.033(2)	0.043(3)	−0.044(3)
C(18c)	0.061(2)	0.103(4)	0.0311(16)	−0.0129(19)	0.0088(16)	−0.043(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 S8. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($\mathring{A}^2$) for [K⊂222][Fe(OEP)(2-MeIm$^-$)]^a

atom	x	y	z	U(eq)
H(m1)	0.2977	0.4419	0.1731	0.030
H(m2)	0.0601	0.2641	0.3433	0.029
H(m3)	0.4610	0.0996	0.4094	0.039
H(m4)	0.7081	0.3136	0.2774	0.036
H(11a)	0.7486	0.4175	0.2209	0.052
H(11b)	0.7032	0.4473	0.1582	0.052
H(12a)	0.7587	0.3069	0.1809	0.099
H(12b)	0.8145	0.3570	0.1374	0.099
H(12c)	0.6990	0.3307	0.1197	0.099
H(21a)	0.5518	0.5033	0.1298	0.041
H(21b)	0.4299	0.5044	0.1384	0.041
H(22a)	0.5282	0.4150	0.0598	0.073
H(22b)	0.4523	0.4765	0.0395	0.073
H(22c)	0.4074	0.4107	0.0706	0.073
H(31a)	0.1403	0.4941	0.1820	0.038
H(31b)	0.0274	0.4812	0.2045	0.038
H(32a)	0.1085	0.4083	0.1081	0.069
H(32b)	0.0224	0.4669	0.1000	0.069
H(32c)	−0.0047	0.3961	0.1304	0.069
H(41a)	−0.0599	0.3280	0.2910	0.036
H(41b)	−0.0746	0.3887	0.2440	0.036
H(42a)	−0.0077	0.4074	0.3661	0.063
H(42b)	−0.1213	0.4253	0.3373	0.063
H(42c)	−0.0232	0.4681	0.3190	0.063
H(51a)	0.0595	0.1064	0.4377	0.035
H(51b)	0.0102	0.1612	0.3913	0.035
H(52a)	0.1020	0.1938	0.5068	0.059
H(52b)	−0.0198	0.1957	0.4878	0.059
H(52c)	0.0562	0.2496	0.4603	0.059
H(61a)	0.3228	0.0332	0.4360	0.044
H(61b)	0.2058	0.0407	0.4537	0.044
H(62a)	0.3810	0.1052	0.5133	0.093
H(62b)	0.3156	0.0445	0.5395	0.093
H(62c)	0.2643	0.1182	0.5297	0.093

Table S8. Continued

atom	x	y	z	$U(\mathrm{eq})$
H(71a)	0.6324	0.0661	0.4165	0.057
H(71b)	0.7475	0.0947	0.4123	0.057
H(72a)	0.7266	0.1650	0.4938	0.099
H(72b)	0.7108	0.0866	0.5104	0.099
H(72c)	0.6121	0.1353	0.4982	0.099
H(81a)	0.8274	0.2391	0.3253	0.054
H(81b)	0.8387	0.1883	0.3809	0.054
H(82a)	0.7856	0.3283	0.3888	0.084
H(82b)	0.8972	0.2972	0.4092	0.084
H(82c)	0.7985	0.2774	0.4443	0.084
H(2)	0.3498	0.0326	0.1726	0.052
H(3)	0.3775	0.0973	0.2650	0.047
H(4a)	0.4059	0.2716	0.1199	0.072
H(4b)	0.2874	0.2804	0.1344	0.072
H(4c)	0.3152	0.2395	0.0764	0.072
H(1ca)	0.3666	0.5593	0.2607	0.063
H(1cb)	0.4726	0.5174	0.2687	0.063
H(2ca)	0.3481	0.5509	0.3610	0.063
H(2cb)	0.3526	0.4777	0.3304	0.063
H(3ca)	0.5714	0.4437	0.3391	0.054
H(3cb)	0.4726	0.4033	0.3600	0.054
H(4ca)	0.5442	0.4152	0.4606	0.060
H(4cb)	0.6131	0.3681	0.4210	0.060
H(5ca)	0.7442	0.3997	0.5008	0.064
H(5cb)	0.6733	0.4579	0.5268	0.064
H(6ca)	0.8500	0.4831	0.5453	0.067
H(6cb)	0.8640	0.4815	0.4757	0.067
H(7ca)	0.5495	0.6790	0.2416	0.056
H(7cb)	0.4975	0.6131	0.2103	0.056
H(8ca)	0.6422	0.5472	0.2532	0.065
H(8cb)	0.6738	0.6021	0.2051	0.065
H(9ca)	0.8458	0.6201	0.2498	0.082
H(9cb)	0.8261	0.5599	0.2956	0.082
H(10a)	0.8789	0.6945	0.3261	0.086

Table S8. Continued

atom	x	y	z	$U(\mathrm{eq})$
H(10b)	0.9548	0.6303	0.3339	0.086
H(11c)	0.9896	0.6271	0.4316	0.065
H(11d)	0.9331	0.5550	0.4203	0.065
H(12d)	0.9437	0.5865	0.5216	0.085
H(12e)	0.8756	0.6526	0.5048	0.085
H(13a)	0.3674	0.6541	0.3386	0.063
H(13b)	0.3785	0.6841	0.2735	0.063
H(14a)	0.4202	0.7661	0.3416	0.073
H(14b)	0.5207	0.7464	0.3083	0.073
H(15a)	0.4336	0.6756	0.4424	0.091
H(15b)	0.4290	0.7571	0.4406	0.091
H(16a)	0.5930	0.7605	0.4964	0.112
H(16b)	0.5050	0.7256	0.5325	0.112
H(17a)	0.6635	0.6698	0.5880	0.092
H(17b)	0.7435	0.6925	0.5409	0.092
H(18a)	0.7969	0.5907	0.5891	0.078
H(18b)	0.6907	0.5550	0.5653	0.078

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

Table S9. Complete Crystallographic Details for $[K \subset 222][Fe(TPP)(2\text{-}MeIm^-)] \cdot 0.5C_6H_5Cl$

formula	$C_{69}H_{71.50}Cl_{0.50}FeKN_8O_6$
FW, amu	1221.52
a, Å	12.431(3)
b, Å	21.078(4)
c, Å	23.879(5)
β, deg	95.74(3)
V, Å^3	6225(2)
space group	P2(1)/n
Z	4
D_c, g/cm^3	1.303
F(000)	2572
μ, mm^{-1}	0.390
crystal dimensions, mm	$0.49 \times 0.21 \times 0.19$
radiation	MoKα, $\bar{\lambda} = 0.71073$ Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.71–31.62
index range	$-18 \leq h \leq 18$
	$-31 \leq k \leq 30$
	$-33 \leq l \leq 35$
total data collected	81972
absorption correction	Semi-empirical from equivalents
relative transmission coefficients (I)	0.9310 and 0.8334
unique data	20698 ($R_{int} = 0.034$)
unique observed data $[I > 2\sigma(I)]$	15677
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	20698/40/835
goodness-of-fit (pased on F^2)	1.046
final R indices $[I > 2\sigma(I)]$	$R_1 = 0.0481$, $wR_2 = 0.1272$
final R indices (all data)	$R_1 = 0.0678$, $wR_2 = 0.1353$

Table S10. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $[\text{K} \subset 222][\text{Fe}(\text{TPP})(2\text{-MeIm}^-)] \cdot 0.5\text{C}_6\text{H}_5\text{Cl}^a$

atom	x	y	z	$U(\text{eq})$
Fe(1)	0.11256(2)	0.32196(1)	0.72286(1)	0.0180(1)
N(1)	0.08668(10)	0.27417(6)	0.79844(6)	0.0180(2)
N(2)	0.26660(11)	0.34518(6)	0.76574(5)	0.0180(2)
N(3)	0.12769(11)	0.40568(7)	0.67627(6)	0.0207(3)
N(4)	−0.05581(11)	0.33915(6)	0.71280(6)	0.0190(2)
C(a1)	−0.01014(13)	0.24782(7)	0.80980(6)	0.0183(3)
C(a2)	0.16431(12)	0.24977(7)	0.83732(6)	0.0179(3)
C(a3)	0.32048(12)	0.31282(7)	0.80991(6)	0.0182(3)
C(a4)	0.34222(13)	0.38426(8)	0.74524(7)	0.0195(3)
C(a5)	0.22242(13)	0.43598(8)	0.66785(7)	0.0213(3)
C(a6)	0.04903(13)	0.43081(8)	0.63814(7)	0.0223(3)
C(a7)	−0.11068(13)	0.37853(8)	0.67419(7)	0.0202(3)
C(a8)	−0.13268(13)	0.30906(7)	0.74041(7)	0.0188(3)
C(b1)	0.00819(13)	0.20323(8)	0.85553(7)	0.0202(3)
C(b2)	0.11569(13)	0.20490(8)	0.87304(7)	0.0203(3)
C(b3)	0.43362(13)	0.33088(8)	0.81646(7)	0.0215(3)
C(b4)	0.44685(13)	0.37501(8)	0.77653(7)	0.0221(3)
C(b5)	0.20378(14)	0.48039(9)	0.62208(7)	0.0260(3)
C(b6)	0.09725(15)	0.47612(9)	0.60274(8)	0.0270(3)
C(b7)	−0.22585(13)	0.37496(8)	0.67895(7)	0.0212(3)
C(b8)	−0.23895(13)	0.33204(8)	0.72010(7)	0.0211(3)
C(m1)	0.27412(12)	0.26813(7)	0.84397(6)	0.0181(3)
C(m2)	0.32240(13)	0.42666(8)	0.70006(7)	0.0206(3)
C(m3)	−0.06257(13)	0.41846(8)	0.63664(7)	0.0211(3)
C(m4)	−0.11219(12)	0.26360(7)	0.78305(6)	0.0184(3)
C(11)	0.34393(13)	0.24130(8)	0.89285(7)	0.0199(3)
C(12)	0.38643(14)	0.28129(9)	0.93620(7)	0.0245(3)
C(13)	0.45018(15)	0.25753(10)	0.98281(8)	0.0299(4)
C(14)	0.47156(15)	0.19318(10)	0.98670(8)	0.0317(4)
C(15)	0.42965(15)	0.15286(9)	0.94418(8)	0.0300(4)
C(16)	0.36644(14)	0.17661(8)	0.89734(7)	0.0235(3)
C(21)	0.41582(13)	0.46697(8)	0.68637(7)	0.0220(3)
C(22)	0.45212(14)	0.51666(9)	0.72157(8)	0.0262(3)
C(23)	0.53921(15)	0.55411(9)	0.70951(9)	0.0304(4)

Table S10. Continued

atom	x	y	z	U(eq)
C(24)	0.59139(15)	0.54186(9)	0.66222(9)	0.0317(4)
C(25)	0.55547(16)	0.49273(9)	0.62675(9)	0.0326(4)
C(26)	0.46782(15)	0.45550(9)	0.63843(8)	0.0270(3)
C(31)	−0.13749(13)	0.45234(8)	0.59358(7)	0.0220(3)
C(32)	−0.20036(15)	0.41890(9)	0.55187(7)	0.0257(3)
C(33)	−0.26869(16)	0.45061(10)	0.51154(8)	0.0319(4)
C(34)	−0.27581(16)	0.51593(10)	0.51226(8)	0.0333(4)
C(35)	−0.21473(16)	0.54991(10)	0.55351(9)	0.0318(4)
C(36)	−0.14601(15)	0.51822(9)	0.59404(8)	0.0275(3)
C(41)	−0.20885(13)	0.22855(8)	0.79993(7)	0.0203(3)
C(42)	−0.25806(13)	0.18279(8)	0.76387(8)	0.0234(3)
C(43)	−0.34924(14)	0.15024(9)	0.77817(9)	0.0303(4)
C(44)	−0.39167(15)	0.16363(9)	0.82796(10)	0.0341(4)
C(45)	−0.34368(16)	0.20878(11)	0.86403(9)	0.0351(4)
C(46)	−0.25162(15)	0.24096(9)	0.85036(8)	0.0289(4)
N(5a)	0.1381(4)	0.2644(2)	0.6590(2)	0.0237(8)
C(1a)	0.1008(3)	0.20437(17)	0.64767(16)	0.0251(8)
N(6a)	0.1387(12)	0.1805(7)	0.5994(5)	0.0292(16)
C(2a)	0.1805(3)	0.22973(19)	0.57571(15)	0.0321(9)
C(3a)	0.1885(3)	0.27987(19)	0.61181(18)	0.0275(8)
C(4a)	0.0439(4)	0.1688(2)	0.6883(2)	0.0293(9)
N(5b)	0.1200(4)	0.2436(2)	0.6681(2)	0.0234(9)
C(1b)	0.1569(3)	0.2359(2)	0.61737(15)	0.0264(9)
N(6b)	0.1203(14)	0.1799(8)	0.5930(6)	0.0292(16)
C(2b)	0.0820(3)	0.1475(2)	0.63401(19)	0.0351(11)
C(3b)	0.0726(4)	0.1869(3)	0.6783(2)	0.0294(11)
C(4b)	0.2178(4)	0.2855(2)	0.5900(2)	0.0328(10)
K(1)	0.01066(3)	0.40097(2)	0.11190(1)	0.0211(1)
N(1c)	−0.07404(13)	0.52098(8)	0.15468(6)	0.0300(3)
N(2c)	0.10513(14)	0.28287(7)	0.06480(7)	0.0314(3)
O(1c)	0.15820(10)	0.50173(6)	0.14661(6)	0.0280(3)
O(2c)	0.24175(10)	0.38145(6)	0.12392(6)	0.0286(3)
O(3c)	−0.15109(11)	0.46853(6)	0.04627(5)	0.0280(3)
O(4c)	−0.04146(11)	0.36935(6)	−0.00426(6)	0.0297(3)

Table S10. Continued

atom	x	y	z	$U(\mathrm{eq})$
O(5c)	$-0.09420(10)$	$0.39619(7)$	$0.21124(5)$	$0.0285(3)$
O(6c)	$-0.04488(11)$	$0.28513(6)$	$0.15154(6)$	$0.0287(3)$
C(1c)	$0.00730(18)$	$0.57133(9)$	$0.15306(9)$	$0.0351(4)$
C(2c)	$0.11936(18)$	$0.55306(10)$	$0.17792(9)$	$0.0367(4)$
C(3c)	$0.26198(16)$	$0.48125(10)$	$0.17046(9)$	$0.0354(4)$
C(4c)	$0.30809(15)$	$0.43670(10)$	$0.13086(10)$	$0.0350(4)$
C(5c)	$0.28268(16)$	$0.33856(10)$	$0.08485(9)$	$0.0345(4)$
C(6c)	$0.22086(18)$	$0.27735(10)$	$0.08485(9)$	$0.0357(4)$
C(7c)	$-0.17415(17)$	$0.54077(11)$	$0.12069(8)$	$0.0362(4)$
C(8c)	$-0.16895(17)$	$0.53357(9)$	$0.05836(8)$	$0.0321(4)$
C(9c)	$-0.16248(16)$	$0.45698(10)$	$-0.01237(8)$	$0.0310(4)$
C(10c)	$-0.15021(17)$	$0.38792(10)$	$-0.02234(9)$	$0.0358(4)$
C(11c)	$-0.0207(2)$	$0.30617(10)$	$-0.02104(10)$	$0.0414(5)$
C(12c)	$0.0912(2)$	$0.28633(10)$	$0.00331(9)$	$0.0390(5)$
C(13c)	$-0.09869(19)$	$0.50989(11)$	$0.21305(8)$	$0.0376(5)$
C(14c)	$-0.15923(17)$	$0.45005(11)$	$0.22082(9)$	$0.0387(5)$
C(15c)	$-0.15744(16)$	$0.33961(11)$	$0.21081(8)$	$0.0343(4)$
C(16c)	$-0.08735(16)$	$0.28311(10)$	$0.20501(8)$	$0.0325(4)$
C(17c)	$0.0252(2)$	$0.23334(10)$	$0.14534(10)$	$0.0401(5)$
C(18c)	$0.0463(2)$	$0.22813(10)$	$0.08486(10)$	$0.0434(5)$
C(1s)	$0.0078(3)$	$0.98808(15)$	$0.52537(12)$	$0.0342(8)$
C(2s)	$0.0449(3)$	$1.04783(14)$	$0.51189(15)$	$0.048(3)$
C(3s)	$0.0282(3)$	$1.06985(14)$	$0.45684(17)$	$0.0480(12)$
C(4s)	$-0.0256(3)$	$1.03213(19)$	$0.41526(13)$	$0.0497(3)$
C(5s)	$-0.0627(3)$	$0.97238(17)$	$0.42874(14)$	$0.0528(12)$
C(6s)	$-0.0460(3)$	$0.95035(13)$	$0.48379(15)$	$0.037(3)$
Cl(1s)	$0.02925(13)$	$0.95999(7)$	$0.59326(6)$	$0.0497(3)$

[a] $U(\mathrm{eq})$ 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 S11. Bond Lengths for [K⊂222][Fe(TPP)(2-MeIm$^-$)]·0.5C$_6$H$_5$Cl^a

bond	length (Å)	bond	length (Å)
Fe(1)–N(5a)	1.999(5)	C(2a)–H(2a)	0.9500
Fe(1)–N(3)	2.1045(14)	C(3a)–H(3a)	0.9500
Fe(1)–N(5b)	2.114(5)	C(4a)–H(4a)	0.9800
Fe(1)–N(4)	2.1140(14)	C(4a)–H(4b)	0.9800
Fe(1)–N(1)	2.1193(14)	C(4a)–H(4c)	0.9800
Fe(1)–N(2)	2.1361(15)	N(5b)–C(1b)	1.348(6)
N(1)–C(a2)	1.371(2)	N(5b)–C(3b)	1.365(7)
N(1)–C(a1)	1.377(2)	C(1b)–N(6b)	1.372(14)
N(2)–C(a3)	1.373(2)	C(1b)–C(4b)	1.481(7)
N(2)–C(a4)	1.376(2)	N(6b)–C(2b)	1.320(14)
N(3)–C(a5)	1.372(2)	C(2b)–C(3b)	1.359(6)
N(3)–C(a6)	1.374(2)	C(2b)–H(2b)	0.9500
N(4)–C(a8)	1.370(2)	C(3b)–H(3b)	0.9500
N(4)–C(a7)	1.371(2)	C(4b)–H(4d)	0.9800
C(a1)–C(m4)	1.402(2)	C(4b)–H(4e)	0.9800
C(a1)–C(b1)	1.442(2)	C(4b)–H(4f)	0.9800
C(a2)–C(m1)	1.412(2)	K(1)–O(6c)	2.7322(14)
C(a2)–C(b2)	1.446(2)	K(1)–O(3c)	2.8101(15)
C(a3)–C(m1)	1.405(2)	K(1)–O(5c)	2.8204(15)
C(a3)–C(b3)	1.450(2)	K(1)–O(4c)	2.8633(15)
C(a4)–C(m2)	1.404(2)	K(1)–O(1c)	2.8735(14)
C(a4)–C(b4)	1.447(2)	K(1)–O(2c)	2.8878(15)
C(a5)–C(m2)	1.408(2)	K(1)–N(1c)	2.9607(16)
C(a5)–C(b5)	1.440(2)	K(1)–N(2c)	3.0174(17)
C(a6)–C(m3)	1.409(2)	N(1c)–C(1c)	1.469(3)
C(a6)–C(b6)	1.445(2)	N(1c)–C(13c)	1.475(2)
C(a7)–C(m3)	1.406(2)	N(1c)–C(7c)	1.476(3)
C(a7)–C(b7)	1.449(2)	N(2c)–C(12c)	1.463(3)
C(a8)–C(m4)	1.403(2)	N(2c)–C(18c)	1.472(3)
C(a8)–C(b8)	1.445(2)	N(2c)–C(6c)	1.475(3)
C(b1)–C(b2)	1.360(2)	O(1c)–C(3c)	1.424(2)
C(b1)–H(b1)	0.9500	O(1c)–C(2c)	1.427(2)
C(b2)–H(b2)	0.9500	O(2c)–C(4c)	1.427(2)
C(b3)–C(b4)	1.354(2)	O(2c)–C(5c)	1.429(2)

Table S11. Continued

bond	length (Å)	bond	length (Å)
C(b3)–H(b3)	0.9500	O(3c)–C(9c)	1.414(2)
C(b4)–H(b4)	0.9500	O(3c)–C(8c)	1.423(2)
C(b5)–C(b6)	1.361(3)	O(4c)–C(11c)	1.422(2)
C(b5)–H(b5)	0.9500	O(4c)–C(10c)	1.432(2)
C(b6)–H(b6)	0.9500	O(5c)–C(14c)	1.425(2)
C(b7)–C(b8)	1.357(2)	O(5c)–C(15c)	1.428(2)
C(b7)–H(b7)	0.9500	O(6c)–C(17c)	1.413(3)
C(b8)–H(b8)	0.9500	O(6c)–C(16c)	1.430(2)
C(m1)–C(11)	1.494(2)	C(1c)–C(2c)	1.509(3)
C(m2)–C(21)	1.501(2)	C(1c)–H(1ca)	0.9900
C(m3)–C(31)	1.498(2)	C(1c)–H(1cb)	0.9900
C(m4)–C(41)	1.500(2)	C(2c)–H(2ca)	0.9900
C(11)–C(16)	1.394(2)	C(2c)–H(2cb)	0.9900
C(11)–C(12)	1.397(2)	C(3c)–C(4c)	1.488(3)
C(12)–C(13)	1.393(3)	C(3c)–H(3ca)	0.9900
C(12)–H(12)	0.9500	C(3c)–H(3cb)	0.9900
C(13)–C(14)	1.384(3)	C(4c)–H(4ca)	0.9900
C(13)–H(13)	0.9500	C(4c)–H(4cb)	0.9900
C(14)–C(15)	1.385(3)	C(5c)–C(6c)	1.502(3)
C(14)–H(14)	0.9500	C(5c)–H(5ca)	0.9900
C(15)–C(16)	1.394(3)	C(5c)–H(5cb)	0.9900
C(15)–H(15)	0.9500	C(6c)–H(6ca)	0.9900
C(16)–H(16)	0.9500	C(6c)–H(6cb)	0.9900
C(21)–C(22)	1.390(3)	C(7c)–C(8c)	1.504(3)
C(21)–C(26)	1.391(2)	C(7c)–H(7ca)	0.9900
C(22)–C(23)	1.393(2)	C(7c)–H(7cb)	0.9900
C(22)–H(22)	0.9500	C(8c)–H(8ca)	0.9900
C(23)–C(24)	1.382(3)	C(8c)–H(8cb)	0.9900
C(23)–H(23)	0.9500	C(9c)–C(10c)	1.485(3)
C(24)–C(25)	1.383(3)	C(9c)–H(9ca)	0.9900
C(24)–H(24)	0.9500	C(9c)–H(9cb)	0.9900
C(25)–C(26)	1.393(3)	C(10c)–H(10a)	0.9900
C(25)–H(25)	0.9500	C(10c)–H(10b)	0.9900
C(26)–H(26)	0.9500	C(11c)–C(12c)	1.512(3)

Table S11. Continued

bond	length (Å)	bond	length (Å)
C(31)–C(36)	1.393(2)	C(11c)–H(11a)	0.9900
C(31)–C(32)	1.394(2)	C(11c)–H(11b)	0.9900
C(32)–C(33)	1.390(3)	C(12c)–H(12a)	0.9900
C(32)–H(32)	0.9500	C(12c)–H(12b)	0.9900
C(33)–C(34)	1.380(3)	C(13c)–C(14c)	1.490(3)
C(33)–H(33)	0.9500	C(13c)–H(13a)	0.9900
C(34)–C(35)	1.382(3)	C(13c)–H(13b)	0.9900
C(34)–H(34)	0.9500	C(14c)–H(14a)	0.9900
C(35)–C(36)	1.395(3)	C(14c)–H(14b)	0.9900
C(35)–H(35)	0.9500	C(15c)–C(16c)	1.490(3)
C(36)–H(36)	0.9500	C(15c)–H(15a)	0.9900
C(41)–C(46)	1.389(2)	C(15c)–H(15b)	0.9900
C(41)–C(42)	1.393(2)	C(16c)–H(16a)	0.9900
C(42)–C(43)	1.396(2)	C(16c)–H(16b)	0.9900
C(42)–H(42)	0.9500	C(17c)–C(18c)	1.497(3)
C(43)–C(44)	1.377(3)	C(17c)–H(17a)	0.9900
C(43)–H(43)	0.9500	C(17c)–H(17b)	0.9900
C(44)–C(45)	1.379(3)	C(18c)–H(18a)	0.9900
C(44)–H(44)	0.9500	C(18c)–H(18b)	0.9900
C(45)–C(46)	1.397(3)	C(1s)–C(2s)	1.3900
C(45)–H(45)	0.9500	C(1s)–C(6s)	1.3900
C(46)–H(46)	0.9500	C(1s)–Cl(1s)	1.721(3)
N(5a)–C(1a)	1.364(5)	C(2s)–C(3s)	1.3900
N(5a)–C(3a)	1.383(7)	C(3s)–C(4s)	1.3900
C(1a)–N(6a)	1.383(14)	C(4s)–C(5s)	1.3900
C(1a)–C(4a)	1.464(6)	C(5s)–C(6s)	1.3900
N(6a)–C(2a)	1.313(13)		
C(2a)–C(3a)	1.361(5)		

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

Table S12. Bond Angles for $[\text{K} \subset 222][\text{Fe(TPP)(2-MeIm}^-)] \cdot 0.5\text{C}_6\text{H}_5\text{Cl}^a$

angle	degree	angle	degree
N(5a)–Fe(1)–N(3)	94.42(13)	C(2b)–C(3b)–H(3b)	125.5
N(5a)–Fe(1)–N(5b)	14.94(13)	N(5b)–C(3b)–H(3b)	125.5
N(3)–Fe(1)–N(5b)	108.46(15)	C(1b)–C(4b)–H(4d)	109.5
N(5a)–Fe(1)–N(4)	104.39(14)	C(1b)–C(4b)–H(4e)	109.5
N(3)–Fe(1)–N(4)	86.33(6)	H(4d)–C(4b)–H(4e)	109.5
N(5b)–Fe(1)–N(4)	99.65(14)	C(1b)–C(4b)–H(4f)	109.5
N(5a)–Fe(1)–N(1)	114.19(13)	H(4d)–C(4b)–H(4f)	109.5
N(3)–Fe(1)–N(1)	151.39(5)	H(4e)–C(4b)–H(4f)	109.5
N(5b)–Fe(1)–N(1)	100.08(15)	O(6c)–K(1)–O(3c)	117.04(4)
N(4)–Fe(1)–N(1)	86.86(6)	O(6c)–K(1)–O(5c)	61.49(4)
N(5a)–Fe(1)–N(2)	107.55(14)	O(3c)–K(1)–O(5c)	97.01(4)
N(3)–Fe(1)–N(2)	86.44(6)	O(6c)–K(1)–O(4c)	95.00(4)
N(5b)–Fe(1)–N(2)	112.52(14)	O(3c)–K(1)–O(4c)	59.85(4)
N(4)–Fe(1)–N(2)	147.68(5)	O(5c)–K(1)–O(4c)	136.69(4)
N(1)–Fe(1)–N(2)	84.60(6)	O(6c)–K(1)–O(1c)	137.45(4)
C(a2)–N(1)–C(a1)	106.57(13)	O(3c)–K(1)–O(1c)	100.76(4)
C(a2)–N(1)–Fe(1)	126.78(10)	O(5c)–K(1)–O(1c)	96.84(4)
C(a1)–N(1)–Fe(1)	124.72(11)	O(4c)–K(1)–O(1c)	121.83(4)
C(a3)–N(2)–C(a4)	105.81(13)	O(6c)–K(1)–O(2c)	96.98(4)
C(a3)–N(2)–Fe(1)	126.83(11)	O(3c)–K(1)–O(2c)	140.97(4)
C(a4)–N(2)–Fe(1)	125.33(11)	O(5c)–K(1)–O(2c)	116.75(5)
C(a5)–N(3)–C(a6)	106.73(13)	O(4c)–K(1)–O(2c)	100.93(5)
C(a5)–N(3)–Fe(1)	126.24(11)	O(1c)–K(1)–O(2c)	58.45(4)
C(a6)–N(3)–Fe(1)	125.33(11)	O(6c)–K(1)–N(1c)	122.22(5)
C(a8)–N(4)–C(a7)	106.26(13)	O(3c)–K(1)–N(1c)	60.01(4)
C(a8)–N(4)–Fe(1)	126.61(11)	O(5c)–K(1)–N(1c)	61.97(4)
C(a7)–N(4)–Fe(1)	126.92(11)	O(4c)–K(1)–N(1c)	118.64(4)
N(1)–C(a1)–C(m4)	125.69(14)	O(1c)–K(1)–N(1c)	60.51(4)
N(1)–C(a1)–C(b1)	109.71(14)	O(2c)–K(1)–N(1c)	118.16(5)
C(m4)–C(a1)–C(b1)	124.54(14)	O(6c)–K(1)–N(2c)	60.86(5)
N(1)–C(a2)–C(m1)	125.47(14)	O(3c)–K(1)–N(2c)	119.58(4)
N(1)–C(a2)–C(b2)	109.73(13)	O(5c)–K(1)–N(2c)	120.92(5)
C(m1)–C(a2)–C(b2)	124.70(14)	O(4c)–K(1)–N(2c)	60.37(4)
N(2)–C(a3)–C(m1)	125.52(14)	O(1c)–K(1)–N(2c)	117.15(5)

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	110.23(14)	O(2c)–K(1)–N(2c)	59.94(5)
C(m1)–C(a3)–C(b3)	124.25(15)	N(1c)–K(1)–N(2c)	176.89(5)
N(2)–C(a4)–C(m2)	125.51(15)	C(1c)–N(1c)–C(13c)	110.35(17)
N(2)–C(a4)–C(b4)	110.27(14)	C(1c)–N(1c)–C(7c)	109.02(16)
C(m2)–C(a4)–C(b4)	124.21(15)	C(13c)–N(1c)–C(7c)	108.72(16)
N(3)–C(a5)–C(m2)	125.35(15)	C(1c)–N(1c)–K(1)	109.80(11)
N(3)–C(a5)–C(b5)	109.78(15)	C(13c)–N(1c)–K(1)	107.77(11)
C(m2)–C(a5)–C(b5)	124.85(15)	C(7c)–N(1c)–K(1)	111.16(11)
N(3)–C(a6)–C(m3)	125.42(15)	C(12c)–N(2c)–C(18c)	110.66(17)
N(3)–C(a6)–C(b6)	109.46(15)	C(12c)–N(2c)–C(6c)	110.09(17)
C(m3)–C(a6)–C(b6)	124.92(16)	C(18c)–N(2c)–C(6c)	109.45(17)
N(4)–C(a7)–C(m3)	125.21(15)	C(12c)–N(2c)–K(1)	108.76(11)
N(4)–C(a7)–C(b7)	110.17(14)	C(18c)–N(2c)–K(1)	107.50(12)
C(m3)–C(a7)–C(b7)	124.58(15)	C(6c)–N(2c)–K(1)	110.34(11)
N(4)–C(a8)–C(m4)	125.52(14)	C(3c)–O(1c)–C(2c)	111.15(15)
N(4)–C(a8)–C(b8)	109.97(14)	C(3c)–O(1c)–K(1)	114.70(11)
C(m4)–C(a8)–C(b8)	124.50(14)	C(2c)–O(1c)–K(1)	118.17(12)
C(b2)–C(b1)–C(a1)	106.98(14)	C(4c)–O(2c)–C(5c)	110.66(15)
C(b2)–C(b1)–H(b1)	126.5	C(4c)–O(2c)–K(1)	116.93(10)
C(a1)–C(b1)–H(b1)	126.5	C(5c)–O(2c)–K(1)	116.16(11)
C(b1)–C(b2)–C(a2)	106.94(14)	C(9c)–O(3c)–C(8c)	111.38(14)
C(b1)–C(b2)–H(b2)	126.5	C(9c)–O(3c)–K(1)	117.39(11)
C(a2)–C(b2)–H(b2)	126.5	C(8c)–O(3c)–K(1)	119.51(11)
C(b4)–C(b3)–C(a3)	106.80(15)	C(11c)–O(4c)–C(10c)	111.31(15)
C(b4)–C(b3)–H(b3)	126.6	C(11c)–O(4c)–K(1)	117.46(12)
C(a3)–C(b3)–H(b3)	126.6	C(10c)–O(4c)–K(1)	110.11(11)
C(b3)–C(b4)–C(a4)	106.86(14)	C(14c)–O(5c)–C(15c)	110.23(15)
C(b3)–C(b4)–H(b4)	126.6	C(14c)–O(5c)–K(1)	115.08(11)
C(a4)–C(b4)–H(b4)	126.6	C(15c)–O(5c)–K(1)	108.92(11)
C(b6)–C(b5)–C(a5)	106.97(15)	C(17c)–O(6c)–C(16c)	110.90(15)
C(b6)–C(b5)–H(b5)	126.5	C(17c)–O(6c)–K(1)	118.31(11)
C(a5)–C(b5)–H(b5)	126.5	C(16c)–O(6c)–K(1)	117.68(11)
C(b5)–C(b6)–C(a6)	106.95(15)	N(1c)–C(1c)–C(2c)	114.59(17)
C(b5)–C(b6)–H(b6)	126.5	N(1c)–C(1c)–H(1ca)	108.6

Table S12. Continued

angle	degree	angle	degree
C(a6)–C(b6)–H(b6)	126.5	C(2c)–C(1c)–H(1ca)	108.6
C(b8)–C(b7)–C(a7)	106.40(15)	N(1c)–C(1c)–H(1cb)	108.6
C(b8)–C(b7)–H(b7)	126.8	C(2c)–C(1c)–H(1cb)	108.6
C(a7)–C(b7)–H(b7)	126.8	H(1ca)–C(1c)–H(1cb)	107.6
C(b7)–C(b8)–C(a8)	107.14(14)	O(1c)–C(2c)–C(1c)	109.58(16)
C(b7)–C(b8)–H(b8)	126.4	O(1c)–C(2c)–H(2ca)	109.8
C(a8)–C(b8)–H(b8)	126.4	C(1c)–C(2c)–H(2ca)	109.8
C(a3)–C(m1)–C(a2)	124.49(15)	O(1c)–C(2c)–H(2cb)	109.8
C(a3)–C(m1)–C(11)	117.79(14)	C(1c)–C(2c)–H(2cb)	109.8
C(a2)–C(m1)–C(11)	117.60(14)	H(2ca)–C(2c)–H(2cb)	108.2
C(a4)–C(m2)–C(a5)	125.87(15)	O(1c)–C(3c)–C(4c)	109.17(16)
C(a4)–C(m2)–C(21)	116.60(15)	O(1c)–C(3c)–H(3ca)	109.8
C(a5)–C(m2)–C(21)	117.50(14)	C(4c)–C(3c)–H(3ca)	109.8
C(a7)–C(m3)–C(a6)	125.10(15)	O(1c)–C(3c)–H(3cb)	109.8
C(a7)–C(m3)–C(31)	116.63(15)	C(4c)–C(3c)–H(3cb)	109.8
C(a6)–C(m3)–C(31)	118.21(14)	H(3ca)–C(3c)–H(3cb)	108.3
C(a1)–C(m4)–C(a8)	125.66(14)	O(2c)–C(4c)–C(3c)	109.51(16)
C(a1)–C(m4)–C(41)	118.26(14)	O(2c)–C(4c)–H(4ca)	109.8
C(a8)–C(m4)–C(41)	116.07(14)	C(3c)–C(4c)–H(4ca)	109.8
C(16)–C(11)–C(12)	118.36(16)	O(2c)–C(4c)–H(4cb)	109.8
C(16)–C(11)–C(m1)	121.80(15)	C(3c)–C(4c)–H(4cb)	109.8
C(12)–C(11)–C(m1)	119.83(15)	H(4ca)–C(4c)–H(4cb)	108.2
C(13)–C(12)–C(11)	121.19(17)	O(2c)–C(5c)–C(6c)	109.14(16)
C(13)–C(12)–H(12)	119.4	O(2c)–C(5c)–H(5ca)	109.9
C(11)–C(12)–H(12)	119.4	C(6c)–C(5c)–H(5ca)	109.9
C(14)–C(13)–C(12)	119.74(18)	O(2c)–C(5c)–H(5cb)	109.9
C(14)–C(13)–H(13)	120.1	C(6c)–C(5c)–H(5cb)	109.9
C(12)–C(13)–H(13)	120.1	H(5ca)–C(5c)–H(5cb)	108.3
C(13)–C(14)–C(15)	119.79(17)	N(2c)–C(6c)–C(5c)	114.50(16)
C(13)–C(14)–H(14)	120.1	N(2c)–C(6c)–H(6ca)	108.6
C(15)–C(14)–H(14)	120.1	C(5c)–C(6c)–H(6ca)	108.6
C(14)–C(15)–C(16)	120.55(18)	N(2c)–C(6c)–H(6cb)	108.6
C(14)–C(15)–H(15)	119.7	C(5c)–C(6c)–H(6cb)	108.6
C(16)–C(15)–H(15)	119.7	H(6ca)–C(6c)–H(6cb)	107.6

angle	degree	angle	degree
C(15)–C(16)–C(11)	120.38(17)	N(1c)–C(7c)–C(8c)	113.47(16)
C(15)–C(16)–H(16)	119.8	N(1c)–C(7c)–H(7ca)	108.9
C(11)–C(16)–H(16)	119.8	C(8c)–C(7c)–H(7ca)	108.9
C(22)–C(21)–C(26)	118.65(16)	N(1c)–C(7c)–H(7cb)	108.9
C(22)–C(21)–C(m2)	120.41(14)	C(8c)–C(7c)–H(7cb)	108.9
C(26)–C(21)–C(m2)	120.94(16)	H(7ca)–C(7c)–H(7cb)	107.7
C(21)–C(22)–C(23)	120.93(17)	O(3c)–C(8c)–C(7c)	108.73(15)
C(21)–C(22)–H(22)	119.5	O(3c)–C(8c)–H(8ca)	109.9
C(23)–C(22)–H(22)	119.5	C(7c)–C(8c)–H(8ca)	109.9
C(24)–C(23)–C(22)	120.07(19)	O(3c)–C(8c)–H(8cb)	109.9
C(24)–C(23)–H(23)	120.0	C(7c)–C(8c)–H(8cb)	109.9
C(22)–C(23)–H(23)	120.0	H(8ca)–C(8c)–H(8cb)	108.3
C(23)–C(24)–C(25)	119.42(17)	O(3c)–C(9c)–C(10c)	109.01(16)
C(23)–C(24)–H(24)	120.3	O(3c)–C(9c)–H(9ca)	109.9
C(25)–C(24)–H(24)	120.3	C(10c)–C(9c)–H(9ca)	109.9
C(24)–C(25)–C(26)	120.67(17)	O(3c)–C(9c)–H(9cb)	109.9
C(24)–C(25)–H(25)	119.7	C(10c)–C(9c)–H(9cb)	109.9
C(26)–C(25)–H(25)	119.7	H(9ca)–C(9c)–H(9cb)	108.3
C(21)–C(26)–C(25)	120.25(18)	O(4c)–C(10c)–C(9c)	109.18(16)
C(21)–C(26)–H(26)	119.9	O(4c)–C(10c)–H(10a)	109.8
C(25)–C(26)–H(26)	119.9	C(9c)–C(10c)–H(10a)	109.8
C(36)–C(31)–C(32)	118.16(16)	O(4c)–C(10c)–H(10b)	109.8
C(36)–C(31)–C(m3)	120.84(16)	C(9c)–C(10c)–H(10b)	109.8
C(32)–C(31)–C(m3)	121.00(15)	H(10a)–C(10c)–H(10b)	108.3
C(33)–C(32)–C(31)	120.79(18)	O(4c)–C(11c)–C(12c)	109.67(17)
C(33)–C(32)–H(32)	119.6	O(4c)–C(11c)–H(11a)	109.7
C(31)–C(32)–H(32)	119.6	C(12c)–C(11c)–H(11a)	109.7
C(34)–C(33)–C(32)	120.44(19)	O(4c)–C(11c)–H(11b)	109.7
C(34)–C(33)–H(33)	119.8	C(12c)–C(11c)–H(11b)	109.7
C(32)–C(33)–H(33)	119.8	H(11a)–C(11c)–H(11b)	108.2
C(33)–C(34)–C(35)	119.64(18)	N(2c)–C(12c)–C(11c)	114.31(18)
C(33)–C(34)–H(34)	120.2	N(2c)–C(12c)–H(12a)	108.7
C(35)–C(34)–H(34)	120.2	C(11c)–C(12c)–H(12a)	108.7
C(34)–C(35)–C(36)	120.06(18)	N(2c)–C(12c)–H(12b)	108.7

Table S12. Continued

angle	degree	angle	degree
C(34)–C(35)–H(35)	120.0	C(11c)–C(12c)–H(12b)	108.7
C(36)–C(35)–H(35)	120.0	H(12a)–C(12c)–H(12b)	107.6
C(31)–C(36)–C(35)	120.90(18)	N(1c)–C(13c)–C(14c)	114.01(18)
C(31)–C(36)–H(36)	119.5	N(1c)–C(13c)–H(13a)	108.7
C(35)–C(36)–H(36)	119.5	C(14c)–C(13c)–H(13a)	108.7
C(46)–C(41)–C(42)	118.93(16)	N(1c)–C(13c)–H(13b)	108.7
C(46)–C(41)–C(m4)	121.78(15)	C(14c)–C(13c)–H(13b)	108.7
C(42)–C(41)–C(m4)	119.28(14)	H(13a)–C(13c)–H(13b)	107.6
C(41)–C(42)–C(43)	120.40(17)	O(5c)–C(14c)–C(13c)	110.65(16)
C(41)–C(42)–H(42)	119.8	O(5c)–C(14c)–H(14a)	109.5
C(43)–C(42)–H(42)	119.8	C(13c)–C(14c)–H(14a)	109.5
C(44)–C(43)–C(42)	120.06(18)	O(5c)–C(14c)–H(14b)	109.5
C(44)–C(43)–H(43)	120.0	C(13c)–C(14c)–H(14b)	109.5
C(42)–C(43)–H(43)	120.0	H(14a)–C(14c)–H(14b)	108.1
C(43)–C(44)–C(45)	120.10(17)	O(5c)–C(15c)–C(16c)	109.98(15)
C(43)–C(44)–H(44)	119.9	O(5c)–C(15c)–H(15a)	109.7
C(45)–C(44)–H(44)	119.9	C(16c)–C(15c)–H(15a)	109.7
C(44)–C(45)–C(46)	120.18(18)	O(5c)–C(15c)–H(15b)	109.7
C(44)–C(45)–H(45)	119.9	C(16c)–C(15c)–H(15b)	109.7
C(46)–C(45)–H(45)	119.9	H(15a)–C(15c)–H(15b)	108.2
C(41)–C(46)–C(45)	120.32(18)	O(6c)–C(16c)–C(15c)	109.30(15)
C(41)–C(46)–H(46)	119.8	O(6c)–C(16c)–H(16a)	109.8
C(45)–C(46)–H(46)	119.8	C(15c)–C(16c)–H(16a)	109.8
C(1a)–N(5a)–C(3a)	103.3(4)	O(6c)–C(16c)–H(16b)	109.8
C(1a)–N(5a)–Fe(1)	129.6(3)	C(15c)–C(16c)–H(16b)	109.8
C(3a)–N(5a)–Fe(1)	126.7(3)	H(16a)–C(16c)–H(16b)	108.3
N(5a)–C(1a)–N(6a)	111.4(6)	O(6c)–C(17c)–C(18c)	109.06(18)
N(5a)–C(1a)–C(4a)	121.3(3)	O(6c)–C(17c)–H(17a)	109.9
N(6a)–C(1a)–C(4a)	126.4(6)	C(18c)–C(17c)–H(17a)	109.9
C(2a)–N(6a)–C(1a)	104.7(10)	O(6c)–C(17c)–H(17b)	109.9
N(6a)–C(2a)–C(3a)	110.3(7)	C(18c)–C(17c)–H(17b)	109.9
N(6a)–C(2a)–H(2a)	124.8	H(17a)–C(17c)–H(17b)	108.3
C(3a)–C(2a)–H(2a)	124.8	N(2c)–C(18c)–C(17c)	113.39(18)
C(2a)–C(3a)–N(5a)	108.8(4)	N(2c)–C(18c)–H(18a)	108.9

Table S12. Continued

angle	degree	angle	degree
C(2a)–C(3a)–H(3a)	125.6	C(17c)–C(18c)–H(18a)	108.9
N(5a)–C(3a)–H(3a)	125.6	N(2c)–C(18c)–H(18b)	108.9
C(1b)–N(5b)–C(3b)	104.2(4)	C(17c)–C(18c)–H(18b)	108.9
C(1b)–N(5b)–Fe(1)	133.6(4)	H(18a)–C(18c)–H(18b)	107.7
C(3b)–N(5b)–Fe(1)	121.9(4)	C(2s)–C(1s)–C(6s)	120.0
N(5b)–C(1b)–N(6b)	110.8(7)	C(2s)–C(1s)–Cl(1s)	120.4(2)
N(5b)–C(1b)–C(4b)	123.2(4)	C(6s)–C(1s)–Cl(1s)	119.6(2)
N(6b)–C(1b)–C(4b)	125.6(7)	C(1s)–C(2s)–C(3s)	120.0
C(2b)–N(6b)–C(1b)	105.1(10)	C(2s)–C(3s)–C(4s)	120.0
N(6b)–C(2b)–C(3b)	109.0(8)	C(5s)–C(4s)–C(3s)	120.0
N(6b)–C(2b)–H(2b)	125.5	C(6s)–C(5s)–C(4s)	120.0
C(3b)–C(2b)–H(2b)	125.5	C(5s)–C(6s)–C(1s)	120.0
C(2b)–C(3b)–N(5b)	109.0(5)		

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

Table S13. Anisotropic Displacement Parameters (Å^2) for $[\text{K} \subset 222][\text{Fe(TPP)(2-MeIm}^-)] \cdot 0.5\text{C}_6\text{H}_5\text{Cl}^a$

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0185(1)	0.0199(1)	0.0158(1)	−0.0004(1)	0.0023(1)	0.0006(1)
N(1)	0.0176(6)	0.0177(6)	0.0185(6)	−0.0010(5)	0.0004(5)	−0.0009(5)
N(2)	0.0199(6)	0.0185(6)	0.0158(6)	0.0003(5)	0.0029(5)	−0.0002(5)
N(3)	0.0205(6)	0.0233(7)	0.0187(6)	0.0026(5)	0.0037(5)	0.0009(5)
N(4)	0.0202(6)	0.0188(6)	0.0181(6)	0.0001(5)	0.0023(5)	−0.0005(5)
C(a1)	0.0207(7)	0.0169(7)	0.0174(7)	−0.0018(5)	0.0028(5)	−0.0017(5)
C(a2)	0.0202(7)	0.0174(7)	0.0160(6)	−0.0019(5)	0.0022(5)	0.0009(5)
C(a3)	0.0189(7)	0.0188(7)	0.0166(7)	−0.0015(5)	0.0010(5)	0.0002(5)
C(a4)	0.0205(7)	0.0196(7)	0.0187(7)	−0.0012(6)	0.0045(6)	−0.0007(5)
C(a5)	0.0222(7)	0.0234(8)	0.0192(7)	0.0023(6)	0.0057(6)	0.0002(6)
C(a6)	0.0229(7)	0.0246(8)	0.0196(7)	0.0034(6)	0.0038(6)	0.0016(6)
C(a7)	0.0212(7)	0.0210(7)	0.0184(7)	−0.0019(6)	0.0012(6)	0.0001(6)
C(a8)	0.0198(7)	0.0179(7)	0.0186(7)	−0.0018(5)	0.0014(5)	−0.0012(5)
C(b1)	0.0228(7)	0.0191(7)	0.0191(7)	−0.0003(6)	0.0040(6)	−0.0025(6)
C(b2)	0.0229(7)	0.0199(7)	0.0182(7)	0.0007(6)	0.0027(6)	0.0001(6)
C(b3)	0.0200(7)	0.0236(8)	0.0205(7)	−0.0011(6)	0.0005(6)	−0.0011(6)
C(b4)	0.0204(7)	0.0240(8)	0.0221(7)	−0.0013(6)	0.0030(6)	−0.0029(6)
C(b5)	0.0261(8)	0.0289(9)	0.0242(8)	0.0073(7)	0.0074(6)	0.0006(6)
C(b6)	0.0272(8)	0.0308(9)	0.0237(8)	0.0086(7)	0.0054(6)	0.0032(7)
C(b7)	0.0196(7)	0.0232(8)	0.0202(7)	−0.0016(6)	−0.0009(6)	0.0005(6)
C(b8)	0.0182(7)	0.0229(8)	0.0219(7)	−0.0014(6)	0.0004(6)	−0.0017(5)
C(m1)	0.0197(7)	0.0182(7)	0.0165(7)	−0.0019(5)	0.0021(5)	0.0004(5)
C(m2)	0.0211(7)	0.0220(7)	0.0195(7)	0.0003(6)	0.0063(6)	−0.0007(6)
C(m3)	0.0245(7)	0.0203(7)	0.0183(7)	−0.0001(6)	0.0011(6)	0.0021(6)
C(m4)	0.0190(7)	0.0182(7)	0.0181(7)	−0.0018(5)	0.0027(5)	−0.0016(5)
C(11)	0.0184(7)	0.0236(7)	0.0178(7)	0.0011(6)	0.0021(5)	−0.0003(6)
C(12)	0.0251(8)	0.0273(8)	0.0211(8)	−0.0020(6)	0.0015(6)	−0.0018(6)
C(13)	0.0262(8)	0.0424(11)	0.0208(8)	−0.0009(7)	0.0004(6)	−0.0034(7)
C(14)	0.0259(8)	0.0456(11)	0.0233(8)	0.0120(8)	0.0000(7)	0.0004(8)
C(15)	0.0266(8)	0.0304(9)	0.0329(9)	0.0105(7)	0.0034(7)	0.0022(7)
C(16)	0.0226(7)	0.0235(8)	0.0244(8)	0.0021(6)	0.0031(6)	−0.0002(6)
C(21)	0.0203(7)	0.0228(8)	0.0234(8)	0.0044(6)	0.0053(6)	0.0003(6)
C(22)	0.0248(8)	0.0280(9)	0.0264(8)	0.0018(7)	0.0059(6)	−0.0028(6)
C(23)	0.0260(8)	0.0268(9)	0.0387(10)	0.0041(7)	0.0041(7)	−0.0032(7)

Table S13. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.0228(8)	0.0287(9)	0.0447(11)	0.0128(8)	0.0098(8)	0.0008(7)
C(25)	0.0306(9)	0.0320(9)	0.0382(10)	0.0096(8)	0.0185(8)	0.0054(7)
C(26)	0.0285(8)	0.0266(8)	0.0275(8)	0.0039(7)	0.0102(7)	0.0026(7)
C(31)	0.0223(7)	0.0253(8)	0.0188(7)	0.0026(6)	0.0029(6)	0.0027(6)
C(32)	0.0300(9)	0.0287(9)	0.0188(7)	−0.0004(6)	0.0034(6)	0.0031(7)
C(33)	0.0313(9)	0.0466(11)	0.0176(8)	−0.0008(7)	0.0009(7)	0.0042(8)
C(34)	0.0310(9)	0.0471(12)	0.0222(8)	0.0118(8)	0.0053(7)	0.0119(8)
C(35)	0.0325(9)	0.0294(9)	0.0345(10)	0.0101(8)	0.0081(8)	0.0079(7)
C(36)	0.0286(9)	0.0260(8)	0.0278(9)	0.0017(7)	0.0030(7)	0.0012(7)
C(41)	0.0180(7)	0.0214(7)	0.0214(7)	0.0026(6)	0.0011(6)	−0.0004(5)
C(42)	0.0196(7)	0.0215(8)	0.0286(8)	0.0015(6)	0.0000(6)	−0.0002(6)
C(43)	0.0215(8)	0.0231(8)	0.0453(11)	0.0046(8)	−0.0017(7)	−0.0038(6)
C(44)	0.0189(8)	0.0316(10)	0.0523(12)	0.0164(9)	0.0060(8)	−0.0010(7)
C(45)	0.0294(9)	0.0428(11)	0.0352(10)	0.0107(9)	0.0133(8)	0.0037(8)
C(46)	0.0267(8)	0.0343(10)	0.0265(8)	0.0000(7)	0.0068(7)	−0.0024(7)
N(5a)	0.0252(19)	0.020(2)	0.0250(19)	−0.0057(15)	−0.0022(13)	0.0003(14)
C(1a)	0.0222(15)	0.0237(17)	0.0279(18)	−0.0061(15)	−0.0055(14)	0.0035(12)
N(6a)	0.021(5)	0.0386(10)	0.025(2)	−0.0145(15)	−0.016(3)	0.001(2)
C(2a)	0.0360(19)	0.038(2)	0.0215(16)	−0.0094(14)	−0.0004(14)	0.0093(15)
C(3a)	0.0308(19)	0.029(2)	0.0227(19)	−0.0038(15)	0.0037(15)	0.0039(15)
C(4a)	0.027(2)	0.028(2)	0.034(2)	−0.0067(17)	0.0033(18)	−0.0011(16)
N(5b)	0.0183(18)	0.023(3)	0.029(2)	−0.0105(19)	0.0009(14)	−0.0002(16)
C(1b)	0.0203(16)	0.038(2)	0.0201(17)	−0.0055(15)	−0.0028(13)	0.0070(15)
N(6b)	0.021(5)	0.0386(10)	0.025(2)	−0.0145(15)	−0.016(3)	0.001(2)
C(2b)	0.0215(18)	0.037(2)	0.047(3)	−0.0219(19)	0.0004(16)	−0.0038(15)
C(3b)	0.021(2)	0.031(3)	0.038(3)	−0.008(2)	0.0122(19)	−0.0064(17)
C(4b)	0.030(2)	0.043(3)	0.025(2)	0.0014(19)	0.0043(17)	0.0095(18)
K(1)	0.0239(2)	0.0203(2)	0.0192(2)	0.0009(1)	0.0033(1)	0.0012(1)
N(1c)	0.0346(8)	0.0337(8)	0.0217(7)	−0.0023(6)	0.0032(6)	0.0121(7)
N(2c)	0.0429(9)	0.0228(7)	0.0283(8)	−0.0019(6)	0.0028(7)	0.0044(6)
O(1c)	0.0286(6)	0.0253(6)	0.0284(6)	−0.0055(5)	−0.0052(5)	0.0017(5)
O(2c)	0.0269(6)	0.0274(6)	0.0318(7)	0.0014(5)	0.0048(5)	0.0025(5)
O(3c)	0.0321(7)	0.0306(7)	0.0214(6)	0.0037(5)	0.0024(5)	0.0057(5)
O(4c)	0.0339(7)	0.0277(6)	0.0263(6)	−0.0077(5)	−0.0035(5)	0.0013(5)

Table S13. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(5c)	0.0230(6)	0.0376(7)	0.0254(6)	0.0035(5)	0.0047(5)	0.0012(5)
O(6c)	0.0290(6)	0.0278(6)	0.0290(6)	0.0088(5)	0.0009(5)	−0.0027(5)
C(1c)	0.0481(12)	0.0248(9)	0.0323(10)	−0.0072(7)	0.0028(8)	0.0089(8)
C(2c)	0.0479(12)	0.0285(10)	0.0324(10)	−0.0112(8)	−0.0029(9)	0.0006(8)
C(3c)	0.0313(10)	0.0315(10)	0.0402(11)	0.0011(8)	−0.0128(8)	−0.0031(8)
C(4c)	0.0215(8)	0.0336(10)	0.0485(12)	0.0059(9)	−0.0032(8)	0.0001(7)
C(5c)	0.0303(9)	0.0392(11)	0.0348(10)	−0.0003(8)	0.0076(8)	0.0104(8)
C(6c)	0.0440(11)	0.0283(9)	0.0350(10)	−0.0008(8)	0.0048(8)	0.0146(8)
C(7c)	0.0382(10)	0.0407(11)	0.0297(9)	−0.0006(8)	0.0040(8)	0.0197(9)
C(8c)	0.0355(10)	0.0316(9)	0.0288(9)	0.0059(7)	0.0013(7)	0.0103(8)
C(9c)	0.0333(9)	0.0376(10)	0.0215(8)	0.0034(7)	−0.0006(7)	0.0045(8)
C(10c)	0.0343(10)	0.0398(11)	0.0312(10)	−0.0051(8)	−0.0067(8)	−0.0033(8)
C(11c)	0.0575(14)	0.0310(10)	0.0334(10)	−0.0120(8)	−0.0067(9)	0.0036(9)
C(12c)	0.0570(13)	0.0321(10)	0.0277(9)	−0.0095(8)	0.0030(9)	0.0117(9)
C(13c)	0.0484(12)	0.0424(11)	0.0231(9)	−0.0023(8)	0.0093(8)	0.0169(9)
C(14c)	0.0355(10)	0.0560(13)	0.0263(9)	0.0044(9)	0.0124(8)	0.0162(9)
C(15c)	0.0260(9)	0.0500(12)	0.0271(9)	0.0055(8)	0.0046(7)	−0.0092(8)
C(16c)	0.0335(10)	0.0375(10)	0.0255(9)	0.0108(8)	−0.0021(7)	−0.0133(8)
C(17c)	0.0510(13)	0.0233(9)	0.0463(12)	0.0108(8)	0.0063(10)	0.0031(8)
C(18c)	0.0609(15)	0.0199(9)	0.0496(13)	−0.0051(8)	0.0071(11)	−0.0022(9)
C(1s)	0.0311(19)	0.032(2)	0.040(2)	0.0040(16)	0.0059(16)	0.0083(15)
C(2s)	0.047(7)	0.019(4)	0.079(6)	0.010(4)	0.011(5)	−0.002(4)
C(3s)	0.033(2)	0.027(2)	0.085(4)	0.013(2)	0.016(2)	0.0090(16)
C(4s)	0.0505(5)	0.0496(6)	0.0492(6)	0.0038(5)	0.0058(5)	0.0149(5)
C(5s)	0.043(3)	0.059(3)	0.058(3)	−0.004(3)	0.008(2)	0.011(2)
C(6s)	0.025(4)	0.044(5)	0.042(4)	−0.016(4)	−0.003(3)	0.006(3)
Cl(1s)	0.0505(5)	0.0496(6)	0.0492(6)	0.0038(5)	0.0058(5)	0.0149(5)

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

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Table S14. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for $[\text{K}{\subset}222][\text{Fe(TPP)(2-MeIm}^-)] \cdot 0.5\text{C}_6\text{H}_5\text{Cl}^a$

atom	x	y	z	U(eq)
H(b1)	−0.0448	0.1776	0.8706	0.024
H(b2)	0.1519	0.1811	0.9030	0.024
H(b3)	0.4880	0.3148	0.8436	0.026
H(b4)	0.5123	0.3959	0.7703	0.027
H(b5)	0.2559	0.5075	0.6081	0.031
H(b6)	0.0614	0.4987	0.5718	0.032
H(b7)	−0.2812	0.3981	0.6575	0.025
H(b8)	−0.3055	0.3195	0.7331	0.025
H(12)	0.3716	0.3255	0.9339	0.029
H(13)	0.4789	0.2854	1.0118	0.036
H(14)	0.5148	0.1767	1.0184	0.038
H(15)	0.4441	0.1087	0.9470	0.036
H(16)	0.3386	0.1485	0.8683	0.028
H(22)	0.4171	0.5252	0.7543	0.031
H(23)	0.5628	0.5881	0.7338	0.037
H(24)	0.6514	0.5670	0.6541	0.038
H(25)	0.5909	0.4843	0.5941	0.039
H(26)	0.4435	0.4222	0.6136	0.032
H(32)	−0.1964	0.3739	0.5510	0.031
H(33)	−0.3108	0.4272	0.4833	0.038
H(34)	−0.3224	0.5374	0.4845	0.040
H(35)	−0.2195	0.5949	0.5543	0.038
H(36)	−0.1045	0.5419	0.6223	0.033
H(42)	−0.2294	0.1737	0.7293	0.028
H(43)	−0.3820	0.1188	0.7535	0.036
H(44)	−0.4541	0.1417	0.8375	0.041
H(45)	−0.3733	0.2180	0.8983	0.042
H(46)	−0.2181	0.2715	0.8757	0.035
H(2a)	0.2022	0.2303	0.5387	0.039
H(3a)	0.2230	0.3191	0.6056	0.033
H(4a)	0.0860	0.1701	0.7253	0.044
H(4b)	0.0350	0.1246	0.6759	0.044
H(4c)	−0.0273	0.1878	0.6910	0.044
H(2b)	0.0639	0.1037	0.6327	0.042

Table S14. Continued

atom	x	y	z	U(eq)
H(3b)	0.0385	0.1767	0.7110	0.035
H(4d)	0.1745	0.3243	0.5859	0.049
H(4e)	0.2335	0.2707	0.5527	0.049
H(4f)	0.2858	0.2942	0.6131	0.049
H(1ca)	−0.0167	0.6087	0.1737	0.042
H(1cb)	0.0108	0.5842	0.1134	0.042
H(2ca)	0.1686	0.5899	0.1768	0.044
H(2cb)	0.1175	0.5403	0.2177	0.044
H(3ca)	0.2555	0.4598	0.2068	0.043
H(3cb)	0.3104	0.5183	0.1775	0.043
H(4ca)	0.3117	0.4577	0.0940	0.042
H(4cb)	0.3824	0.4246	0.1458	0.042
H(5ca)	0.3604	0.3305	0.0957	0.041
H(5cb)	0.2747	0.3573	0.0467	0.041
H(6ca)	0.2546	0.2464	0.0608	0.043
H(6cb)	0.2275	0.2602	0.1236	0.043
H(7ca)	−0.1890	0.5857	0.1290	0.043
H(7cb)	−0.2352	0.5152	0.1319	0.043
H(8ca)	−0.2376	0.5481	0.0377	0.039
H(8cb)	−0.1094	0.5597	0.0462	0.039
H(9ca)	−0.1067	0.4808	−0.0305	0.037
H(9cb)	−0.2345	0.4714	−0.0289	0.037
H(10a)	−0.2012	0.3638	−0.0012	0.043
H(10b)	−0.1669	0.3785	−0.0629	0.043
H(11a)	−0.0261	0.3036	−0.0626	0.050
H(11b)	−0.0752	0.2772	−0.0076	0.050
H(12a)	0.1076	0.2442	−0.0121	0.047
H(12b)	0.1444	0.3169	−0.0092	0.047
H(13a)	−0.1417	0.5461	0.2251	0.045
H(13b)	−0.0300	0.5088	0.2379	0.045
H(14a)	−0.1809	0.4484	0.2596	0.046
H(14b)	−0.2257	0.4493	0.1943	0.046
H(15a)	−0.2150	0.3410	0.1790	0.041
H(15b)	−0.1923	0.3365	0.2462	0.041

Table S14. Continued

atom	x	y	z	$U(\mathrm{eq})$
H(16a)	-0.0273	0.2830	0.2355	0.039
H(16b)	-0.1300	0.2438	0.2081	0.039
H(17a)	-0.0083	0.1937	0.1575	0.048
H(17b)	0.0941	0.2399	0.1692	0.048
H(18a)	0.0886	0.1891	0.0799	0.052
H(18b)	-0.0237	0.2239	0.0614	0.052

[a] $U(\mathrm{eq})$ 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

Table S1. Variable temperature Mössbauer Parameters for two Imidazolate-Ligated Iron(II).

Table S2. High magnetic field fitting Mössbauer Parameters for two Imidazolate-Ligated Iron(II).

Table S3. Complete Crystallographic Details for $[\text{K}\subset222][\text{Fe(OEP)(2-MeIm}^-)]$.

Table S4. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for $[\text{K}\subset222][\text{Fe(OEP)(2-MeIm}^-)]$.

Table S5. Bond Lengths for $[\text{K}\subset222][\text{Fe(OEP)(2-MeIm}^-)]$.

Table S6. Bond Angles for $[\text{K}\subset222][\text{Fe(OEP)(2-MeIm}^-)]$.

Table S7. Anisotropic Isotropic Displacement Parameters for $[\text{K}\subset222][\text{Fe(OEP)(2-MeIm}^-)]$.

Table S8. Hydrogen Coordinates and Isotropic Displacement Parameters for $[\text{K}\subset222][\text{Fe(OEP)(2-MeIm}^-)]$.

Table S9. Complete Crystallographic Details for $[\text{K}\subset222][\text{Fe(TPP)(2-MeIm}^-)]\cdot0.5\text{C}_6\text{H}_5\text{Cl}$.

Table S10. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for $[\text{K}\subset222][\text{Fe(TPP)(2-MeIm}^-)]\cdot0.5\text{C}_6\text{H}_5\text{Cl}$.

Table S11. Bond Lengths for $[\text{K}\subset222][\text{Fe(TPP)(2-MeIm}^-)]\cdot0.5\text{C}_6\text{H}_5\text{Cl}$.

Table S12. Bond Angles for $[\text{K}\subset222][\text{Fe(TPP)(2-MeIm}^-)]\cdot0.5\text{C}_6\text{H}_5\text{Cl}$.

Table S13. Anisotropic Isotropic Displacement Parameters for $[\text{K}\subset222][\text{Fe(TPP)(2-MeIm}^-)]\cdot0.5\text{C}_6\text{H}_5\text{Cl}$.

Table S14. Hydrogen Coordinates and Isotropic Displacement Parameters for $[\text{K}\subset222][\text{Fe(TPP)(2-MeIm}^-)]\cdot0.5\text{C}_6\text{H}_5\text{Cl}$.