Supporting Information for

Just a Proton: Distinguishing the Two Electronic States of Five-Coordinate High-Spin Iron(II) Porphyrinates with Imidazole/ate Coordination

Chuanjiang Hu, Corinne D. Sulok, Florian Paulat, Nicolai Lehnert, Anna I. Twigg, Michael P. Hendrich, Charles E. Schulz, and W. Robert Scheidt

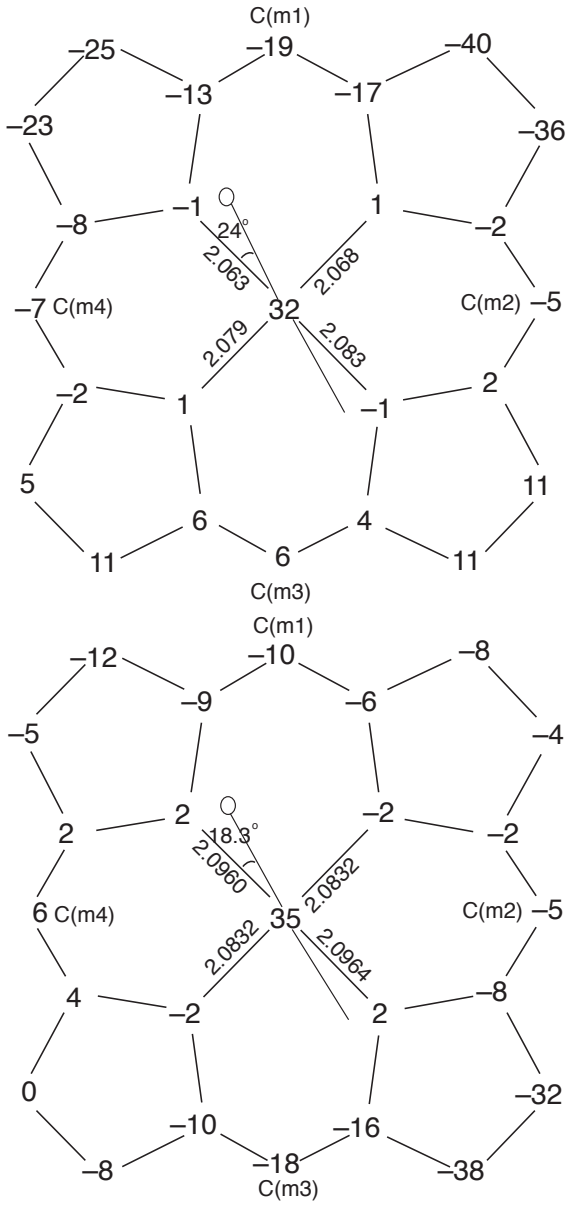

Figure S1. Formal core diagrams of [Fe(TPP)(2-MeHIm)] comparing the experimental structure determination (top) and calculated, optimized structure (bottom). Atomic displacements from the four nitrogen mean plane are shown in units of 0.01 ÅThe orientation of the imidazole ligand is shown with the circle denoting the methyl group position. The axial Fe–N_{Im} distances are 2.127(3) (obsd) and 2.1827 (calcd) Å.

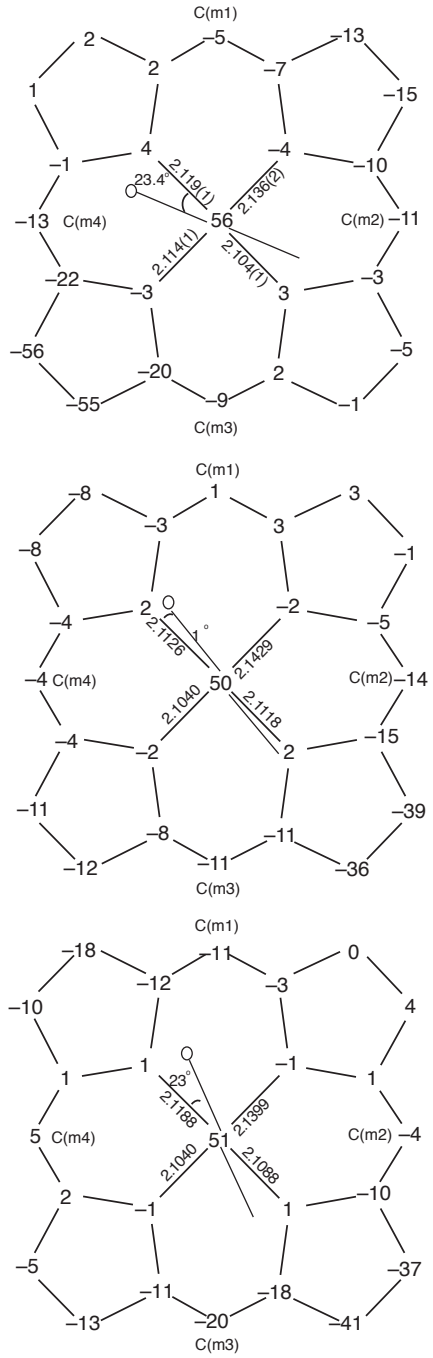

Figure S2. Formal core diagrams of $[Fe(TPP)(2\text{-}MeIm^{-})]^{-}$ comparing the experimental structure determination (top), calculated optimized structure (middle), calculated optimized structure (bottom) with fixed imidazole orientation. Atomic displacements from the four nitrogen mean plane are shown in units of 0.01 ÅṪhe orientation of the imidazole ligand is shown with the circle denoting the methyl group position. The axial $Fe–N_{Im}$ distances are 2.056(81) (obsd), 2.048 (calcd), and 2.051 (calcd-fixed).

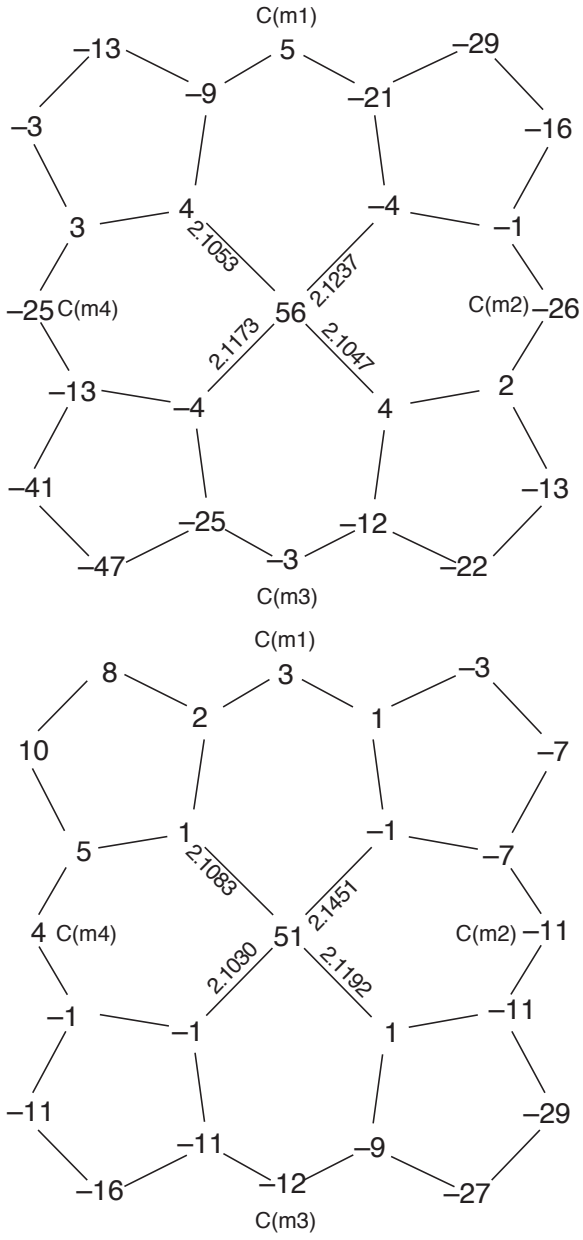

Figure S3. Formal core diagrams of $[Fe(TPP)Cl]^-$ comparing the experimental structure determination (top) and calculated, optimized structure (bottom). Atomic displacements from the four nitrogen mean plane are shown in units of 0.01 ÅṪhe axial Fe–Cl distances are 2.3400(5) (obsd) and 2.300 Å.

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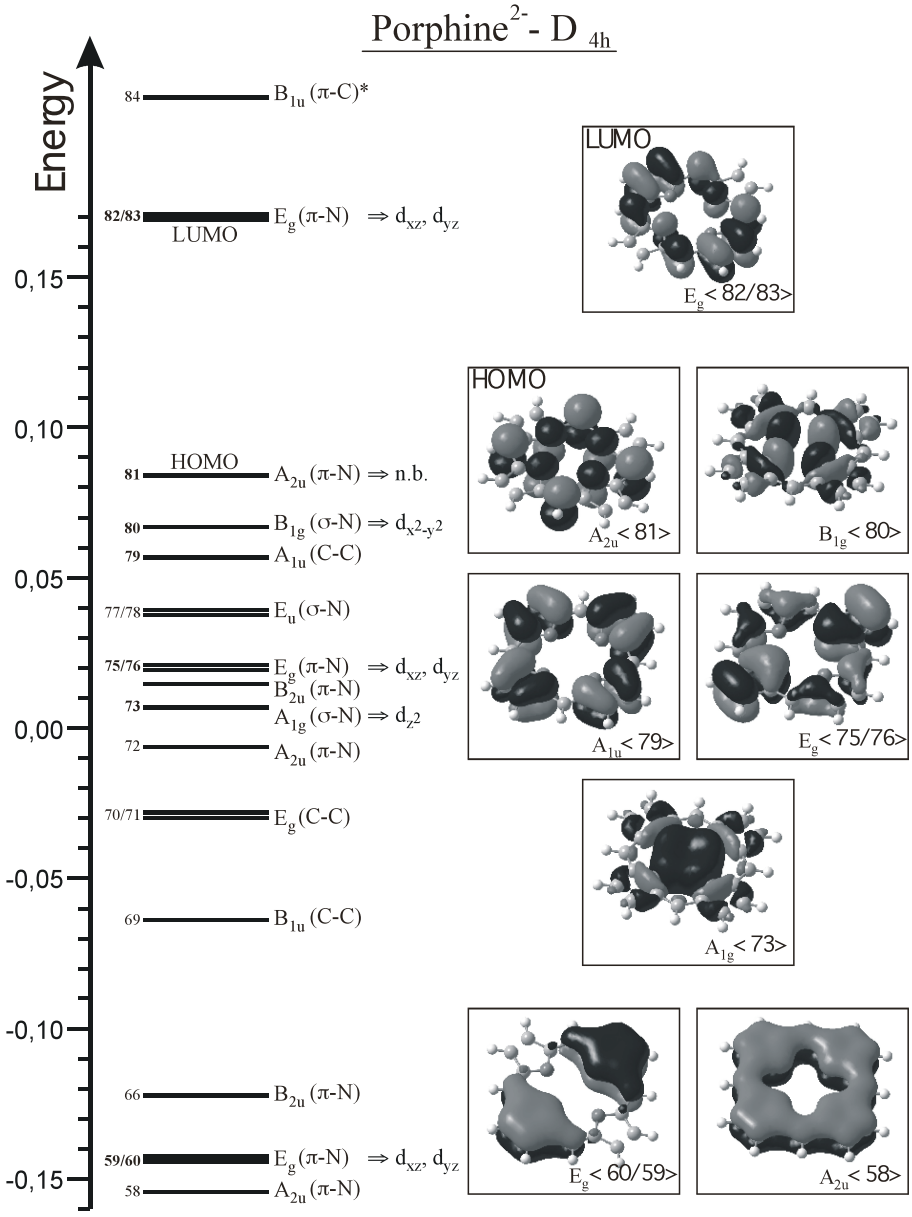

Figure S4. MO diagram of the free porphine(2-) ligand and contour plots. Energies are given in Hartrees. Metal d orbitals that could potentially interact with these MOs are indicated (using the coordinate system described in the text, where the z axis is orthogonal to the porphyrin ring).

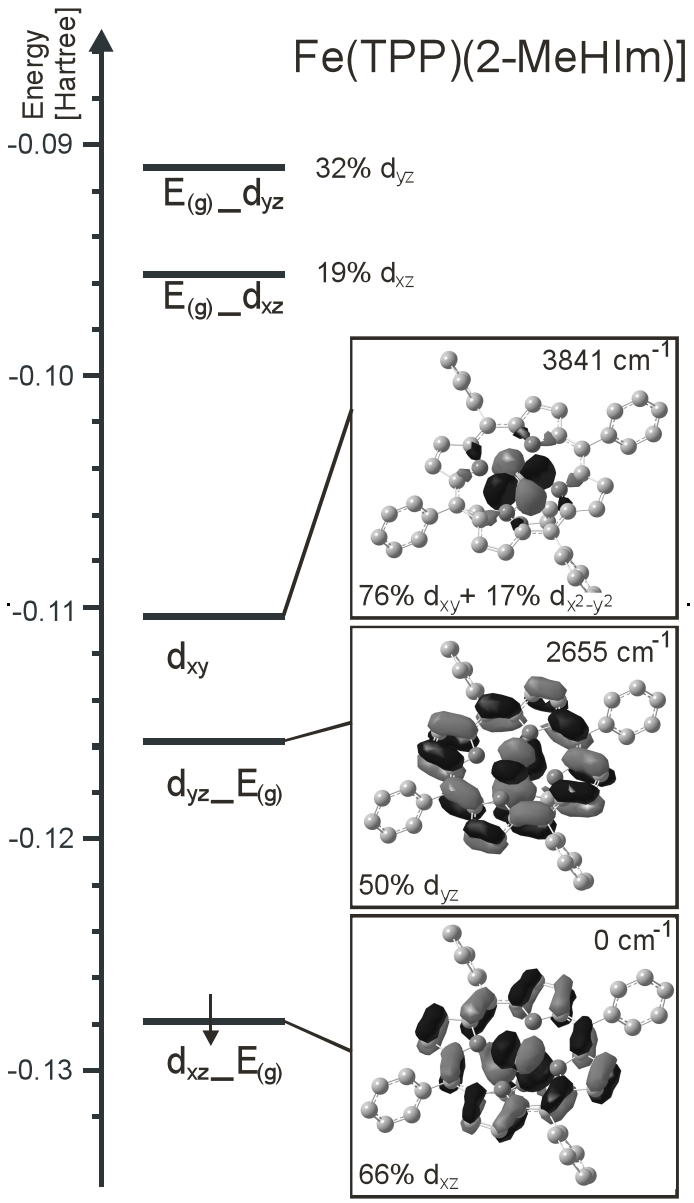

Figure S5. Frontier β-MO diagram of the fully optimized structure of [Fe(TPP)(2-MeHIm)] calculated with BP86/TZVP. The applied coordinate system is chosen such that x and y are located in the porphyrin plane, and z is orthogonal to the porphyrin ring in direction of the axial ligand. $E_{(g)}$ refers to the LUMO of the porphyrin as shown in Figure S4 (the index 'g' is put in brackets because of the low symmetry of the porphyrin core). The nomenclature a_b indicates that orbital a interacts with b and that a has a larger contribution to the resulting MO.

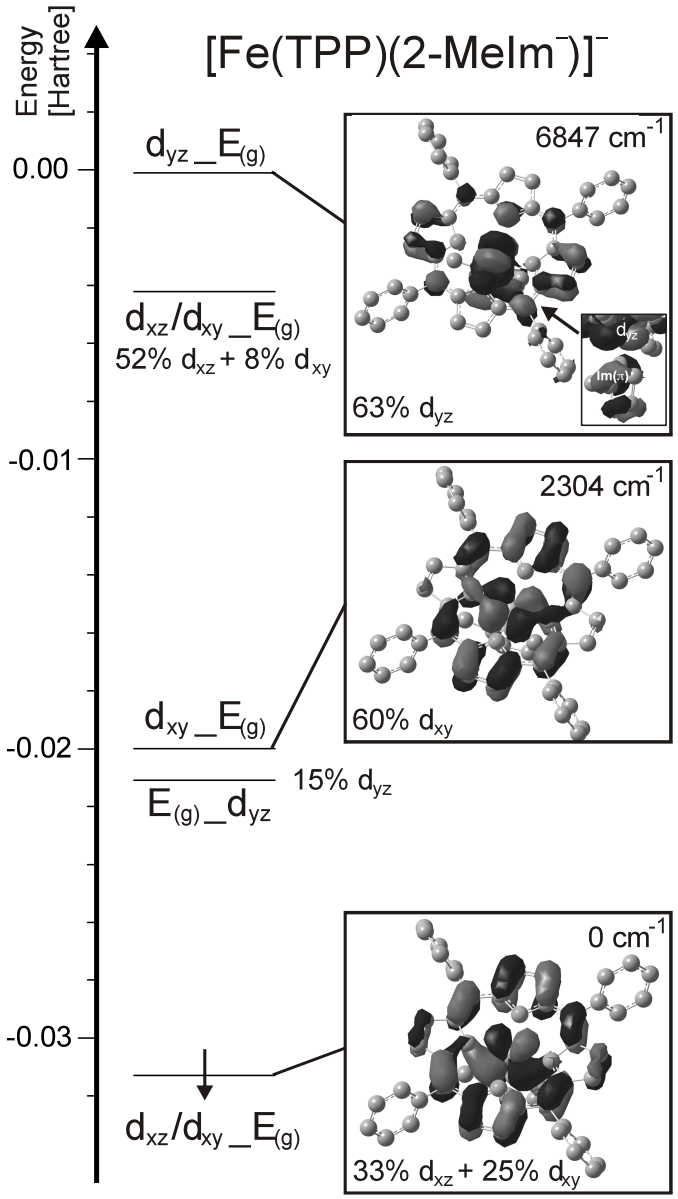

Figure S6. Frontier β-MO diagram of the fully optimized structure of [Fe(TPP)(2-MeIm$^-$)]$^-$ calculated with BP86/TZVP. The applied coordinate system is chosen such that x and y are located in the porphyrin plane, and z is orthogonal to the porphyrin ring in direction of the axial ligand. $E_{(g)}$ refers to the LUMO of the porphyrin as shown in Figure S4 (the index 'g' is put in brackets because of the low symmetry of the porphyrin core). The nomenclature a_b indicates that orbital a interacts with b and that a has a larger contribution to the resulting MO.

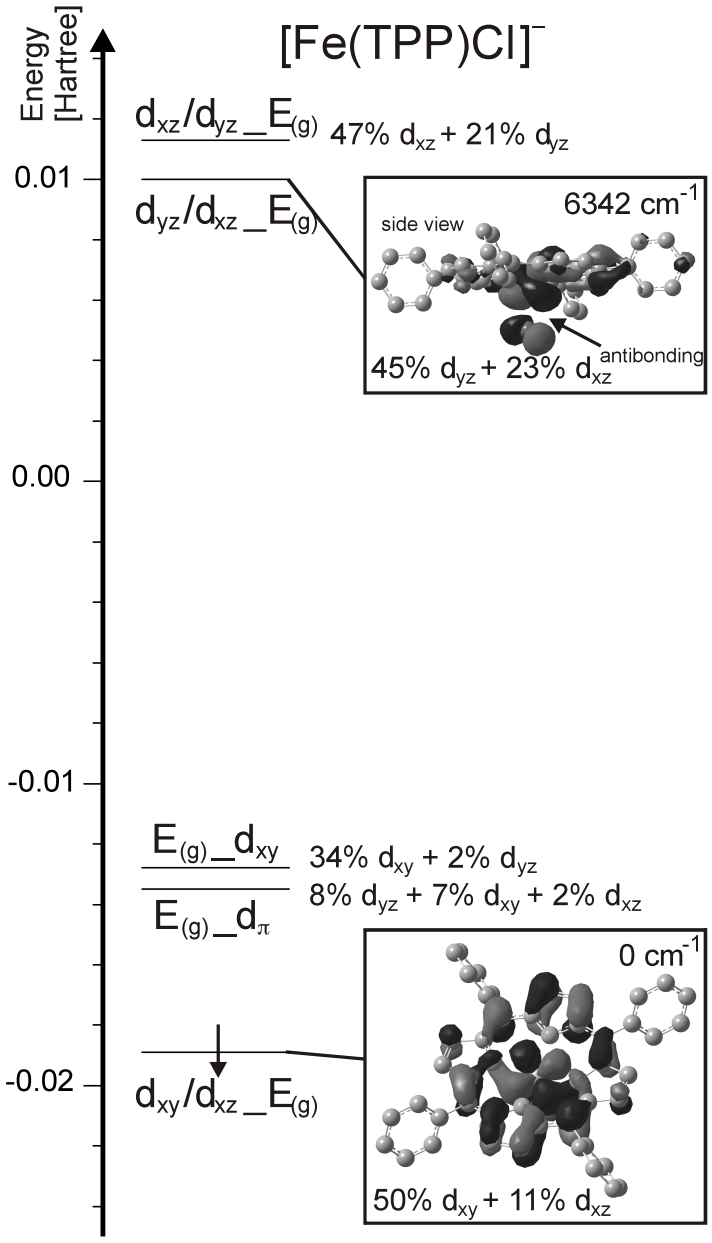

Figure S7. Frontier β-MO diagram of the fully optimized structure of $[Fe(TPP)(Cl)]^-$ calculated with BP86/TZVP. The applied coordinate system is chosen such that x and y are located in the porphyrin plane, and z is orthogonal to the porphyrin ring in direction of the axial ligand. $E_{(g)}$ refers to the LUMO of the porphyrin as shown in Figure S4 (the index 'g' is put in brackets because of the low symmetry of the porphyrin core). The nomenclature a_b indicates that orbital a interacts with b and that a has a larger contribution to the resulting MO.

X-ray Structure Determination of Na(222)[Fe(TPP)Cl].

Single crystal experiment was carried out on a Bruker Apex system with graphite monochromated Mo-K radiation ($\lambda = 0.71073$ Å). A red crystal with the dimensions $0.30 \times 0.50 \times 0.60$ mm^3 was used for the structure determination. It was glued to a glass fiber by epoxy cement and measured at room temperature. The structure was solved by direct methods using SHELXS-97[1] and refined against F^2 using SHELXL-97;[2, 3] subsequent difference Fourier syntheses led to the location of most of the remaining nonhydrogen atoms. For the structure refinement all data were used including negative intensities. The asymmetric unit contains one porphyrin molecule, one Na(222) cation and three methylenechloride solvate molecules. These solvate molecules are all disordered over two positions. In the same molecule, their C–Cl and Cl···Cl distances were constrained at 1.77 Å and 2.88 Å. The final refinement gave the occupancy as 0.61 for the major component of second methylenechloride and 0.57 for the major component of third one. Checkcif pointed out the short distances for Cl(3b)···Cl(6a) and Cl(3b)···C(3sa). These atoms are belong to different disordered methylenechloride solvate molecules, the sum of their occupancies is less than 1, so it is reasonable they can exist in the close region at different time. All nonhydrogen atoms were refined anisotropically if not remarked otherwise below. Hydrogen atoms were added with the standard SHELXL-97 idealization methods. The program SADABS[4] was applied for the absorption correction. The highest peak, 1.49 e/Å^3, is located 0.66 Å from the heavy atom Fe(1). Complete crystallographic details, atomic coordinates, anisotropic thermal parameters, and fixed hydrogen atom coordinates are given in the Supporting Information.

References and Notes

(1) Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467.

(2) Sheldrick, G. M.: Program for the Refinement of Crystal Structures. Universität Göttingen, Germany, 1997.

(3) $R_1 = \sum \parallel F_o| - |F_c \parallel / \sum |F_o|$ and $wR_2 = \left\{ \sum \left[w \left({F_o}^2 - {F_c}^2 \right)^2 \right] / \sum \left[w({F_o}^2)^2 \right] \right\}^{1/2}$. The conventional R-factors R_1 are based on F, with F set to zero for negative F^2. The criterion of $F^2 > 2\sigma(F^2)$ was used only for calculating R_1. R-factors based on F^2 (wR_2) are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

(4) Sheldrick, G. M.: Program for Empirical Absorption Correction of Area Detector Data. Universität Göttingen, Germany, 1996.

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Gaussian, Inc.: Pittsburgh, PA, 2003.

Table S1. Complete Crystallographic Details for Na(222)[Fe(TPP)Cl]

formula	$C_{65}H_{70}Cl_7FeN_6NaO_6$
FW, amu	1358.26
a, Å	12.720(2)
b, Å	12.902(2)
c, Å	22.267(4)
α, deg	85.756(8)
β, deg	83.340(7)
γ, deg	63.273(7)
V, Å^3	3241.0(9)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.392
F(000)	1412
μ, mm^{-1}	0.584
crystal dimensions, mm	0.60 × 0.50 × 0.30
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	0.92–30.88
index range	$-18 \leq h \leq 18$
	$-18 \leq k \leq 18$
	$-31 \leq l \leq 31$
total data collected	94826
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.8444 and 0.7209
unique data	19830 (R_{int} = 0.031)
unique observed data [I > 2σ(I)]	17903
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	19830/12/838
goodness-of-fit (pased on F^2)	1.044
final R indices [I > 2σ(I)]	R_1 = 0.0383, wR_2 = 0.1032
final R indices (all data)	R_1 = 0.0447, wR_2 = 0.1190

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for Na(222)[Fe(TPP)Cl][a]

atom	x	y	z	U(eq)
Fe(1)	0.24671(2)	0.11612(2)	0.24910(1)	0.0142(1)
N(1)	0.29849(9)	0.04821(9)	0.33572(5)	0.0149(2)
N(2)	0.31265(9)	−0.05999(9)	0.22491(5)	0.0146(2)
N(3)	0.28767(9)	0.14890(9)	0.15734(5)	0.0150(2)
N(4)	0.28600(9)	0.25337(9)	0.26724(5)	0.0153(2)
C(a1)	0.29380(11)	0.11306(11)	0.38309(5)	0.0159(2)
C(a2)	0.31890(10)	−0.05964(11)	0.35959(5)	0.0152(2)
C(a3)	0.33610(11)	−0.15490(10)	0.26306(5)	0.0153(2)
C(a4)	0.31329(11)	−0.09600(10)	0.16811(5)	0.0153(2)
C(a5)	0.29452(11)	0.08303(11)	0.11010(5)	0.0160(2)
C(a6)	0.29244(11)	0.24737(11)	0.13186(5)	0.0158(2)
C(a7)	0.29658(11)	0.33514(11)	0.22715(6)	0.0166(2)
C(a8)	0.29197(11)	0.28565(11)	0.32374(6)	0.0166(2)
C(b1)	0.30590(12)	0.04582(11)	0.43887(6)	0.0187(2)
C(b2)	0.32348(11)	−0.06197(11)	0.42444(6)	0.0181(2)
C(b3)	0.35132(12)	−0.25347(11)	0.22929(6)	0.0180(2)
C(b4)	0.33570(11)	−0.21625(11)	0.17067(6)	0.0177(2)
C(b5)	0.30077(13)	0.14261(12)	0.05322(6)	0.0209(2)
C(b6)	0.30024(13)	0.24413(12)	0.06661(6)	0.0209(2)
C(b7)	0.30878(13)	0.42196(12)	0.25934(6)	0.0214(2)
C(b8)	0.30707(13)	0.39101(12)	0.31894(6)	0.0211(2)
C(m1)	0.34078(11)	−0.15683(11)	0.32597(5)	0.0154(2)
C(m2)	0.30144(11)	−0.02881(11)	0.11465(5)	0.0158(2)
C(m3)	0.29679(11)	0.33507(10)	0.16401(6)	0.0160(2)
C(m4)	0.28978(11)	0.22411(11)	0.37813(6)	0.0163(2)
C(11)	0.37975(12)	−0.27161(11)	0.35857(6)	0.0177(2)
C(12)	0.30634(14)	−0.29374(13)	0.40411(7)	0.0249(3)
C(13)	0.34636(17)	−0.40113(16)	0.43466(8)	0.0335(3)
C(14)	0.45881(18)	−0.48772(14)	0.41945(8)	0.0353(4)
C(15)	0.53252(16)	−0.46716(13)	0.37400(8)	0.0311(3)
C(16)	0.49357(13)	−0.35939(12)	0.34405(6)	0.0231(3)
C(21)	0.29928(12)	−0.07895(11)	0.05644(5)	0.0171(2)
C(22)	0.19187(14)	−0.06192(16)	0.03798(7)	0.0293(3)
C(23)	0.18687(17)	−0.10199(19)	−0.01761(8)	0.0371(4)

Table S2. Continued

atom	x	y	z	U(eq)
C(24)	0.28888(16)	−0.15865(14)	−0.05541(7)	0.0290(3)
C(25)	0.39598(15)	−0.17498(13)	−0.03779(6)	0.0260(3)
C(26)	0.40130(13)	−0.13572(12)	0.01794(6)	0.0226(2)
C(31)	0.31431(12)	0.42836(11)	0.12668(6)	0.0184(2)
C(32)	0.22907(14)	0.50532(12)	0.08998(7)	0.0257(3)
C(33)	0.25333(18)	0.58339(14)	0.05101(7)	0.0332(3)
C(34)	0.36088(18)	0.58652(14)	0.04915(7)	0.0347(4)
C(35)	0.44478(16)	0.51263(15)	0.08618(8)	0.0320(3)
C(36)	0.42214(13)	0.43337(12)	0.12473(7)	0.0240(3)
C(41)	0.28715(11)	0.28058(11)	0.43504(6)	0.0172(2)
C(42)	0.18415(12)	0.37604(12)	0.45576(6)	0.0208(2)
C(43)	0.17989(14)	0.43281(13)	0.50736(6)	0.0250(3)
C(44)	0.27829(15)	0.39430(14)	0.53932(6)	0.0267(3)
C(45)	0.38099(15)	0.29868(15)	0.51975(7)	0.0295(3)
C(46)	0.38546(13)	0.24187(13)	0.46787(7)	0.0257(3)
Cl(1)	0.04051(3)	0.19186(3)	0.25907(2)	0.0254(1)
Na(1)	0.83104(5)	0.79629(5)	0.24711(3)	0.0210(1)
N(5)	0.94077(11)	0.79002(11)	0.34784(6)	0.0259(2)
N(6)	0.72095(12)	0.80110(12)	0.14957(6)	0.0268(2)
O(1)	0.94420(10)	0.92097(10)	0.23795(5)	0.0278(2)
O(2)	0.96321(11)	0.75697(11)	0.15071(6)	0.0323(2)
O(3)	0.97877(10)	0.60152(9)	0.27285(5)	0.0278(2)
O(4)	0.74767(11)	0.63688(10)	0.24822(5)	0.0294(2)
O(5)	0.69800(9)	0.86038(10)	0.33942(5)	0.0257(2)
O(6)	0.65197(9)	0.99557(10)	0.22735(5)	0.0280(2)
C(1C)	0.97987(15)	0.88167(14)	0.34170(8)	0.0307(3)
C(2C)	1.03267(14)	0.89268(14)	0.27898(9)	0.0328(3)
C(3C)	0.9918(2)	0.92108(17)	0.17683(9)	0.0404(4)
C(4C)	1.04952(18)	0.79946(19)	0.15220(10)	0.0445(5)
C(5C)	0.91174(17)	0.78055(16)	0.09490(8)	0.0363(4)
C(6C)	0.81505(16)	0.74153(15)	0.10166(7)	0.0325(3)
C(7C)	1.03989(15)	0.67373(14)	0.35081(9)	0.0335(3)
C(8C)	1.00752(15)	0.58106(14)	0.33399(8)	0.0312(3)
C(9C)	0.95675(16)	0.51212(14)	0.25118(8)	0.0333(3)

Table S2. Continued

atom	x	y	z	U(eq)
C(10C)	0.83274(16)	0.52895(15)	0.27174(8)	0.0328(3)
C(11C)	0.70657(16)	0.62389(15)	0.19375(8)	0.0317(3)
C(12C)	0.64503(16)	0.74212(16)	0.16350(8)	0.0336(3)
C(13C)	0.85455(16)	0.80874(16)	0.40108(7)	0.0324(3)
C(14C)	0.73284(15)	0.89899(16)	0.38836(7)	0.0307(3)
C(15C)	0.58250(13)	0.94101(15)	0.32440(8)	0.0297(3)
C(16C)	0.58621(14)	1.03877(14)	0.28426(8)	0.0312(3)
C(17C)	0.57610(13)	0.99733(14)	0.18413(8)	0.0304(3)
C(18C)	0.64991(15)	0.92305(15)	0.13171(8)	0.0319(3)
C(1S)	0.98001(19)	0.14126(19)	0.41938(10)	0.0462(5)
Cl(1a)	0.8803(2)	0.0945(2)	0.46443(13)	0.0564(4)
Cl(2a)	0.96360(15)	0.27039(14)	0.44444(10)	0.0730(4)
Cl(1b)	0.8627(6)	0.1225(5)	0.4566(3)	0.0564(4)
Cl(2b)	0.9382(4)	0.3017(3)	0.4167(2)	0.0730(4)
C(2Sa)	0.9896(6)	0.3169(6)	0.1173(4)	0.0281(12)
Cl(3a)	0.9761(4)	0.4250(3)	0.0603(2)	0.0425(6)
Cl(4a)	0.95794(15)	0.21178(10)	0.08969(6)	0.0621(4)
C(2Sb)	1.0059(9)	0.2975(9)	0.1092(7)	0.036(3)
Cl(3b)	0.8779(2)	0.2761(2)	0.11678(9)	0.0667(9)
Cl(4b)	0.9633(6)	0.4304(5)	0.0665(3)	0.0464(11)
C(3Sa)	0.7692(7)	0.2017(7)	0.2419(3)	0.0315(11)
Cl(5a)	0.7386(2)	0.2141(2)	0.32094(10)	0.0422(4)
Cl(6a)	0.69532(12)	0.33548(8)	0.20368(7)	0.0524(5)
C(3Sb)	0.7596(10)	0.2047(11)	0.2611(4)	0.0369(19)
Cl(6b)	0.63713(18)	0.3156(2)	0.22965(9)	0.0885(11)
Cl(5b)	0.7410(3)	0.2094(3)	0.34018(12)	0.0402(5)

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

Table S3. Bond Lengths for Na(222)[Fe(TPP)Cl][a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(1)	2.1088(11)	Na(1)–O(1)	2.5822(13)
Fe(1)–N(3)	2.1091(11)	Na(1)–O(6)	2.6057(13)
Fe(1)–N(4)	2.1207(11)	Na(1)–N(6)	2.6999(15)
Fe(1)–N(2)	2.1257(11)	Na(1)–O(4)	2.7025(14)
Fe(1)–Cl(1)	2.3400(5)	Na(1)–N(5)	2.7537(15)
N(1)–C(a2)	1.3725(16)	N(5)–C(7C)	1.466(2)
N(1)–C(a1)	1.3739(15)	N(5)–C(1C)	1.468(2)
N(2)–C(a3)	1.3734(15)	N(5)–C(13C)	1.473(2)
N(2)–C(a4)	1.3773(15)	N(6)–C(6C)	1.469(2)
N(3)–C(a5)	1.3713(15)	N(6)–C(18C)	1.470(2)
N(3)–C(a6)	1.3765(15)	N(6)–C(12C)	1.471(2)
N(4)–C(a7)	1.3743(16)	O(1)–C(3C)	1.424(2)
N(4)–C(a8)	1.3749(15)	O(1)–C(2C)	1.433(2)
C(a1)–C(m4)	1.4069(17)	O(2)–C(5C)	1.421(2)
C(a1)–C(b1)	1.4436(17)	O(2)–C(4C)	1.435(2)
C(a2)–C(m1)	1.4095(17)	O(3)–C(8C)	1.425(2)
C(a2)–C(b2)	1.4495(17)	O(3)–C(9C)	1.430(2)
C(a3)–C(m1)	1.4069(17)	O(4)–C(11C)	1.424(2)
C(a3)–C(b3)	1.4515(17)	O(4)–C(10C)	1.433(2)
C(a4)–C(m2)	1.4009(17)	O(5)–C(14C)	1.4223(19)
C(a4)–C(b4)	1.4438(17)	O(5)–C(15C)	1.4284(19)
C(a5)–C(m2)	1.4022(17)	O(6)–C(17C)	1.4318(19)
C(a5)–C(b5)	1.4454(17)	O(6)–C(16C)	1.434(2)
C(a6)–C(m3)	1.4076(17)	C(1C)–C(2C)	1.503(3)
C(a6)–C(b6)	1.4473(17)	C(1C)–H(1a)	0.9900
C(a7)–C(m3)	1.4056(17)	C(1C)–H(1b)	0.9900
C(a7)–C(b7)	1.4469(17)	C(2C)–H(2a)	0.9900
C(a8)–C(m4)	1.4028(18)	C(2C)–H(2b)	0.9900
C(a8)–C(b8)	1.4508(18)	C(3C)–C(4C)	1.517(3)
C(b1)–C(b2)	1.3629(18)	C(3C)–H(3a)	0.9900
C(b1)–H(b1)	0.9500	C(3C)–H(3b)	0.9900
C(b2)–H(b2)	0.9500	C(4C)–H(4a)	0.9900
C(b3)–C(b4)	1.3622(17)	C(4C)–H(4b)	0.9900
C(b3)–H(b3)	0.9500	C(5C)–C(6C)	1.514(3)

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(b4)–H(b4)	0.9500	C(5C)–H(5a)	0.9900
C(b5)–C(b6)	1.3616(18)	C(5C)–H(5b)	0.9900
C(b5)–H(b5)	0.9500	C(6C)–H(6a)	0.9900
C(b6)–H(b6)	0.9500	C(6C)–H(6b)	0.9900
C(b7)–C(b8)	1.3579(19)	C(7C)–C(8C)	1.511(2)
C(b7)–H(b7)	0.9500	C(7C)–H(7a)	0.9900
C(b8)–H(b8)	0.9500	C(7C)–H(7b)	0.9900
C(m1)–C(11)	1.4932(17)	C(8C)–H(8a)	0.9900
C(m2)–C(21)	1.4992(17)	C(8C)–H(8b)	0.9900
C(m3)–C(31)	1.4966(17)	C(9C)–C(10C)	1.511(3)
C(m4)–C(41)	1.4975(17)	C(9C)–H(9a)	0.9900
C(11)–C(16)	1.3979(19)	C(9C)–H(9b)	0.9900
C(11)–C(12)	1.3997(19)	C(10C)–H(10a)	0.9900
C(12)–C(13)	1.396(2)	C(10C)–H(10b)	0.9900
C(12)–H(12)	0.9500	C(11C)–C(12C)	1.513(2)
C(13)–C(14)	1.384(3)	C(11C)–H(11a)	0.9900
C(13)–H(13)	0.9500	C(11C)–H(11b)	0.9900
C(14)–C(15)	1.392(3)	C(12C)–H(12a)	0.9900
C(14)–H(14)	0.9500	C(12C)–H(12b)	0.9900
C(15)–C(16)	1.394(2)	C(13C)–C(14C)	1.505(2)
C(15)–H(15)	0.9500	C(13C)–H(13a)	0.9900
C(16)–H(16)	0.9500	C(13C)–H(13b)	0.9900
C(21)–C(22)	1.3896(19)	C(14C)–H(14a)	0.9900
C(21)–C(26)	1.3912(19)	C(14C)–H(14b)	0.9900
C(22)–C(23)	1.395(2)	C(15C)–C(16C)	1.506(3)
C(22)–H(22)	0.9500	C(15C)–H(15a)	0.9900
C(23)–C(24)	1.382(3)	C(15C)–H(15b)	0.9900
C(23)–H(23)	0.9500	C(16C)–H(16a)	0.9900
C(24)–C(25)	1.381(2)	C(16C)–H(16b)	0.9900
C(24)–H(24)	0.9500	C(17C)–C(18C)	1.505(3)
C(25)–C(26)	1.3945(18)	C(17C)–H(17a)	0.9900
C(25)–H(25)	0.9500	C(17C)–H(17b)	0.9900
C(26)–H(26)	0.9500	C(18C)–H(18a)	0.9900
C(31)–C(32)	1.395(2)	C(18C)–H(18b)	0.9900

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(31)–C(36)	1.3974(19)	C(1S)–Cl(2a)	1.711(2)
C(32)–C(33)	1.397(2)	C(1S)–Cl(1b)	1.727(6)
C(32)–H(32)	0.9500	C(1S)–Cl(1a)	1.812(3)
C(33)–C(34)	1.382(3)	C(1S)–Cl(2b)	1.889(4)
C(33)–H(33)	0.9500	C(1S)–H(1S1)	0.9900
C(34)–C(35)	1.378(3)	C(1S)–H(1S2)	0.9900
C(34)–H(34)	0.9500	C(2Sa)–Cl(4a)	1.746(6)
C(35)–C(36)	1.394(2)	C(2Sa)–Cl(3a)	1.776(6)
C(35)–H(35)	0.9500	C(2Sa)–H(2Sa)	0.9900
C(36)–H(36)	0.9500	C(2Sa)–H(2Sb)	0.9900
C(41)–C(42)	1.3925(18)	C(2Sb)–Cl(3b)	1.756(9)
C(41)–C(46)	1.3943(18)	C(2Sb)–Cl(4b)	1.784(8)
C(42)–C(43)	1.3906(18)	C(2Sb)–H(2SC)	0.9900
C(42)–H(42)	0.9500	C(2Sb)–H(2Sd)	0.9900
C(43)–C(44)	1.384(2)	C(3Sa)–Cl(6a)	1.759(8)
C(43)–H(43)	0.9500	C(3Sa)–Cl(5a)	1.762(6)
C(44)–C(45)	1.384(2)	C(3Sa)–H(3Sa)	0.9900
C(44)–H(44)	0.9500	C(3Sa)–H(3Sb)	0.9900
C(45)–C(46)	1.395(2)	C(3Sb)–Cl(5b)	1.750(8)
C(45)–H(45)	0.9500	C(3Sb)–Cl(6b)	1.751(12)
C(46)–H(46)	0.9500	C(3Sb)–H(3SC)	0.9900
Na(1)–O(5)	2.4410(12)	C(3Sb)–H(3Sd)	0.9900
Na(1)–O(3)	2.4420(12)		
Na(1)–O(2)	2.4997(13)		

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

Table S4. Bond Angles for Na(222)[Fe(TPP)Cl][a]

angle	degree	angle	degree
N(1)–Fe(1)–N(3)	151.13(4)	O(6)–Na(1)–N(5)	113.94(4)
N(1)–Fe(1)–N(4)	86.75(4)	N(6)–Na(1)–N(5)	178.99(5)
N(3)–Fe(1)–N(4)	85.58(4)	O(4)–Na(1)–N(5)	114.82(4)
N(1)–Fe(1)–N(2)	85.42(4)	C(7C)–N(5)–C(1C)	112.30(13)
N(3)–Fe(1)–N(2)	86.18(4)	C(7C)–N(5)–C(13C)	110.48(13)
N(4)–Fe(1)–N(2)	147.34(4)	C(1C)–N(5)–C(13C)	110.70(14)
N(1)–Fe(1)–Cl(1)	105.00(3)	C(7C)–N(5)–Na(1)	106.28(10)
N(3)–Fe(1)–Cl(1)	103.86(3)	C(1C)–N(5)–Na(1)	109.07(9)
N(4)–Fe(1)–Cl(1)	106.53(3)	C(13C)–N(5)–Na(1)	107.80(9)
N(2)–Fe(1)–Cl(1)	106.13(3)	C(6C)–N(6)–C(18C)	110.37(13)
C(a2)–N(1)–C(a1)	106.38(10)	C(6C)–N(6)–C(12C)	110.94(14)
C(a2)–N(1)–Fe(1)	127.61(8)	C(18C)–N(6)–C(12C)	110.33(13)
C(a1)–N(1)–Fe(1)	124.76(8)	C(6C)–N(6)–Na(1)	106.11(9)
C(a3)–N(2)–C(a4)	106.19(10)	C(18C)–N(6)–Na(1)	108.33(10)
C(a3)–N(2)–Fe(1)	127.53(8)	C(12C)–N(6)–Na(1)	110.64(9)
C(a4)–N(2)–Fe(1)	124.72(8)	C(3C)–O(1)–C(2C)	111.18(14)
C(a5)–N(3)–C(a6)	106.23(10)	C(3C)–O(1)–Na(1)	108.84(10)
C(a5)–N(3)–Fe(1)	125.12(8)	C(2C)–O(1)–Na(1)	116.73(9)
C(a6)–N(3)–Fe(1)	127.79(8)	C(5C)–O(2)–C(4C)	113.55(15)
C(a7)–N(4)–C(a8)	106.28(10)	C(5C)–O(2)–Na(1)	118.80(10)
C(a7)–N(4)–Fe(1)	127.85(8)	C(4C)–O(2)–Na(1)	111.34(10)
C(a8)–N(4)–Fe(1)	125.46(8)	C(8C)–O(3)–C(9C)	112.57(12)
N(1)–C(a1)–C(m4)	125.67(11)	C(8C)–O(3)–Na(1)	116.46(9)
N(1)–C(a1)–C(b1)	109.93(11)	C(9C)–O(3)–Na(1)	112.81(9)
C(m4)–C(a1)–C(b1)	124.12(11)	C(11C)–O(4)–C(10C)	112.69(13)
N(1)–C(a2)–C(m1)	125.41(11)	C(11C)–O(4)–Na(1)	117.29(9)
N(1)–C(a2)–C(b2)	110.04(10)	C(10C)–O(4)–Na(1)	108.82(9)
C(m1)–C(a2)–C(b2)	124.41(11)	C(14C)–O(5)–C(15C)	111.67(12)
N(2)–C(a3)–C(m1)	125.71(11)	C(14C)–O(5)–Na(1)	119.73(9)
N(2)–C(a3)–C(b3)	109.95(10)	C(15C)–O(5)–Na(1)	109.68(9)
C(m1)–C(a3)–C(b3)	124.29(11)	C(17C)–O(6)–C(16C)	111.01(12)
N(2)–C(a4)–C(m2)	125.38(11)	C(17C)–O(6)–Na(1)	116.43(9)
N(2)–C(a4)–C(b4)	110.22(11)	C(16C)–O(6)–Na(1)	108.31(9)
C(m2)–C(a4)–C(b4)	124.29(11)	N(5)–C(1C)–C(2C)	113.14(14)

Table S4. Continued

angle	degree	angle	degree
N(3)–C(a5)–C(m2)	126.12(11)	N(5)–C(1C)–H(1a)	109.0
N(3)–C(a5)–C(b5)	110.16(11)	C(2C)–C(1C)–H(1a)	109.0
C(m2)–C(a5)–C(b5)	123.63(11)	N(5)–C(1C)–H(1b)	109.0
N(3)–C(a6)–C(m3)	125.26(11)	C(2C)–C(1C)–H(1b)	109.0
N(3)–C(a6)–C(b6)	110.00(11)	H(1a)–C(1C)–H(1b)	107.8
C(m3)–C(a6)–C(b6)	124.63(11)	O(1)–C(2C)–C(1C)	108.23(12)
N(4)–C(a7)–C(m3)	125.58(11)	O(1)–C(2C)–H(2a)	110.1
N(4)–C(a7)–C(b7)	110.03(11)	C(1C)–C(2C)–H(2a)	110.1
C(m3)–C(a7)–C(b7)	124.39(12)	O(1)–C(2C)–H(2b)	110.1
N(4)–C(a8)–C(m4)	125.81(11)	C(1C)–C(2C)–H(2b)	110.1
N(4)–C(a8)–C(b8)	109.90(11)	H(2a)–C(2C)–H(2b)	108.4
C(m4)–C(a8)–C(b8)	124.22(11)	O(1)–C(3C)–C(4C)	110.75(15)
C(b2)–C(b1)–C(a1)	107.07(11)	O(1)–C(3C)–H(3a)	109.5
C(b2)–C(b1)–H(b1)	126.5	C(4C)–C(3C)–H(3a)	109.5
C(a1)–C(b1)–H(b1)	126.5	O(1)–C(3C)–H(3b)	109.5
C(b1)–C(b2)–C(a2)	106.51(11)	C(4C)–C(3C)–H(3b)	109.5
C(b1)–C(b2)–H(b2)	126.7	H(3a)–C(3C)–H(3b)	108.1
C(a2)–C(b2)–H(b2)	126.7	O(2)–C(4C)–C(3C)	110.43(15)
C(b4)–C(b3)–C(a3)	106.82(11)	O(2)–C(4C)–H(4a)	109.6
C(b4)–C(b3)–H(b3)	126.6	C(3C)–C(4C)–H(4a)	109.6
C(a3)–C(b3)–H(b3)	126.6	O(2)–C(4C)–H(4b)	109.6
C(b3)–C(b4)–C(a4)	106.80(11)	C(3C)–C(4C)–H(4b)	109.6
C(b3)–C(b4)–H(b4)	126.6	H(4a)–C(4C)–H(4b)	108.1
C(a4)–C(b4)–H(b4)	126.6	O(2)–C(5C)–C(6C)	107.88(13)
C(b6)–C(b5)–C(a5)	106.87(11)	O(2)–C(5C)–H(5a)	110.1
C(b6)–C(b5)–H(b5)	126.6	C(6C)–C(5C)–H(5a)	110.1
C(a5)–C(b5)–H(b5)	126.6	O(2)–C(5C)–H(5b)	110.1
C(b5)–C(b6)–C(a6)	106.73(11)	C(6C)–C(5C)–H(5b)	110.1
C(b5)–C(b6)–H(b6)	126.6	H(5a)–C(5C)–H(5b)	108.4
C(a6)–C(b6)–H(b6)	126.6	N(6)–C(6C)–C(5C)	113.51(14)
C(b8)–C(b7)–C(a7)	106.95(12)	N(6)–C(6C)–H(6a)	108.9
C(b8)–C(b7)–H(b7)	126.5	C(5C)–C(6C)–H(6a)	108.9
C(a7)–C(b7)–H(b7)	126.5	N(6)–C(6C)–H(6b)	108.9
C(b7)–C(b8)–C(a8)	106.82(11)	C(5C)–C(6C)–H(6b)	108.9

Table S4. Continued

angle	degree	angle	degree
C(b7)–C(b8)–H(b8)	126.6	H(6a)–C(6C)–H(6b)	107.7
C(a8)–C(b8)–H(b8)	126.6	N(5)–C(7C)–C(8C)	111.94(13)
C(a3)–C(m1)–C(a2)	124.60(11)	N(5)–C(7C)–H(7a)	109.2
C(a3)–C(m1)–C(11)	117.46(11)	C(8C)–C(7C)–H(7a)	109.2
C(a2)–C(m1)–C(11)	117.80(11)	N(5)–C(7C)–H(7b)	109.2
C(a4)–C(m2)–C(a5)	125.22(11)	C(8C)–C(7C)–H(7b)	109.2
C(a4)–C(m2)–C(21)	119.04(11)	H(7a)–C(7C)–H(7b)	107.9
C(a5)–C(m2)–C(21)	115.71(11)	O(3)–C(8C)–C(7C)	108.58(13)
C(a7)–C(m3)–C(a6)	124.92(11)	O(3)–C(8C)–H(8a)	110.0
C(a7)–C(m3)–C(31)	118.63(11)	C(7C)–C(8C)–H(8a)	110.0
C(a6)–C(m3)–C(31)	116.19(11)	O(3)–C(8C)–H(8b)	110.0
C(a8)–C(m4)–C(a1)	125.34(11)	C(7C)–C(8C)–H(8b)	110.0
C(a8)–C(m4)–C(41)	116.64(11)	H(8a)–C(8C)–H(8b)	108.4
C(a1)–C(m4)–C(41)	117.98(11)	O(3)–C(9C)–C(10C)	111.38(14)
C(16)–C(11)–C(12)	118.69(12)	O(3)–C(9C)–H(9a)	109.4
C(16)–C(11)–C(m1)	119.30(12)	C(10C)–C(9C)–H(9a)	109.4
C(12)–C(11)–C(m1)	122.00(12)	O(3)–C(9C)–H(9b)	109.4
C(13)–C(12)–C(11)	120.61(15)	C(10C)–C(9C)–H(9b)	109.4
C(13)–C(12)–H(12)	119.7	H(9a)–C(9C)–H(9b)	108.0
C(11)–C(12)–H(12)	119.7	O(4)–C(10C)–C(9C)	110.35(13)
C(14)–C(13)–C(12)	120.14(15)	O(4)–C(10C)–H(10a)	109.6
C(14)–C(13)–H(13)	119.9	C(9C)–C(10C)–H(10a)	109.6
C(12)–C(13)–H(13)	119.9	O(4)–C(10C)–H(10b)	109.6
C(13)–C(14)–C(15)	119.87(14)	C(9C)–C(10C)–H(10b)	109.6
C(13)–C(14)–H(14)	120.1	H(10a)–C(10C)–H(10b)	108.1
C(15)–C(14)–H(14)	120.1	O(4)–C(11C)–C(12C)	108.77(14)
C(14)–C(15)–C(16)	120.15(16)	O(4)–C(11C)–H(11a)	109.9
C(14)–C(15)–H(15)	119.9	C(12C)–C(11C)–H(11a)	109.9
C(16)–C(15)–H(15)	119.9	O(4)–C(11C)–H(11b)	109.9
C(15)–C(16)–C(11)	120.53(15)	C(12C)–C(11C)–H(11b)	109.9
C(15)–C(16)–H(16)	119.7	H(11a)–C(11C)–H(11b)	108.3
C(11)–C(16)–H(16)	119.7	N(6)–C(12C)–C(11C)	113.51(14)
C(22)–C(21)–C(26)	118.46(12)	N(6)–C(12C)–H(12a)	108.9
C(22)–C(21)–C(m2)	119.57(12)	C(11C)–C(12C)–H(12a)	108.9

Table S4. Continued

angle	degree	angle	degree
C(26)–C(21)–C(m2)	121.82(12)	N(6)–C(12C)–H(12b)	108.9
C(21)–C(22)–C(23)	120.65(15)	C(11C)–C(12C)–H(12b)	108.9
C(21)–C(22)–H(22)	119.7	H(12a)–C(12C)–H(12b)	107.7
C(23)–C(22)–H(22)	119.7	N(5)–C(13C)–C(14C)	111.74(13)
C(24)–C(23)–C(22)	120.39(15)	N(5)–C(13C)–H(13a)	109.3
C(24)–C(23)–H(23)	119.8	C(14C)–C(13C)–H(13a)	109.3
C(22)–C(23)–H(23)	119.8	N(5)–C(13C)–H(13b)	109.3
C(25)–C(24)–C(23)	119.44(13)	C(14C)–C(13C)–H(13b)	109.3
C(25)–C(24)–H(24)	120.3	H(13a)–C(13C)–H(13b)	107.9
C(23)–C(24)–H(24)	120.3	O(5)–C(14C)–C(13C)	107.86(13)
C(24)–C(25)–C(26)	120.28(14)	O(5)–C(14C)–H(14a)	110.1
C(24)–C(25)–H(25)	119.9	C(13C)–C(14C)–H(14a)	110.1
C(26)–C(25)–H(25)	119.9	O(5)–C(14C)–H(14b)	110.1
C(21)–C(26)–C(25)	120.78(13)	C(13C)–C(14C)–H(14b)	110.1
C(21)–C(26)–H(26)	119.6	H(14a)–C(14C)–H(14b)	108.4
C(25)–C(26)–H(26)	119.6	O(5)–C(15C)–C(16C)	111.28(12)
C(32)–C(31)–C(36)	118.77(13)	O(5)–C(15C)–H(15a)	109.4
C(32)–C(31)–C(m3)	121.63(12)	C(16C)–C(15C)–H(15a)	109.4
C(36)–C(31)–C(m3)	119.42(12)	O(5)–C(15C)–H(15b)	109.4
C(31)–C(32)–C(33)	120.07(15)	C(16C)–C(15C)–H(15b)	109.4
C(31)–C(32)–H(32)	120.0	H(15a)–C(15C)–H(15b)	108.0
C(33)–C(32)–H(32)	120.0	O(6)–C(16C)–C(15C)	110.51(13)
C(34)–C(33)–C(32)	120.47(16)	O(6)–C(16C)–H(16a)	109.5
C(34)–C(33)–H(33)	119.8	C(15C)–C(16C)–H(16a)	109.5
C(32)–C(33)–H(33)	119.8	O(6)–C(16C)–H(16b)	109.5
C(35)–C(34)–C(33)	119.95(14)	C(15C)–C(16C)–H(16b)	109.5
C(35)–C(34)–H(34)	120.0	H(16a)–C(16C)–H(16b)	108.1
C(33)–C(34)–H(34)	120.0	O(6)–C(17C)–C(18C)	109.33(13)
C(34)–C(35)–C(36)	120.10(16)	O(6)–C(17C)–H(17a)	109.8
C(34)–C(35)–H(35)	120.0	C(18C)–C(17C)–H(17a)	109.8
C(36)–C(35)–H(35)	120.0	O(6)–C(17C)–H(17b)	109.8
C(35)–C(36)–C(31)	120.62(15)	C(18C)–C(17C)–H(17b)	109.8
C(35)–C(36)–H(36)	119.7	H(17a)–C(17C)–H(17b)	108.3
C(31)–C(36)–H(36)	119.7	N(6)–C(18C)–C(17C)	113.06(13)

Table S4. Continued

angle	degree	angle	degree
C(42)–C(41)–C(46)	118.41(12)	N(6)–C(18C)–H(18a)	109.0
C(42)–C(41)–C(m4)	119.41(11)	C(17C)–C(18C)–H(18a)	109.0
C(46)–C(41)–C(m4)	122.17(12)	N(6)–C(18C)–H(18b)	109.0
C(43)–C(42)–C(41)	120.88(13)	C(17C)–C(18C)–H(18b)	109.0
C(43)–C(42)–H(42)	119.6	H(18a)–C(18C)–H(18b)	107.8
C(41)–C(42)–H(42)	119.6	Cl(2a)–C(1S)–Cl(1b)	104.7(3)
C(44)–C(43)–C(42)	120.23(13)	Cl(2a)–C(1S)–Cl(1a)	110.43(15)
C(44)–C(43)–H(43)	119.9	Cl(1b)–C(1S)–Cl(2b)	107.8(3)
C(42)–C(43)–H(43)	119.9	Cl(1a)–C(1S)–Cl(2b)	117.23(18)
C(43)–C(44)–C(45)	119.63(13)	Cl(2a)–C(1S)–H(1S1)	109.6
C(43)–C(44)–H(44)	120.2	Cl(1b)–C(1S)–H(1S1)	121.3
C(45)–C(44)–H(44)	120.2	Cl(1a)–C(1S)–H(1S1)	109.6
C(44)–C(45)–C(46)	120.17(14)	Cl(2b)–C(1S)–H(1S1)	122.1
C(44)–C(45)–H(45)	119.9	Cl(2a)–C(1S)–H(1S2)	109.6
C(46)–C(45)–H(45)	119.9	Cl(1b)–C(1S)–H(1S2)	103.2
C(41)–C(46)–C(45)	120.66(14)	Cl(1a)–C(1S)–H(1S2)	109.6
C(41)–C(46)–H(46)	119.7	Cl(2b)–C(1S)–H(1S2)	86.9
C(45)–C(46)–H(46)	119.7	H(1S1)–C(1S)–H(1S2)	108.1
O(5)–Na(1)–O(3)	104.38(5)	Cl(4a)–C(2Sa)–Cl(3a)	109.9(4)
O(5)–Na(1)–O(2)	172.67(5)	Cl(4a)–C(2Sa)–H(2Sa)	109.7
O(3)–Na(1)–O(2)	81.55(5)	Cl(3a)–C(2Sa)–H(2Sa)	109.7
O(5)–Na(1)–O(1)	104.69(4)	Cl(4a)–C(2Sa)–H(2Sb)	109.7
O(3)–Na(1)–O(1)	104.36(4)	Cl(3a)–C(2Sa)–H(2Sb)	109.7
O(2)–Na(1)–O(1)	69.28(4)	H(2Sa)–C(2Sa)–H(2Sb)	108.2
O(5)–Na(1)–O(6)	69.96(4)	Cl(3b)–C(2Sb)–Cl(4b)	103.5(6)
O(3)–Na(1)–O(6)	172.09(4)	Cl(3b)–C(2Sb)–H(2SC)	111.1
O(2)–Na(1)–O(6)	104.55(5)	Cl(4b)–C(2Sb)–H(2SC)	111.1
O(1)–Na(1)–O(6)	82.72(4)	Cl(3b)–C(2Sb)–H(2Sd)	111.1
O(5)–Na(1)–N(6)	113.63(5)	Cl(4b)–C(2Sb)–H(2Sd)	111.1
O(3)–Na(1)–N(6)	112.82(5)	H(2SC)–C(2Sb)–H(2Sd)	109.0
O(2)–Na(1)–N(6)	66.98(5)	Cl(6a)–C(3Sa)–Cl(5a)	112.0(4)
O(1)–Na(1)–N(6)	115.81(4)	Cl(6a)–C(3Sa)–H(3Sa)	109.2
O(6)–Na(1)–N(6)	66.08(4)	Cl(5a)–C(3Sa)–H(3Sa)	109.2
O(5)–Na(1)–O(4)	83.50(4)	Cl(6a)–C(3Sa)–H(3Sb)	109.2

Table S4. Continued

angle	degree	angle	degree
O(3)–Na(1)–O(4)	67.81(4)	Cl(5a)–C(3Sa)–H(3Sb)	109.2
O(2)–Na(1)–O(4)	102.93(4)	H(3Sa)–C(3Sa)–H(3Sb)	107.9
O(1)–Na(1)–O(4)	170.16(4)	Cl(5b)–C(3Sb)–Cl(6b)	110.8(6)
O(6)–Na(1)–O(4)	105.51(4)	Cl(5b)–C(3Sb)–H(3SC)	109.5
N(6)–Na(1)–O(4)	64.31(4)	Cl(6b)–C(3Sb)–H(3SC)	109.5
O(5)–Na(1)–N(5)	65.58(4)	Cl(5b)–C(3Sb)–H(3Sd)	109.5
O(3)–Na(1)–N(5)	67.00(4)	Cl(6b)–C(3Sb)–H(3Sd)	109.5
O(2)–Na(1)–N(5)	113.89(5)	H(3SC)–C(3Sb)–H(3Sd)	108.1
O(1)–Na(1)–N(5)	65.15(4)		

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

Table S5. Anisotropic Displacement Parameters (Å^2) for Na(222)[Fe(TPP)Cl][a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0165(1)	0.0136(1)	0.0128(1)	−0.0007(1)	−0.0021(1)	−0.0069(1)
N(1)	0.0162(4)	0.0144(4)	0.0137(4)	−0.0014(3)	−0.0013(3)	−0.0064(4)
N(2)	0.0176(4)	0.0143(4)	0.0122(4)	−0.0003(3)	−0.0013(3)	−0.0073(4)
N(3)	0.0178(4)	0.0141(4)	0.0143(4)	−0.0011(3)	−0.0014(3)	−0.0080(4)
N(4)	0.0174(4)	0.0153(4)	0.0139(4)	−0.0010(3)	−0.0028(3)	−0.0074(4)
C(A1)	0.0166(5)	0.0159(5)	0.0137(5)	−0.0019(4)	−0.0014(4)	−0.0058(4)
C(A2)	0.0156(5)	0.0164(5)	0.0136(5)	0.0000(4)	−0.0012(4)	−0.0073(4)
C(A3)	0.0174(5)	0.0142(5)	0.0152(5)	−0.0010(4)	−0.0014(4)	−0.0078(4)
C(A4)	0.0168(5)	0.0150(5)	0.0151(5)	−0.0026(4)	−0.0011(4)	−0.0078(4)
C(A5)	0.0196(5)	0.0165(5)	0.0128(5)	−0.0003(4)	−0.0019(4)	−0.0087(4)
C(A6)	0.0189(5)	0.0156(5)	0.0131(5)	0.0006(4)	−0.0010(4)	−0.0082(4)
C(A7)	0.0189(5)	0.0150(5)	0.0169(5)	−0.0018(4)	−0.0016(4)	−0.0083(4)
C(A8)	0.0169(5)	0.0157(5)	0.0167(5)	−0.0038(4)	−0.0021(4)	−0.0062(4)
C(B1)	0.0232(6)	0.0196(5)	0.0129(5)	−0.0014(4)	−0.0009(4)	−0.0091(5)
C(B2)	0.0218(5)	0.0188(5)	0.0137(5)	0.0007(4)	−0.0015(4)	−0.0093(4)
C(B3)	0.0235(6)	0.0155(5)	0.0170(5)	−0.0004(4)	−0.0029(4)	−0.0103(4)
C(B4)	0.0227(6)	0.0158(5)	0.0166(5)	−0.0023(4)	−0.0022(4)	−0.0100(4)
C(B5)	0.0319(7)	0.0197(6)	0.0131(5)	−0.0003(4)	−0.0017(5)	−0.0133(5)
C(B6)	0.0301(6)	0.0194(6)	0.0150(5)	0.0000(4)	−0.0009(5)	−0.0128(5)
C(B7)	0.0302(6)	0.0189(6)	0.0194(6)	−0.0030(4)	−0.0011(5)	−0.0146(5)
C(B8)	0.0283(6)	0.0196(6)	0.0189(6)	−0.0041(4)	−0.0016(5)	−0.0135(5)
C(M1)	0.0169(5)	0.0156(5)	0.0144(5)	0.0007(4)	−0.0018(4)	−0.0080(4)
C(M2)	0.0181(5)	0.0160(5)	0.0141(5)	−0.0024(4)	−0.0014(4)	−0.0080(4)
C(M3)	0.0179(5)	0.0149(5)	0.0154(5)	−0.0005(4)	−0.0008(4)	−0.0076(4)
C(M4)	0.0160(5)	0.0156(5)	0.0160(5)	−0.0040(4)	−0.0018(4)	−0.0054(4)
C(11)	0.0242(6)	0.0166(5)	0.0154(5)	0.0020(4)	−0.0052(4)	−0.0114(5)
C(12)	0.0313(7)	0.0280(7)	0.0222(6)	0.0060(5)	−0.0056(5)	−0.0197(6)
C(13)	0.0508(10)	0.0371(8)	0.0273(7)	0.0140(6)	−0.0124(7)	−0.0327(8)
C(14)	0.0574(11)	0.0232(7)	0.0348(8)	0.0128(6)	−0.0228(8)	−0.0240(7)
C(15)	0.0419(8)	0.0166(6)	0.0330(8)	0.0022(5)	−0.0155(6)	−0.0089(6)
C(16)	0.0283(6)	0.0174(6)	0.0218(6)	−0.0001(5)	−0.0061(5)	−0.0079(5)
C(21)	0.0236(6)	0.0175(5)	0.0134(5)	−0.0007(4)	−0.0027(4)	−0.0116(4)
C(22)	0.0270(7)	0.0469(9)	0.0206(6)	−0.0050(6)	−0.0023(5)	−0.0217(7)
C(23)	0.0392(9)	0.0600(11)	0.0251(7)	−0.0065(7)	−0.0087(6)	−0.0314(9)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.0483(9)	0.0317(7)	0.0167(6)	−0.0021(5)	−0.0067(6)	−0.0253(7)
C(25)	0.0373(8)	0.0229(6)	0.0179(6)	−0.0065(5)	0.0006(5)	−0.0133(6)
C(26)	0.0255(6)	0.0230(6)	0.0192(6)	−0.0062(5)	−0.0013(5)	−0.0100(5)
C(31)	0.0244(6)	0.0157(5)	0.0158(5)	−0.0025(4)	0.0010(4)	−0.0097(4)
C(32)	0.0328(7)	0.0199(6)	0.0243(6)	0.0019(5)	−0.0051(5)	−0.0114(5)
C(33)	0.0531(10)	0.0205(6)	0.0234(7)	0.0031(5)	−0.0043(6)	−0.0145(7)
C(34)	0.0611(11)	0.0246(7)	0.0230(7)	−0.0050(5)	0.0106(7)	−0.0258(7)
C(35)	0.0406(8)	0.0304(7)	0.0326(8)	−0.0098(6)	0.0124(6)	−0.0249(7)
C(36)	0.0269(6)	0.0221(6)	0.0259(6)	−0.0054(5)	0.0037(5)	−0.0142(5)
C(41)	0.0210(5)	0.0167(5)	0.0144(5)	−0.0023(4)	−0.0019(4)	−0.0086(4)
C(42)	0.0235(6)	0.0187(6)	0.0182(5)	−0.0034(4)	−0.0022(4)	−0.0072(5)
C(43)	0.0315(7)	0.0225(6)	0.0204(6)	−0.0078(5)	0.0032(5)	−0.0117(5)
C(44)	0.0396(8)	0.0313(7)	0.0171(6)	−0.0066(5)	−0.0002(5)	−0.0225(6)
C(45)	0.0331(7)	0.0353(8)	0.0242(7)	−0.0038(6)	−0.0105(6)	−0.0167(6)
C(46)	0.0237(6)	0.0264(6)	0.0247(6)	−0.0059(5)	−0.0070(5)	−0.0073(5)
Cl(1)	0.0167(1)	0.0264(2)	0.0323(2)	0.0027(1)	−0.0026(1)	−0.0093(1)
Na(1)	0.0184(2)	0.0204(2)	0.0208(3)	0.0014(2)	0.0003(2)	−0.0064(2)
N(5)	0.0230(5)	0.0241(6)	0.0309(6)	0.0052(5)	−0.0067(5)	−0.0106(5)
N(6)	0.0270(6)	0.0271(6)	0.0247(6)	0.0052(5)	−0.0065(5)	−0.0105(5)
O(1)	0.0262(5)	0.0262(5)	0.0289(5)	−0.0018(4)	0.0062(4)	−0.0116(4)
O(2)	0.0309(6)	0.0364(6)	0.0330(6)	−0.0057(5)	0.0073(4)	−0.0195(5)
O(3)	0.0267(5)	0.0208(5)	0.0323(6)	0.0044(4)	−0.0032(4)	−0.0079(4)
O(4)	0.0332(6)	0.0291(5)	0.0263(5)	0.0018(4)	−0.0061(4)	−0.0139(5)
O(5)	0.0229(5)	0.0313(5)	0.0238(5)	−0.0055(4)	0.0020(4)	−0.0130(4)
O(6)	0.0172(4)	0.0288(5)	0.0361(6)	0.0008(4)	−0.0041(4)	−0.0084(4)
C(1C)	0.0296(7)	0.0273(7)	0.0392(8)	0.0012(6)	−0.0107(6)	−0.0148(6)
C(2C)	0.0217(6)	0.0269(7)	0.0510(10)	0.0005(7)	−0.0005(6)	−0.0128(6)
C(3C)	0.0558(11)	0.0388(9)	0.0348(9)	−0.0080(7)	0.0181(8)	−0.0323(9)
C(4C)	0.0383(9)	0.0490(11)	0.0542(11)	−0.0243(9)	0.0239(8)	−0.0297(9)
C(5C)	0.0402(9)	0.0351(8)	0.0267(7)	0.0018(6)	0.0089(6)	−0.0139(7)
C(6C)	0.0405(8)	0.0333(8)	0.0203(6)	0.0005(6)	−0.0049(6)	−0.0132(7)
C(7C)	0.0259(7)	0.0270(7)	0.0476(10)	0.0097(7)	−0.0157(7)	−0.0106(6)
C(8C)	0.0282(7)	0.0237(7)	0.0394(8)	0.0102(6)	−0.0121(6)	−0.0092(6)
C(9C)	0.0356(8)	0.0195(6)	0.0394(9)	−0.0006(6)	−0.0036(7)	−0.0076(6)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(10C)	0.0410(9)	0.0290(7)	0.0340(8)	0.0105(6)	−0.0103(7)	−0.0206(7)
C(11C)	0.0388(8)	0.0327(8)	0.0293(7)	0.0026(6)	−0.0091(6)	−0.0199(7)
C(12C)	0.0337(8)	0.0359(8)	0.0358(8)	0.0067(7)	−0.0141(6)	−0.0183(7)
C(13C)	0.0367(8)	0.0392(8)	0.0233(7)	0.0047(6)	−0.0071(6)	−0.0183(7)
C(14C)	0.0313(7)	0.0401(8)	0.0219(6)	−0.0070(6)	0.0018(5)	−0.0169(7)
C(15C)	0.0185(6)	0.0381(8)	0.0331(8)	−0.0090(6)	0.0048(5)	−0.0135(6)
C(16C)	0.0207(6)	0.0265(7)	0.0423(9)	−0.0074(6)	−0.0022(6)	−0.0062(5)
C(17C)	0.0210(6)	0.0300(7)	0.0368(8)	0.0074(6)	−0.0092(6)	−0.0080(5)
C(18C)	0.0296(7)	0.0320(8)	0.0296(7)	0.0102(6)	−0.0102(6)	−0.0097(6)
C(1S)	0.0434(10)	0.0504(11)	0.0483(11)	−0.0217(9)	0.0105(8)	−0.0244(9)
Cl(1A)	0.0694(9)	0.0678(13)	0.0392(8)	−0.0096(7)	0.0156(6)	−0.0406(10)
Cl(2A)	0.0907(8)	0.0619(7)	0.0863(11)	−0.0335(7)	0.0087(8)	−0.0507(7)
Cl(1B)	0.0694(9)	0.0678(13)	0.0392(8)	−0.0096(7)	0.0156(6)	−0.0406(10)
Cl(2B)	0.0907(8)	0.0619(7)	0.0863(11)	−0.0335(7)	0.0087(8)	−0.0507(7)
C(2SA)	0.029(2)	0.0234(19)	0.037(2)	0.0010(16)	−0.0113(18)	−0.0140(18)
Cl(3A)	0.0541(8)	0.0431(12)	0.0412(12)	0.0123(9)	−0.0159(10)	−0.0305(9)
Cl(4A)	0.0919(10)	0.0469(6)	0.0726(7)	−0.0020(5)	−0.0237(7)	−0.0493(7)
C(2SB)	0.032(4)	0.032(4)	0.041(5)	0.011(4)	−0.008(3)	−0.013(3)
Cl(3B)	0.0796(15)	0.1005(18)	0.0634(11)	0.0335(12)	−0.0391(11)	−0.0759(16)
Cl(4B)	0.076(2)	0.0251(11)	0.0338(11)	0.0017(7)	−0.0026(11)	−0.0198(11)
C(3SA)	0.029(2)	0.0280(17)	0.040(3)	−0.001(2)	−0.006(2)	−0.0144(14)
Cl(5A)	0.0429(6)	0.0422(7)	0.0485(10)	−0.0106(8)	−0.0030(8)	−0.0238(5)
Cl(6A)	0.0506(7)	0.0368(5)	0.0732(8)	0.0113(4)	−0.0350(7)	−0.0175(4)
C(3SB)	0.024(3)	0.041(3)	0.044(5)	0.002(4)	−0.007(3)	−0.013(2)
Cl(6B)	0.0407(10)	0.1172(17)	0.0574(10)	0.0011(10)	−0.0243(8)	0.0131(10)
Cl(5B)	0.0408(7)	0.0317(6)	0.0489(13)	−0.0026(10)	−0.0123(11)	−0.0145(5)

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

Table S6. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for Na(222)[Fe(TPP)Cl][a]

atom	x	y	z	U(eq)
H(B1	0.3023	0.0718	0.4782	0.022
H(B2	0.3362	−0.1260	0.4516	0.022
H(B3	0.3688	−0.3294	0.2450	0.022
H(B4	0.3389	−0.2608	0.1378	0.021
H(B5	0.3045	0.1160	0.0140	0.025
H(B6	0.3042	0.3017	0.0385	0.025
H(B7	0.3165	0.4880	0.2421	0.026
H(B8	0.3144	0.4307	0.3513	0.025
H(12)	0.2286	−0.2351	0.4143	0.030
H(13)	0.2963	−0.4148	0.4660	0.040
H(14)	0.4856	−0.5611	0.4400	0.042
H(15)	0.6096	−0.5267	0.3634	0.037
H(16)	0.5448	−0.3455	0.3135	0.028
H(22)	0.1211	−0.0226	0.0635	0.035
H(23)	0.1129	−0.0903	−0.0296	0.045
H(24)	0.2853	−0.1861	−0.0932	0.035
H(25)	0.4663	−0.2131	−0.0637	0.031
H(26)	0.4755	−0.1479	0.0298	0.027
H(32)	0.1544	0.5046	0.0915	0.031
H(33)	0.1955	0.6347	0.0256	0.040
H(34)	0.3770	0.6395	0.0224	0.042
H(35)	0.5181	0.5157	0.0854	0.038
H(36)	0.4806	0.3823	0.1499	0.029
H(42)	0.1159	0.4028	0.4344	0.025
H(43)	0.1092	0.4983	0.5207	0.030
H(44)	0.2754	0.4333	0.5745	0.032
H(45)	0.4486	0.2717	0.5417	0.035
H(46)	0.4562	0.1762	0.4548	0.031
H(1A)	1.0393	0.8650	0.3707	0.037
H(1B)	0.9115	0.9567	0.3525	0.037
H(2A)	1.0590	0.9544	0.2774	0.039
H(2B)	1.1021	0.8187	0.2677	0.039
H(3A)	1.0511	0.9516	0.1746	0.049
H(3B)	0.9279	0.9728	0.1518	0.049

Table S6. Continued

atom	x	y	z	U(eq)
H(4A)	1.0874	0.8003	0.1109	0.053
H(4B)	1.1116	0.7471	0.1781	0.053
H(5A)	0.9724	0.7381	0.0620	0.044
H(5B)	0.8783	0.8647	0.0848	0.044
H(6A)	0.7797	0.7555	0.0627	0.039
H(6B)	0.8506	0.6569	0.1106	0.039
H(7A)	1.0649	0.6575	0.3923	0.040
H(7B)	1.1075	0.6713	0.3230	0.040
H(8A)	1.0748	0.5034	0.3384	0.037
H(8B)	0.9390	0.5836	0.3611	0.037
H(9A)	1.0144	0.4357	0.2662	0.040
H(9B)	0.9680	0.5125	0.2064	0.040
H(10A)	0.8211	0.4642	0.2575	0.039
H(10B)	0.8213	0.5284	0.3165	0.039
H(11A)	0.6509	0.5893	0.2029	0.038
H(11B)	0.7740	0.5716	0.1664	0.038
H(12A)	0.6169	0.7332	0.1255	0.040
H(12B)	0.5749	0.7916	0.1903	0.040
H(13A)	0.8806	0.8338	0.4351	0.039
H(13B)	0.8517	0.7346	0.4133	0.039
H(14A)	0.6765	0.9092	0.4246	0.037
H(14B)	0.7338	0.9744	0.3776	0.037
H(15A)	0.5311	0.9732	0.3620	0.036
H(15B)	0.5480	0.9002	0.3035	0.036
H(16A)	0.5046	1.0966	0.2774	0.037
H(16B)	0.6235	1.0779	0.3044	0.037
H(17A)	0.5292	1.0780	0.1696	0.036
H(17B)	0.5206	0.9674	0.2033	0.036
H(18A)	0.5972	0.9265	0.1014	0.038
H(18B)	0.7034	0.9551	0.1123	0.038
H(1S1)	1.0626	0.0816	0.4221	0.055
H(1S2)	0.9633	0.1504	0.3765	0.055
H(2SA)	1.0710	0.2800	0.1298	0.034
H(2SB)	0.9342	0.3530	0.1531	0.034

Table S6. Continued

atom	x	y	z	U(eq)
H(2SC)	1.0727	0.2329	0.0874	0.043
H(2SD)	1.0287	0.3041	0.1492	0.043
H(3SA)	0.8554	0.1716	0.2313	0.038
H(3SB)	0.7447	0.1451	0.2283	0.038
H(3SC)	0.7699	0.1285	0.2484	0.044
H(3SD)	0.8317	0.2132	0.2461	0.044

[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.