Supporting Information for

Tetragonal to Triclinic — A Phase Change for [Fe(TPP)(NO)]

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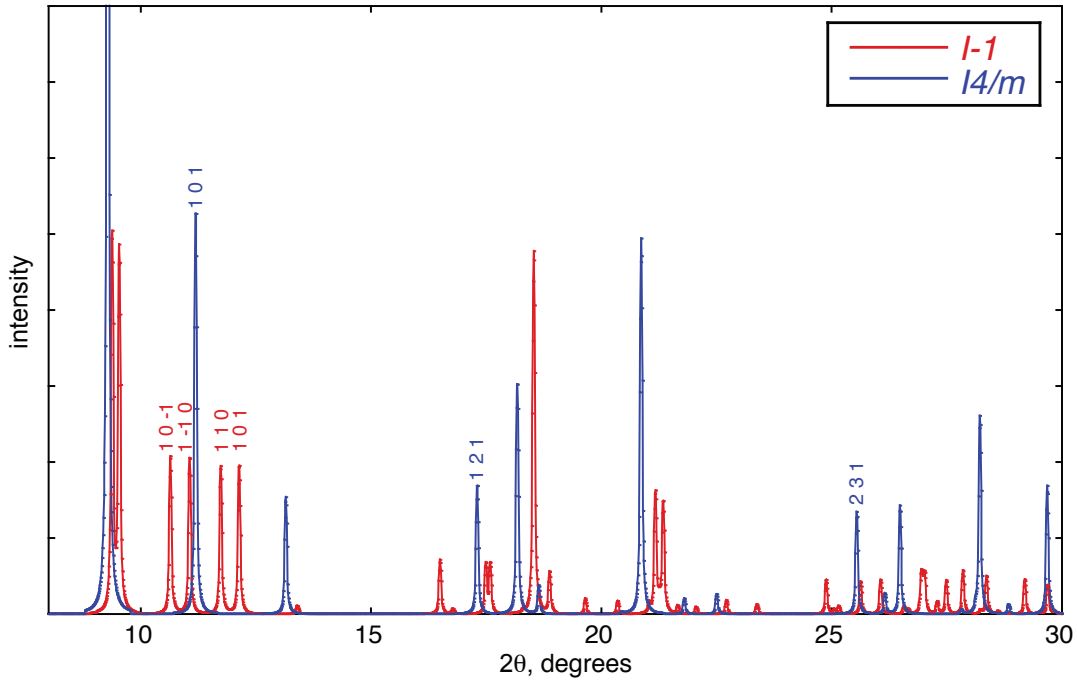

Figure S1. Simulated X-ray powder diffraction spectra of [Fe(TPP)(NO)] in the $I-1$ and $I4/m$ crystalline phases.

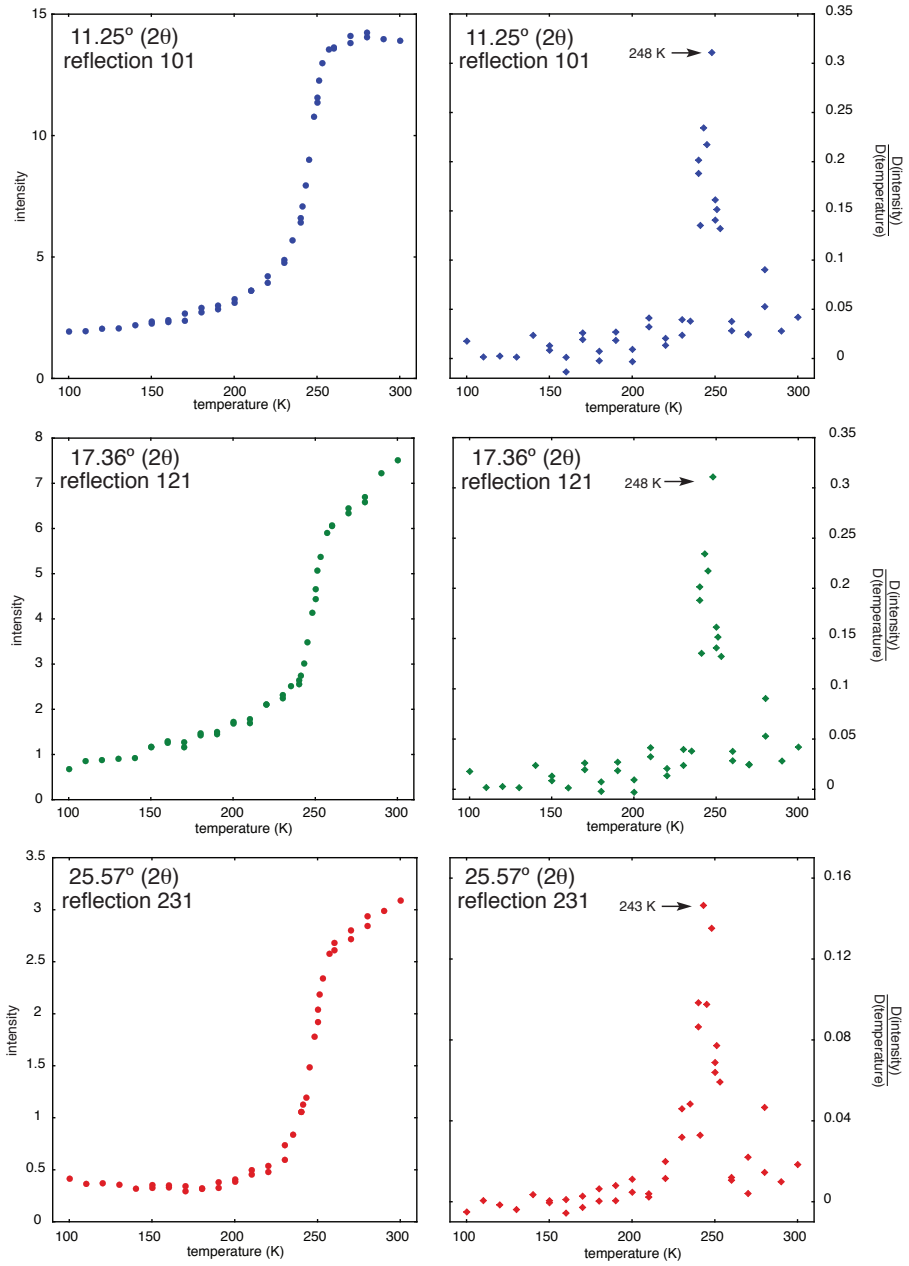

Figure S2. X-ray powder diffraction intensity vs. T for the 101, 121, and 231 reflections of [Fe(TPP)(NO)] ($I4/m$) are given in the left-hand panels. The right-hand panels show the derivatives of intensity vs. T.

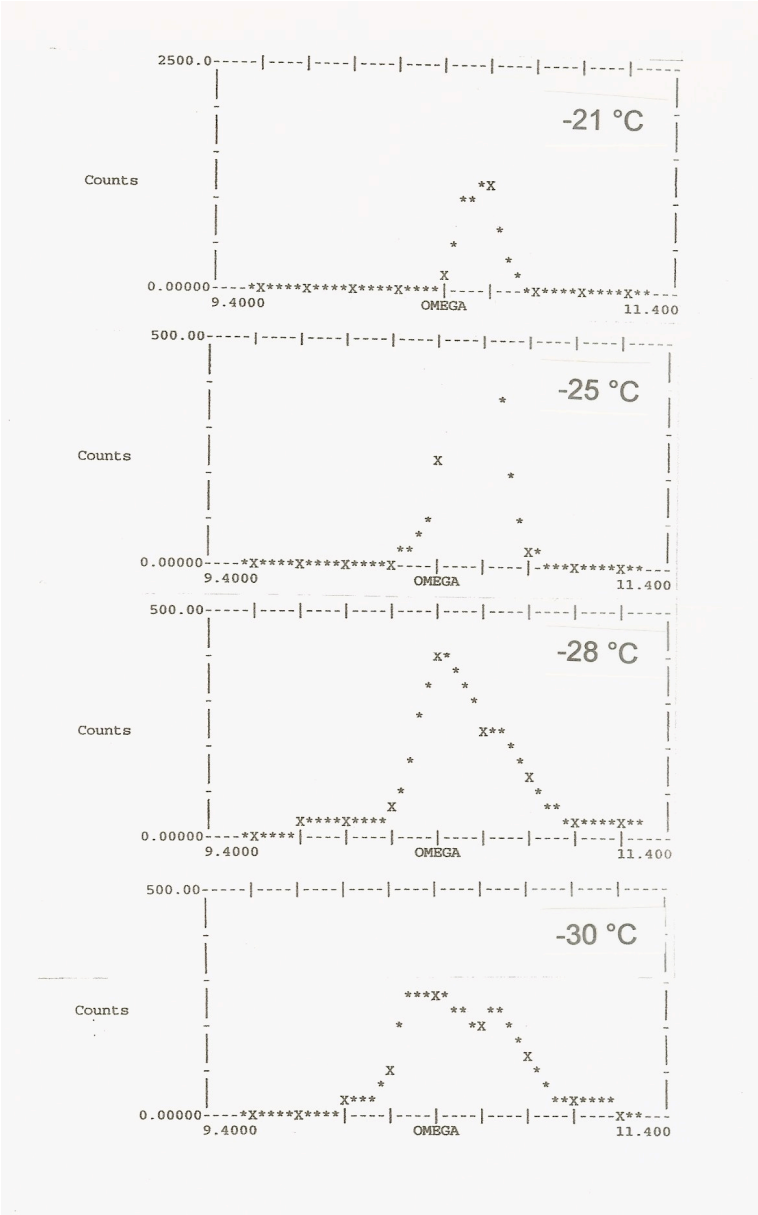

Figure S3. Series of ω-scans of the (3 1 0) reflection using a serial detector and a single crystal of Fe(TPP)(NO).
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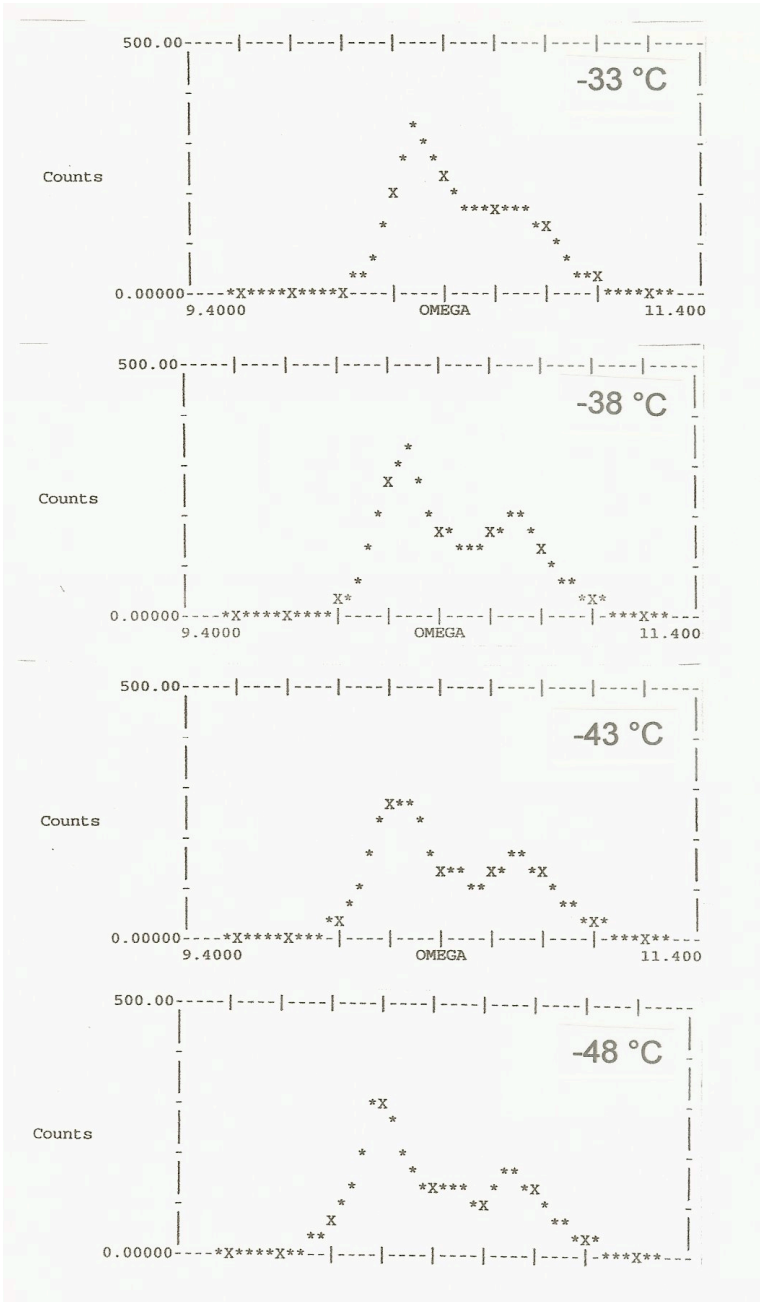


Figure S3. continued.

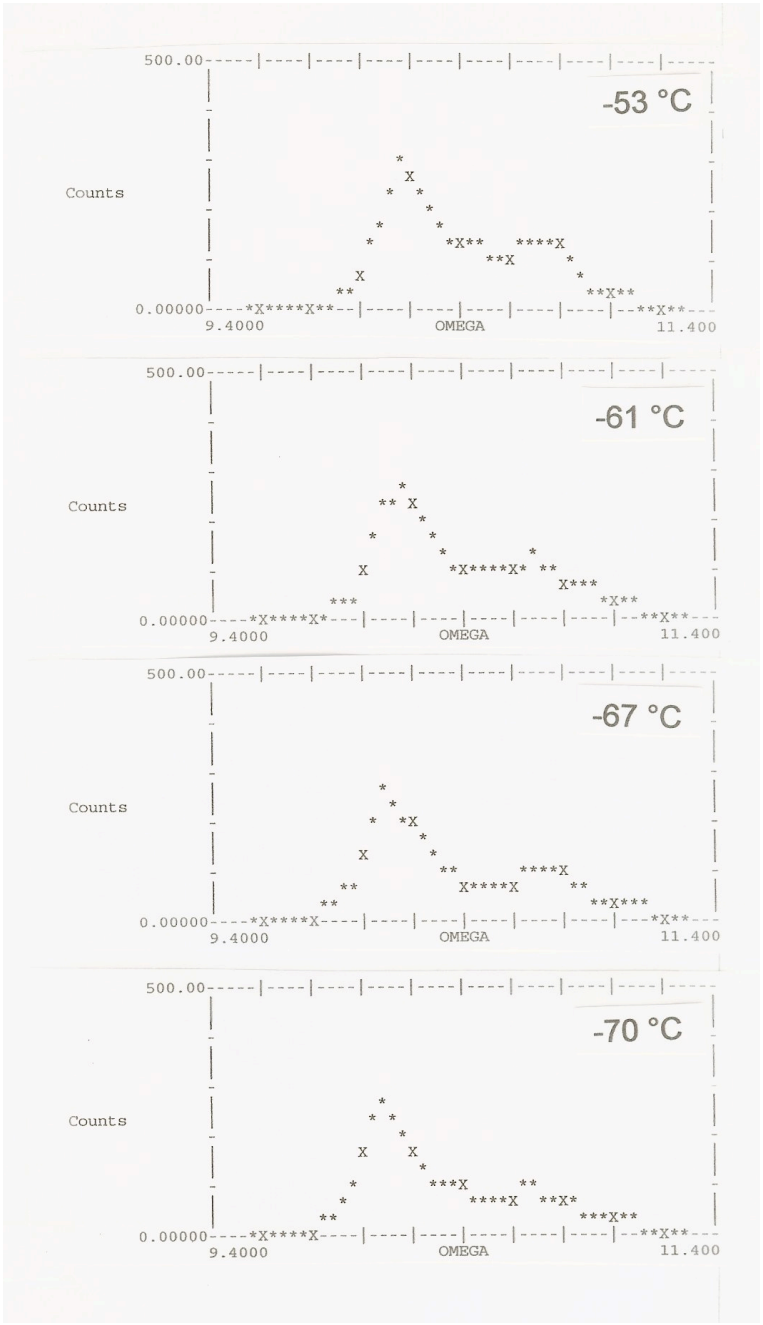


Figure S3. continued.

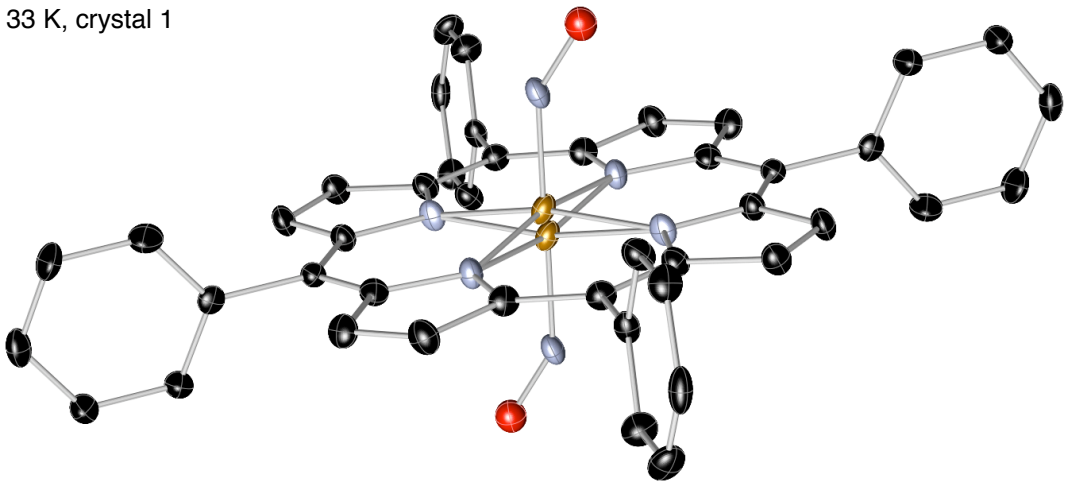


Figure S4. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 33 K. Hydrogen atoms are omitted for clarity.

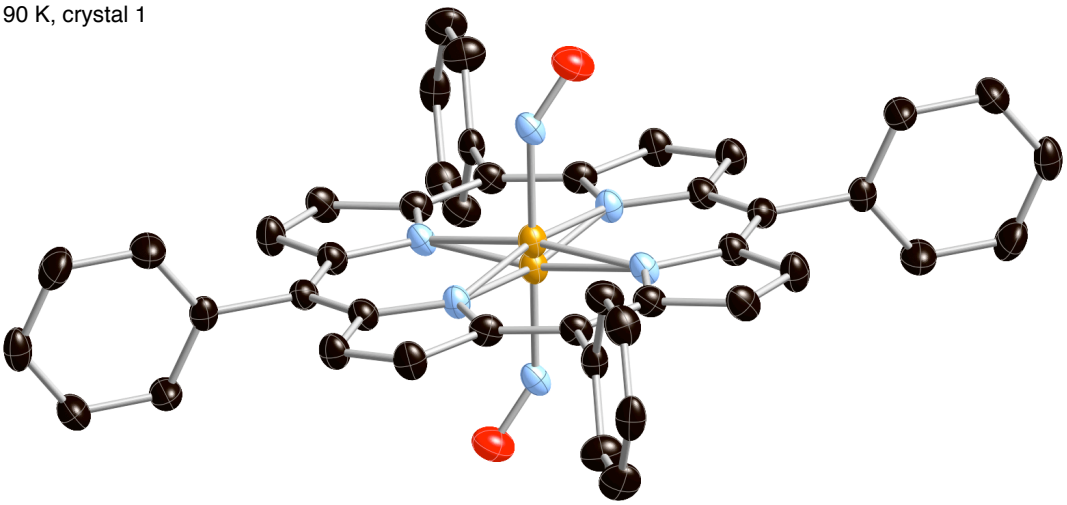


Figure S5. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 90 K. Hydrogen atoms are omitted for clarity.

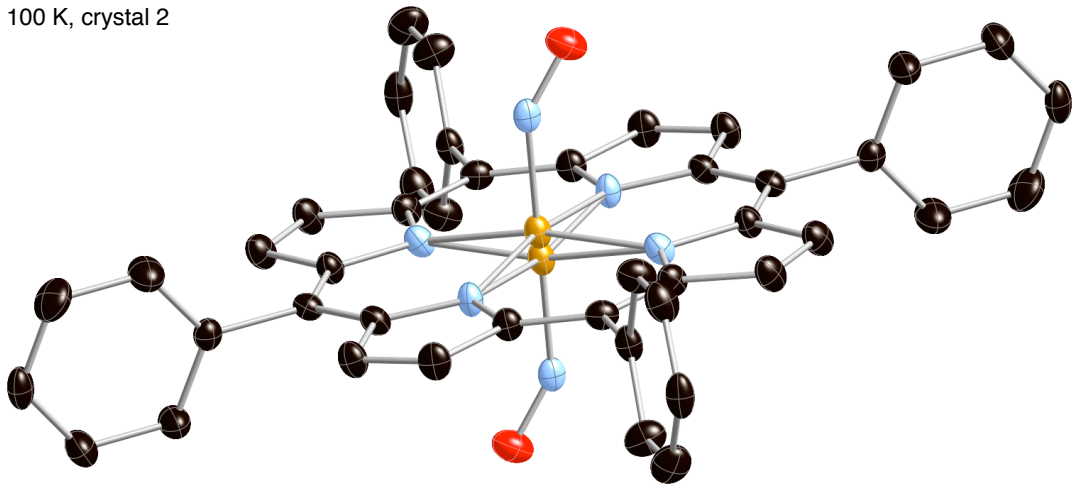


Figure S6. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 100 K. Hydrogen atoms are omitted for clarity.

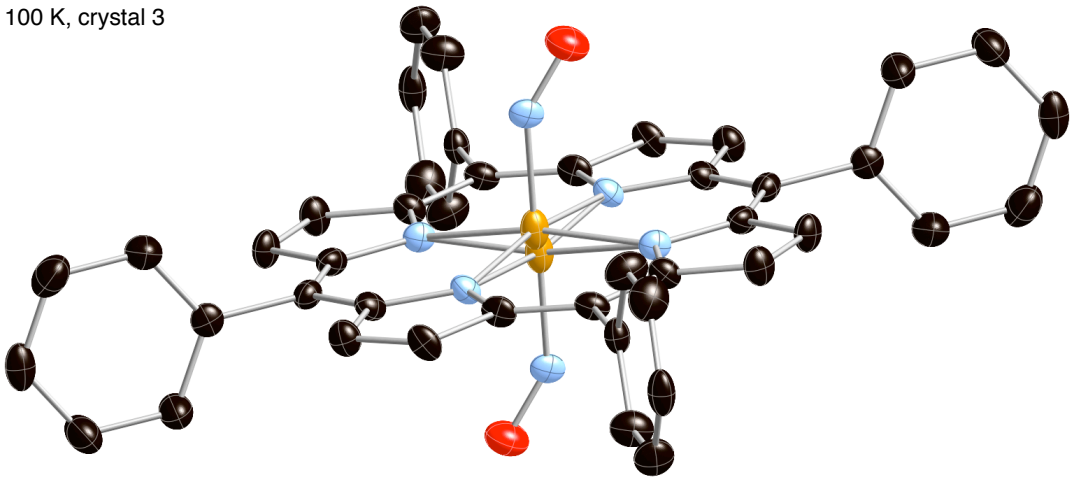


Figure S7. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 100 K. Hydrogen atoms are omitted for clarity.

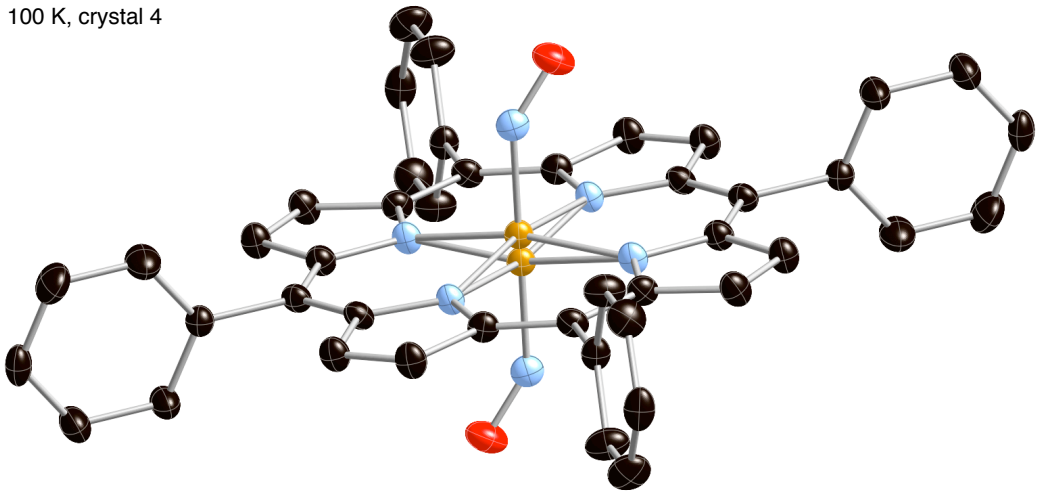


Figure S8. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 100 K. Hydrogen atoms are omitted for clarity.

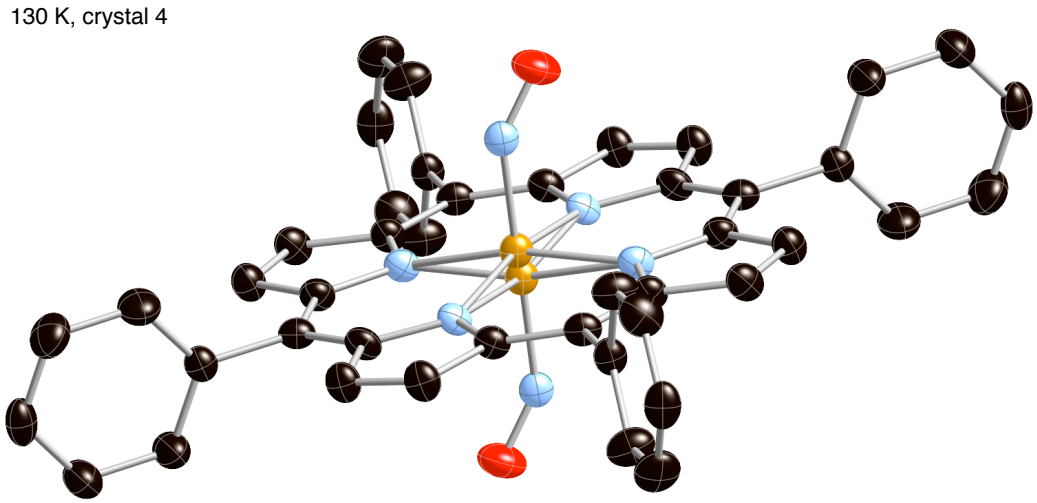


Figure S9. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 130 K. Hydrogen atoms are omitted for clarity.

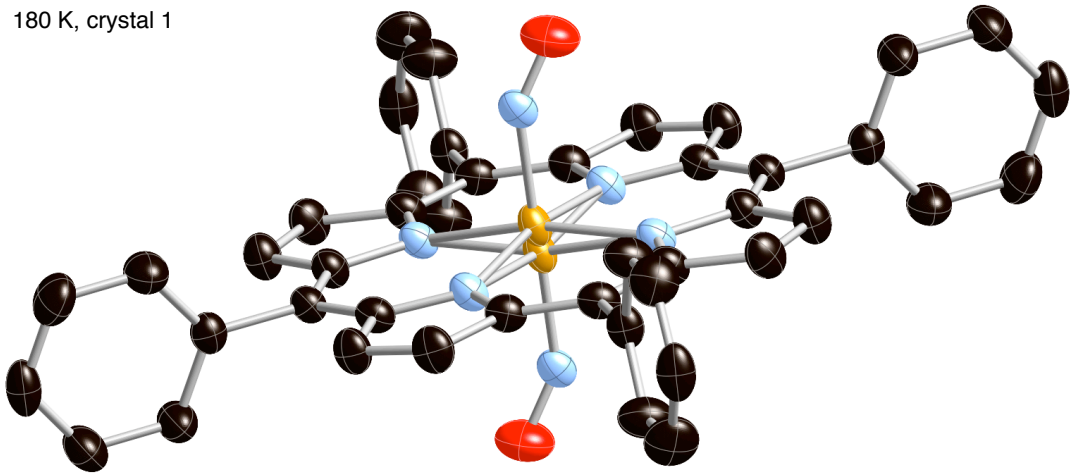


Figure S10. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 180 K. Hydrogen atoms are omitted for clarity.

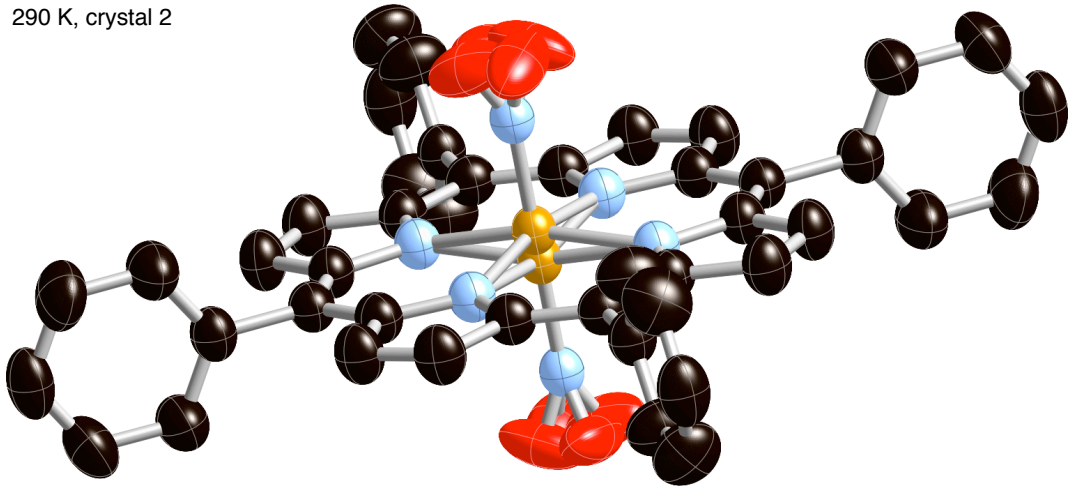


Figure S11. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 290 K. Hydrogen atoms are omitted for clarity.

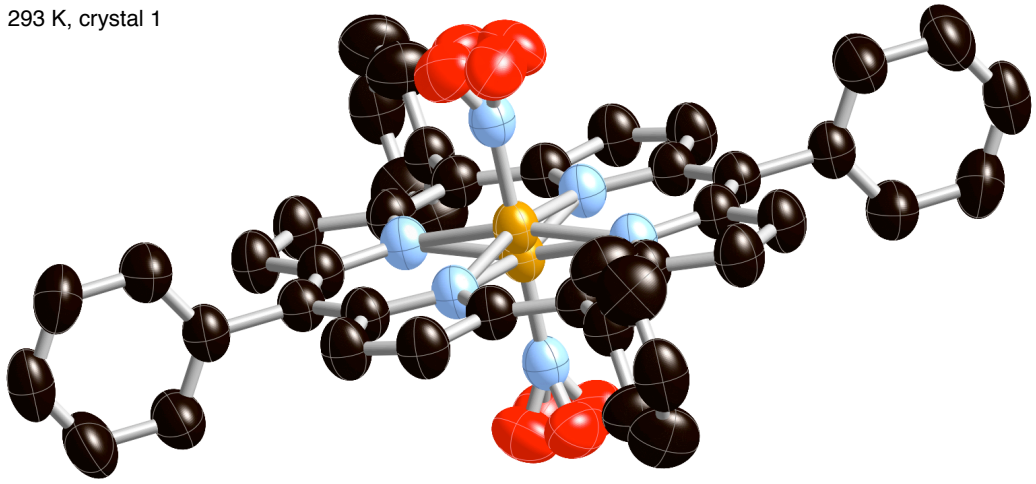


Figure S12. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 293 K. Hydrogen atoms are omitted for clarity.

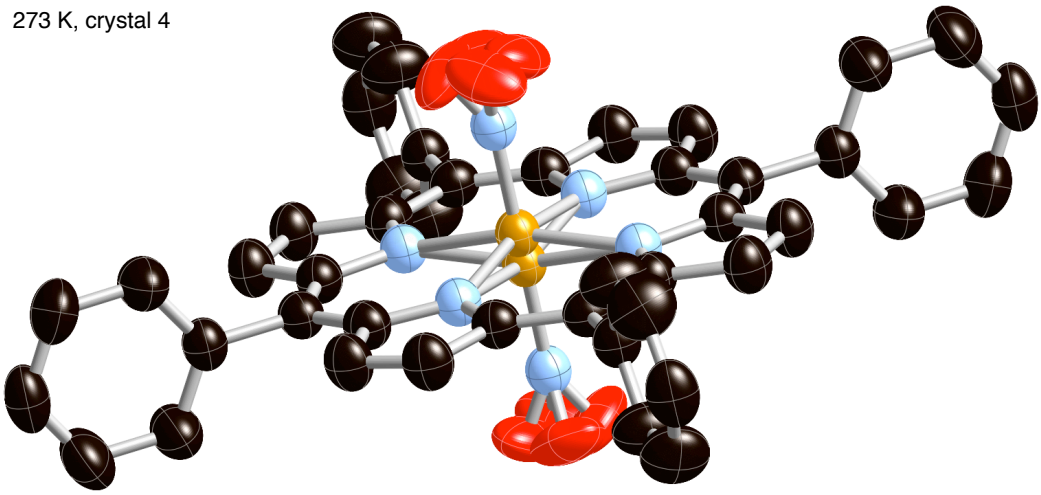


Figure S13. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 273 K. Hydrogen atoms are omitted for clarity.

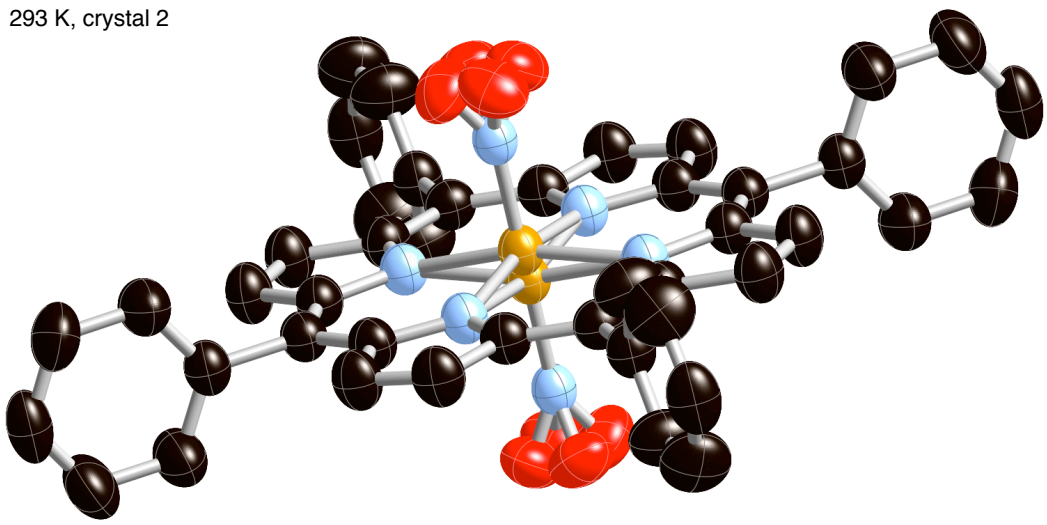


Figure S14. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 293 K. Hydrogen atoms are omitted for clarity.

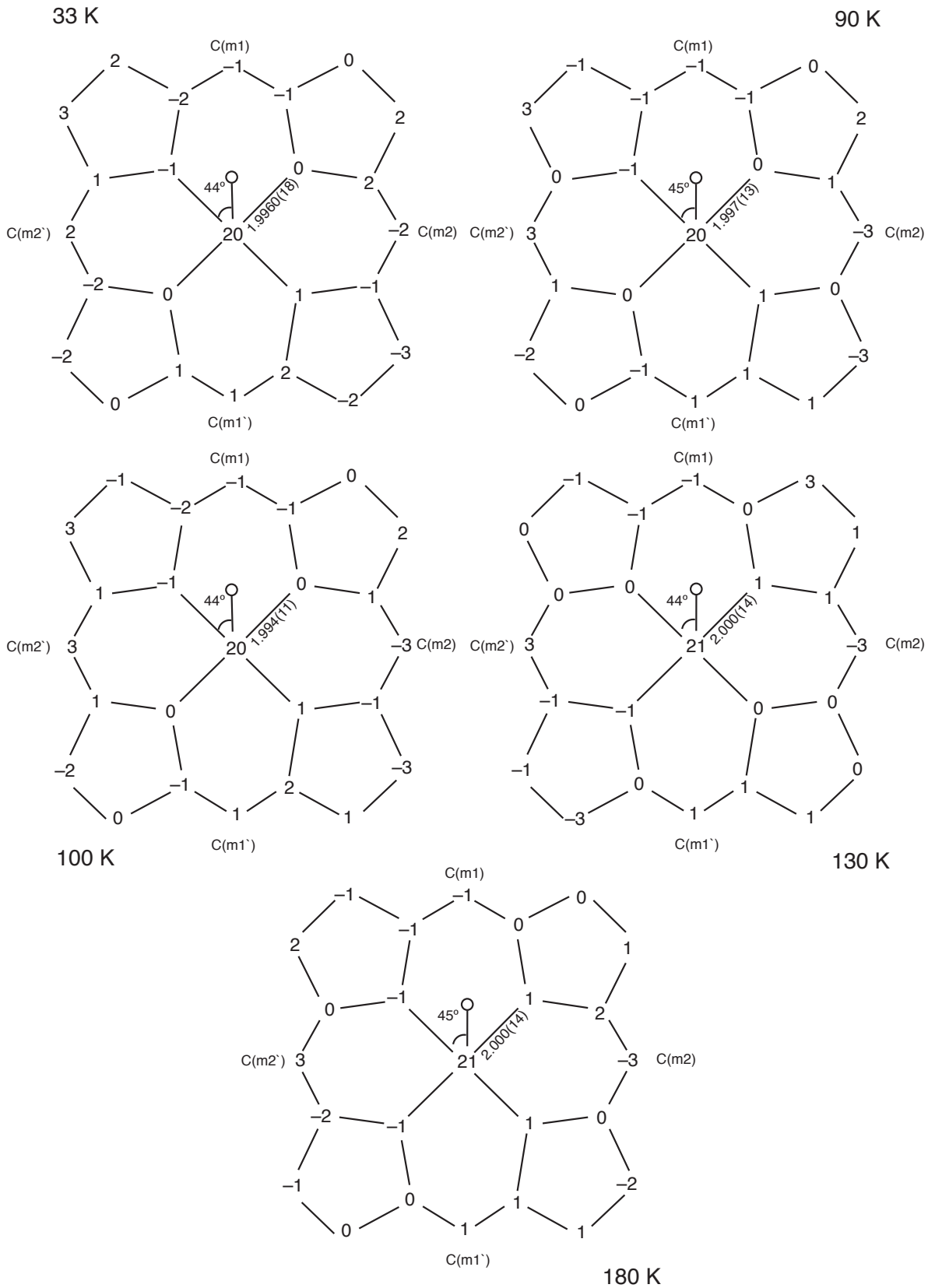
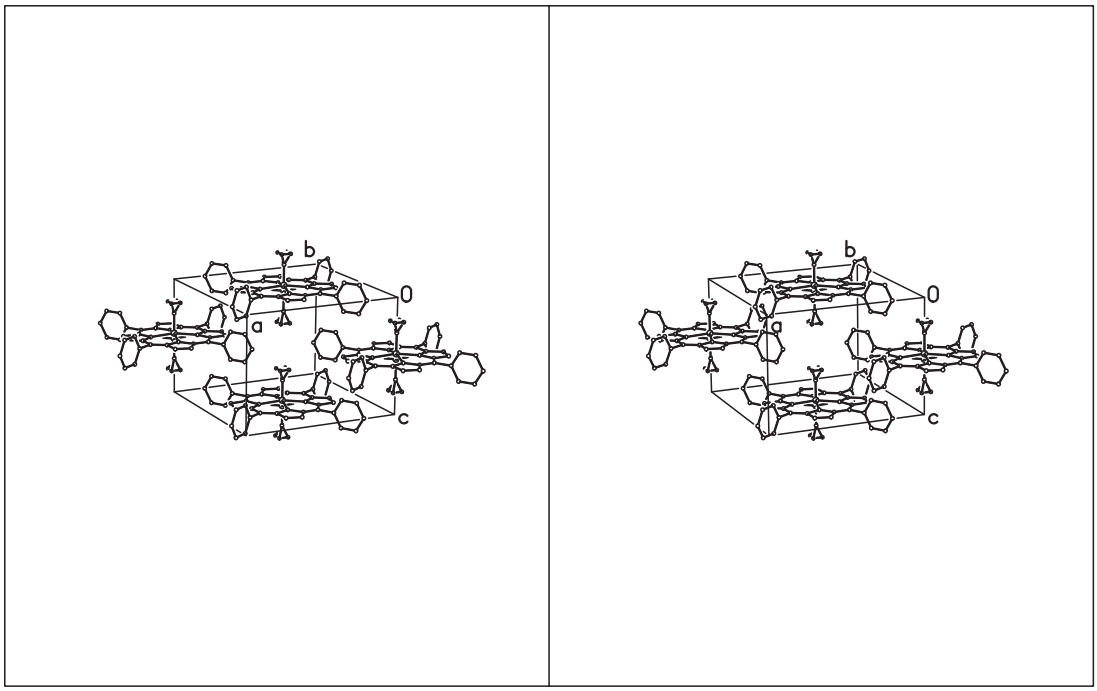
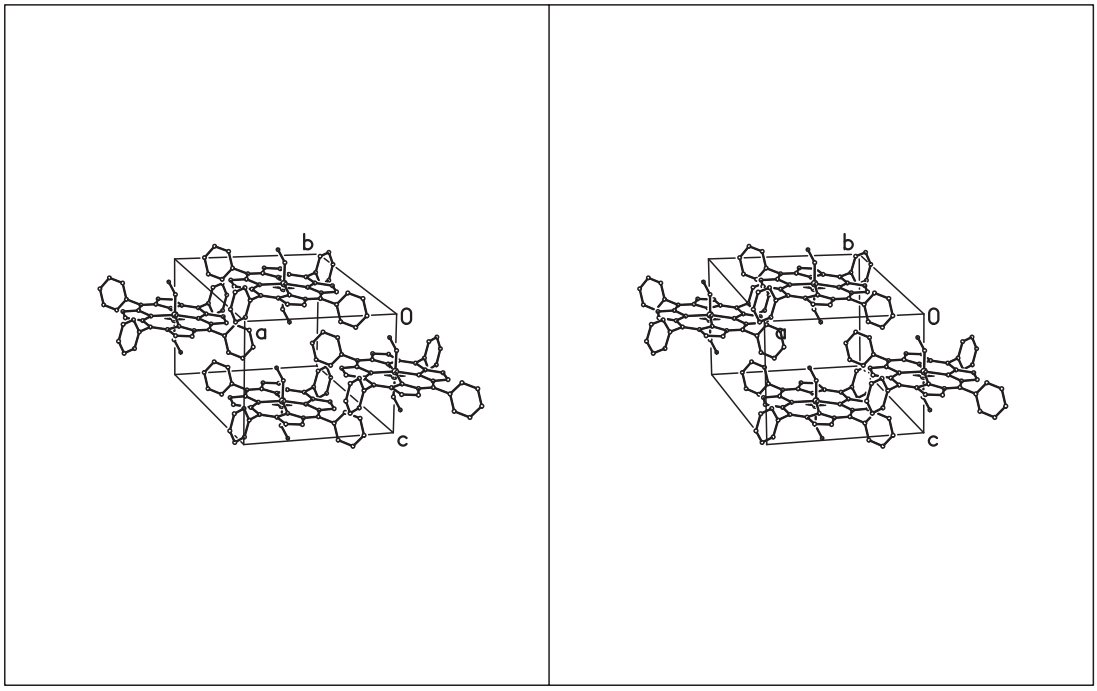


Figure S15. Formal diagram of the porphyrinato cores of [Fe(TPP)(NO)] at 33, 90, 100, 130, and 180 K displaying the perpendicular displacements (in units of 0.01 Å) of the core atoms from the 24-atom mean plane. Positive displacements are toward the nitrosyl-coordinated face. The location of the nitrosyl oxygen atom projection onto the porphyrin core is indicated by the small circle.

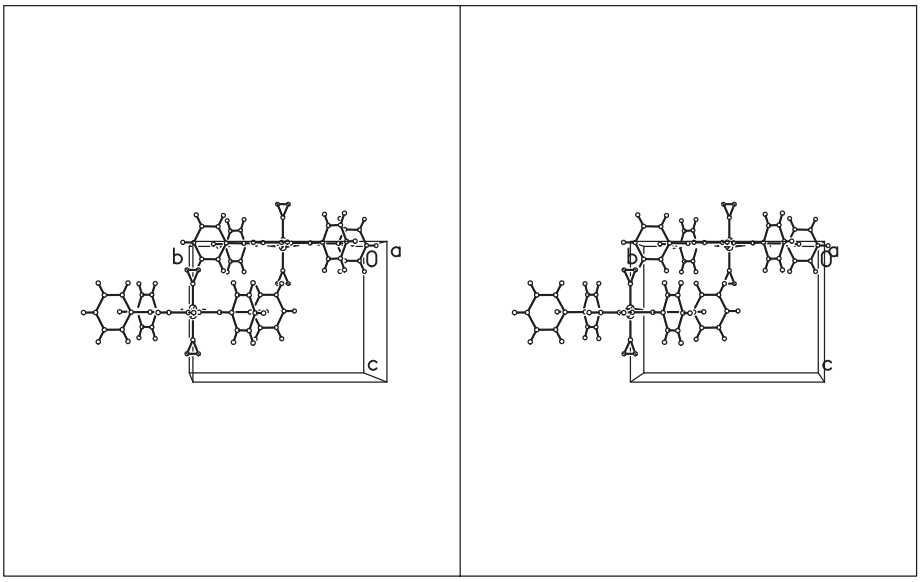


Tetragonal I4/m



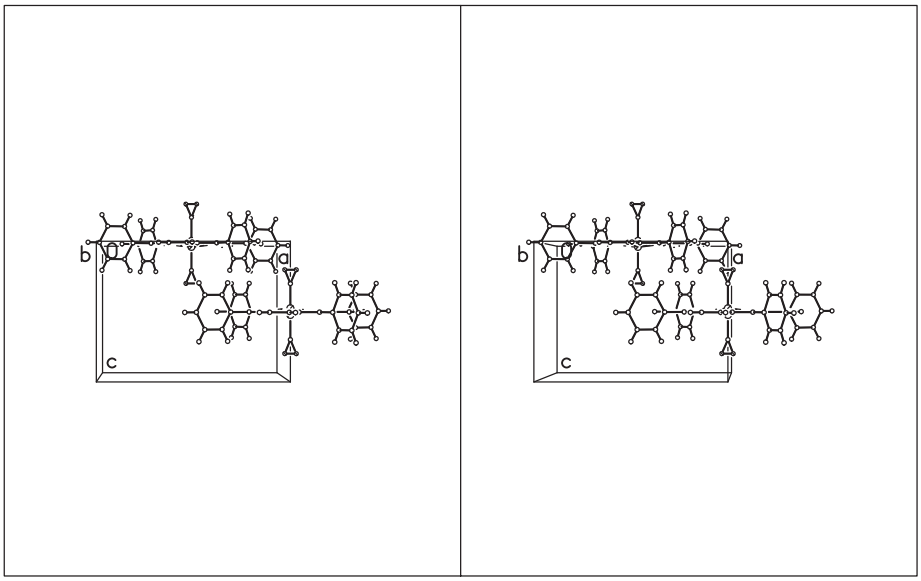
Triclinic I-1

Figure S16. Stereo diagrams of the two I-centered cells (3 pages).

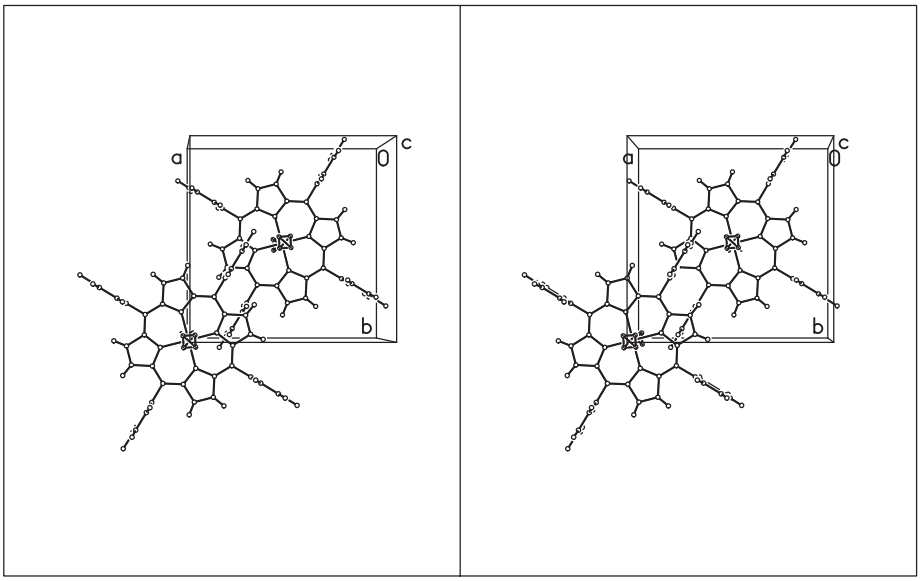


view down a

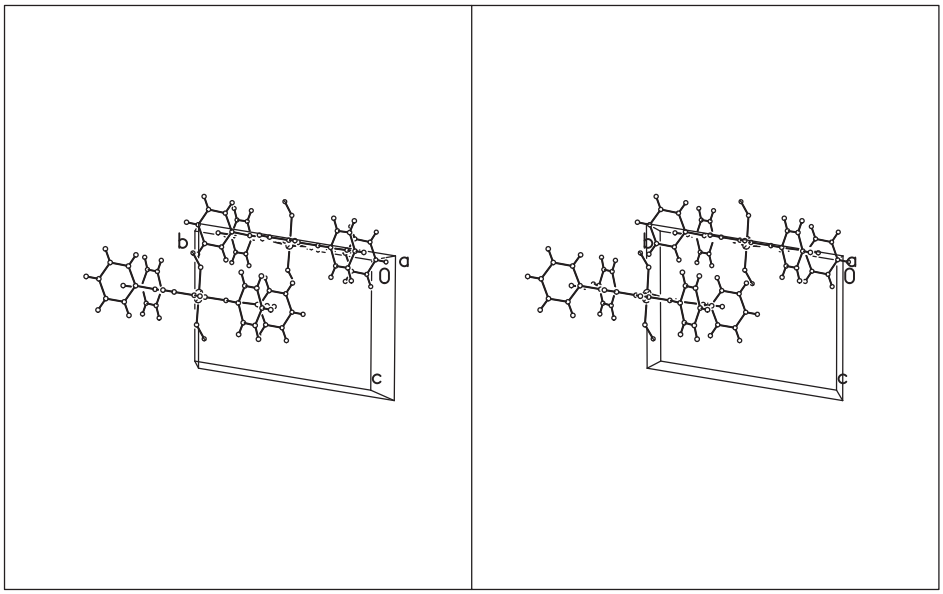
Tetragonal



view down b

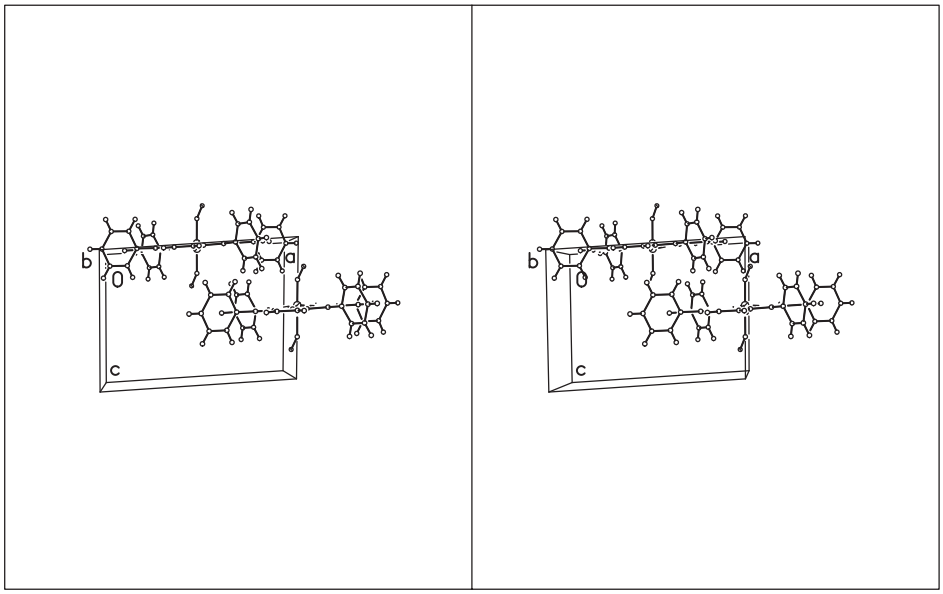


view down c

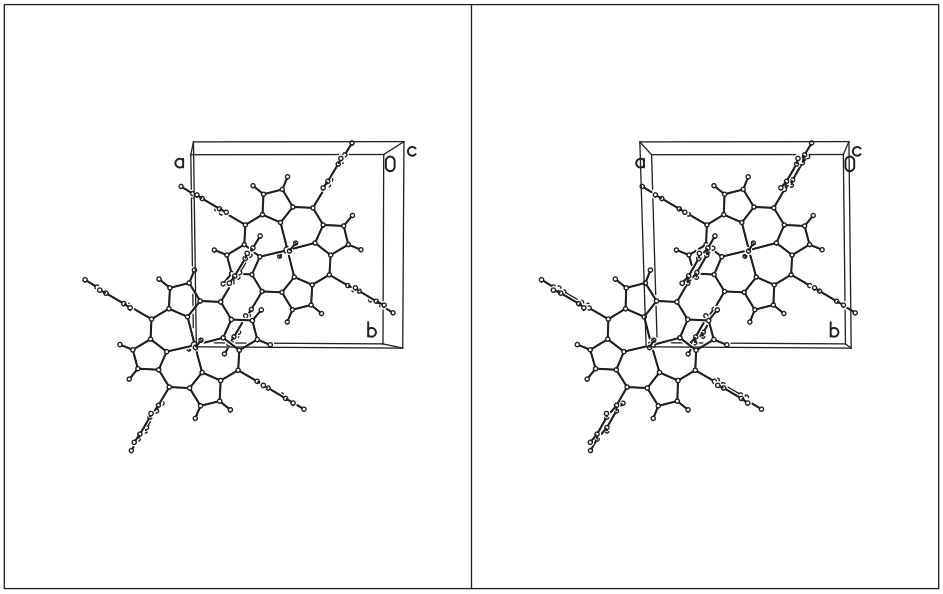


view down a

Triclinic I



view down b



view down c

Supporting Information

Table S1. Complete Crystallographic Details for [Fe(TPP)(NO)] at 33 K, crystal 1

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	9.745(2)
b, Å	9.867(2)
c, Å	10.375(3)
α, deg	82.66(2)
β, deg	66.010(2)
γ, deg	70.05(2)
V, Å^3	856.7(4)
space group	$P\bar{1}$
Z	1
D_c, g/cm^3	1.354
F(000)	361
μ, mm^{-1}	0.484
crystal dimensions, mm	0.21 × 0.17 × 0.08
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	33(2)
diffractometer	Bruker SMART Apex II
θ range for collected data, deg	3.05–27.50
index range	$-11 \leq h \leq 12$
	$-12 \leq k \leq 12$
	$0 \leq l \leq 13$
total data collected	4221
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9623 and 0.9052
unique data	4221 (R_{int} = 0.0806)
unique observed data [I > 2σ(I)]	2476
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	4221/0/247
goodness-of-fit (pased on F^2)	0.827
final R indices [I > 2σ(I)]	R_1 = 0.0486, wR_2 = 0.0806
final R indices (all data)	R_1 = 0.0940, wR_2 = 0.0884

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 33 K, crystal 1[a]

atom	x	y	z	U(eq)
Fe(1)	0.4811(7)	0.4971(9)	0.4985(9)	0.0146(7)
N(1)	0.4642(2)	0.6814(2)	0.3923(2)	0.0147(5)
N(2)	0.3571(3)	0.6095(2)	0.67951(19)	0.0153(5)
C(m1)	0.6313(3)	0.5875(3)	0.1493(2)	0.0152(6)
C(m2)	0.2814(3)	0.8561(3)	0.5877(2)	0.0134(6)
C(a1)	0.5281(3)	0.6986(3)	0.2469(2)	0.0155(6)
C(a2)	0.3689(3)	0.8190(3)	0.4448(3)	0.0157(6)
C(a3)	0.2790(3)	0.7565(3)	0.6961(2)	0.0145(6)
C(a4)	0.3166(3)	0.5565(3)	0.8149(2)	0.0153(6)
C(b1)	0.4726(3)	0.8464(3)	0.2107(3)	0.0190(6)
C(b2)	0.3742(3)	0.9206(3)	0.3330(2)	0.0176(6)
C(b3)	0.1910(3)	0.7945(3)	0.8430(2)	0.0177(6)
C(b4)	0.2145(3)	0.6707(3)	0.9159(2)	0.0183(6)
C(10)	0.6924(3)	0.6269(2)	−0.0040(2)	0.0138(6)
C(11)	0.8411(3)	0.6458(3)	−0.0682(3)	0.0193(7)
C(12)	0.8985(3)	0.6816(3)	−0.2106(3)	0.0196(7)
C(13)	0.8081(3)	0.6981(2)	−0.2892(2)	0.0195(7)
C(14)	0.6593(3)	0.6821(3)	−0.2252(3)	0.0227(7)
C(15)	0.6017(3)	0.6468(3)	−0.0829(3)	0.0203(7)
C(20)	0.1827(3)	1.0105(3)	0.6267(2)	0.0133(6)
C(21)	0.0223(3)	1.0567(3)	0.6517(3)	0.0217(7)
C(22)	−0.0695(3)	1.1995(3)	0.6876(3)	0.0231(7)
C(23)	−0.0021(3)	1.2979(3)	0.6993(2)	0.0205(7)
C(24)	0.1566(3)	1.2531(3)	0.6756(3)	0.0273(7)
C(25)	0.2482(3)	1.1104(3)	0.6389(3)	0.0253(7)
N(3)	0.3092(5)	0.4894(4)	0.4901(4)	0.0166(10)
O(1)	0.1804(4)	0.5563(4)	0.5027(4)	0.0214(9)

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

Table S3. Bond Lengths for [Fe(TPP)(NO)] at 33 K, crystal 1[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.405(7)	C(b3)–H(b3)	0.9500
Fe(1)–N(3)	1.739(6)	C(b4)–H(b4)	0.9500
Fe(1)–N(1)	1.995(9)	C(10)–C(15)	1.385(4)
Fe(1)–N(2)	1.997(9)	C(10)–C(11)	1.394(3)
Fe(1)–N(2)#1)	2.000(9)	C(11)–C(12)	1.397(3)
Fe(1)–N(1)#1)	2.004(9)	C(11)–H(11)	0.9500
Fe(1)–N(3)#1)	2.143(5)	C(12)–C(13)	1.385(4)
N(1)–C(a2)	1.385(3)	C(12)–H(12)	0.9500
N(1)–C(a1)	1.391(3)	C(13)–C(14)	1.384(4)
N(1)–Fe(1)#1)	2.003(9)	C(13)–H(13)	0.9500
N(2)–C(a4)	1.380(3)	C(14)–C(15)	1.394(3)
N(2)–C(a3)	1.385(3)	C(14)–H(14)	0.9500
N(2)–Fe(1)#1)	2.000(9)	C(15)–H(15)	0.9500
C(m1)–C(a1)	1.393(3)	C(20)–C(25)	1.386(4)
C(m1)–C(a4#1)	1.393(3)	C(20)–C(21)	1.391(4)
C(m1)–C(10)	1.505(3)	C(21)–C(22)	1.388(3)
C(m2)–C(a3)	1.394(3)	C(21)–H(21)	0.9500
C(m2)–C(a2)	1.400(3)	C(22)–C(23)	1.385(4)
C(m2)–C(20)	1.500(3)	C(22)–H(22)	0.9500
C(a1)–C(b1)	1.431(3)	C(23)–C(24)	1.378(4)
C(a2)–C(b2)	1.429(3)	C(23)–H(23)	0.9500
C(a3)–C(b3)	1.436(3)	C(24)–C(25)	1.388(3)
C(a4)–C(m1#1)	1.393(3)	C(24)–H(24)	0.9500
C(a4)–C(b4)	1.430(3)	C(25)–H(25)	0.9500
C(b1)–C(b2)	1.355(3)	N(3)–O(1)	1.163(5)
C(b1)–H(b1)	0.9500	N(3)–Fe(1)#1)	2.143(5)
C(b2)–H(b2)	0.9500		
C(b3)–C(b4)	1.353(3)		

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

Table S4. Bond Angles for [Fe(TPP)(NO)] at 33 K, crystal 1[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(3)	175(3)	C(b2)–C(b1)–H(b1)	126.5
Fe(1)#1–Fe(1)–N(1)	85(3)	C(a1)–C(b1)–H(b1)	126.5
N(3)–Fe(1)–N(1)	90.9(4)	C(b1)–C(b2)–C(a2)	107.1(2)
Fe(1)#1–Fe(1)–N(2)	85(2)	C(b1)–C(b2)–H(b2)	126.5
N(3)–Fe(1)–N(2)	91.5(3)	C(a2)–C(b2)–H(b2)	126.5
N(1)–Fe(1)–N(2)	89.6(4)	C(b4)–C(b3)–C(a3)	106.8(2)
Fe(1)#1–Fe(1)–N(2)#1	84(2)	C(b4)–C(b3)–H(b3)	126.6
N(3)–Fe(1)–N(2)#1	100.1(4)	C(a3)–C(b3)–H(b3)	126.6
N(1)–Fe(1)–N(2)#1	89.5(4)	C(b3)–C(b4)–C(a4)	107.2(2)
N(2)–Fe(1)–N(2)#1	168.4(2)	C(b3)–C(b4)–H(b4)	126.4
Fe(1)#1–Fe(1)–N(1)#1	83(3)	C(a4)–C(b4)–H(b4)	126.4
N(3)–Fe(1)–N(1)#1	100.7(4)	C(15)–C(10)–C(11)	119.0(2)
N(1)–Fe(1)–N(1)#1	168.4(2)	C(15)–C(10)–C(m1)	120.8(2)
N(2)–Fe(1)–N(1)#1	89.3(4)	C(11)–C(10)–C(m1)	120.2(2)
N(2)#1–Fe(1)–N(1)#1	89.3(3)	C(10)–C(11)–C(12)	120.4(3)
Fe(1)#1–Fe(1)–N(3)#1	4(2)	C(10)–C(11)–H(11)	119.8
N(3)–Fe(1)–N(3)#1	179.0(5)	C(12)–C(11)–H(11)	119.8
N(1)–Fe(1)–N(3)#1	88.4(3)	C(13)–C(12)–C(11)	120.1(3)
N(2)–Fe(1)–N(3)#1	87.7(3)	C(13)–C(12)–H(12)	119.9
N(2)#1–Fe(1)–N(3)#1	80.7(3)	C(11)–C(12)–H(12)	119.9
N(1)#1–Fe(1)–N(3)#1	80.0(3)	C(14)–C(13)–C(12)	119.7(2)
C(a2)–N(1)–C(a1)	104.3(2)	C(14)–C(13)–H(13)	120.2
C(a2)–N(1)–Fe(1)	127.6(3)	C(12)–C(13)–H(13)	120.2
C(a1)–N(1)–Fe(1)	127.6(3)	C(13)–C(14)–C(15)	120.2(3)
C(a2)–N(1)–Fe(1)#1	127.8(3)	C(13)–C(14)–H(14)	119.9
C(a1)–N(1)–Fe(1)#1	127.5(3)	C(15)–C(14)–H(14)	119.9
C(a4)–N(2)–C(a3)	104.8(2)	C(10)–C(15)–C(14)	120.6(3)
C(a4)–N(2)–Fe(1)	127.7(3)	C(10)–C(15)–H(15)	119.7
C(a3)–N(2)–Fe(1)	127.2(3)	C(14)–C(15)–H(15)	119.7
C(a4)–N(2)–Fe(1)#1	127.4(3)	C(25)–C(20)–C(21)	118.3(2)
C(a3)–N(2)–Fe(1)#1	127.2(3)	C(25)–C(20)–C(m2)	121.3(2)
C(a1)–C(m1)–C(a4#1	124.2(2)	C(21)–C(20)–C(m2)	120.4(2)
C(a1)–C(m1)–C(10)	117.6(2)	C(22)–C(21)–C(20)	120.6(3)
C(a4#1–C(m1)–C(10)	118.2(2)	C(22)–C(21)–H(21)	119.7

Table S4. Continued

angle	degree	angle	degree
C(a3)–C(m2)–C(a2)	123.4(2)	C(20)–C(21)–H(21)	119.7
C(a3)–C(m2)–C(20)	118.1(2)	C(23)–C(22)–C(21)	120.3(3)
C(a2)–C(m2)–C(20)	118.5(2)	C(23)–C(22)–H(22)	119.9
N(1)–C(a1)–C(m1)	124.9(2)	C(21)–C(22)–H(22)	119.9
N(1)–C(a1)–C(b1)	110.7(2)	C(24)–C(23)–C(22)	119.6(2)
C(m1)–C(a1)–C(b1)	124.4(2)	C(24)–C(23)–H(23)	120.2
N(1)–C(a2)–C(m2)	125.3(2)	C(22)–C(23)–H(23)	120.2
N(1)–C(a2)–C(b2)	110.9(2)	C(23)–C(24)–C(25)	120.0(3)
C(m2)–C(a2)–C(b2)	123.8(2)	C(23)–C(24)–H(24)	120.0
N(2)–C(a3)–C(m2)	126.0(2)	C(25)–C(24)–H(24)	120.0
N(2)–C(a3)–C(b3)	110.50(19)	C(20)–C(25)–C(24)	121.2(3)
C(m2)–C(a3)–C(b3)	123.5(2)	C(20)–C(25)–H(25)	119.4
N(2)–C(a4)–C(m1#1	125.4(2)	C(24)–C(25)–H(25)	119.4
N(2)–C(a4)–C(b4)	110.7(2)	O(1)–N(3)–Fe(1)	144.4(5)
C(m1#1–C(a4)–C(b4)	123.9(2)	O(1)–N(3)–Fe(1)#1	143.3(4)
C(b2)–C(b1)–C(a1)	107.0(2)		

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

Table S5. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 33 K, crystal 1[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.022(2)	0.0127(6)	0.0105(4)	0.0003(4)	−0.0061(16)	−0.0070(15)
N(1)	0.0170(13)	0.0109(12)	0.0127(11)	0.0000(9)	−0.0044(10)	−0.0017(10)
N(2)	0.0175(13)	0.0124(12)	0.0116(11)	0.0043(9)	−0.0053(10)	−0.0013(10)
C(m1)	0.0166(15)	0.0172(14)	0.0118(13)	0.0030(10)	−0.0056(12)	−0.0062(12)
C(m2)	0.0126(14)	0.0131(14)	0.0147(13)	0.0000(10)	−0.0058(12)	−0.0036(11)
C(a1)	0.0159(15)	0.0176(15)	0.0103(13)	0.0023(11)	−0.0031(12)	−0.0053(12)
C(a2)	0.0123(14)	0.0169(14)	0.0174(13)	−0.0005(11)	−0.0044(12)	−0.0052(12)
C(a3)	0.0159(15)	0.0126(14)	0.0136(13)	0.0010(11)	−0.0066(12)	−0.0020(12)
C(a4)	0.0133(15)	0.0165(14)	0.0135(13)	0.0009(10)	−0.0038(12)	−0.0038(12)
C(b1)	0.0189(16)	0.0170(15)	0.0173(14)	0.0043(11)	−0.0066(13)	−0.0032(12)
C(b2)	0.0213(16)	0.0119(14)	0.0185(14)	0.0038(11)	−0.0070(13)	−0.0065(12)
C(b3)	0.0165(15)	0.0139(14)	0.0173(14)	−0.0024(11)	−0.0055(12)	0.0012(12)
C(b4)	0.0199(16)	0.0191(15)	0.0124(13)	0.0003(11)	−0.0064(12)	−0.0021(13)
C(10)	0.0173(15)	0.0115(13)	0.0087(12)	0.0021(10)	−0.0048(12)	−0.0011(12)
C(11)	0.0180(15)	0.0200(15)	0.0169(14)	0.0004(11)	−0.0071(12)	−0.0020(12)
C(12)	0.0193(16)	0.0203(16)	0.0155(14)	0.0003(12)	−0.0027(13)	−0.0069(12)
C(13)	0.0299(17)	0.0090(13)	0.0108(13)	0.0001(10)	−0.0011(13)	−0.0041(12)
C(14)	0.0363(18)	0.0208(16)	0.0179(15)	0.0038(12)	−0.0180(14)	−0.0096(14)
C(15)	0.0227(16)	0.0223(16)	0.0177(15)	0.0035(12)	−0.0083(13)	−0.0102(13)
C(20)	0.0184(16)	0.0145(14)	0.0066(12)	0.0022(10)	−0.0045(12)	−0.0058(12)
C(21)	0.0187(16)	0.0198(16)	0.0311(16)	−0.0031(13)	−0.0134(13)	−0.0059(13)
C(22)	0.0179(16)	0.0194(16)	0.0327(17)	−0.0050(13)	−0.0121(14)	−0.0023(13)
C(23)	0.0267(17)	0.0137(14)	0.0143(13)	−0.0018(11)	−0.0044(13)	−0.0021(13)
C(24)	0.0317(18)	0.0181(16)	0.0389(18)	−0.0046(13)	−0.0156(15)	−0.0120(14)
C(25)	0.0161(16)	0.0282(18)	0.0341(17)	−0.0053(14)	−0.0095(14)	−0.0084(13)
N(3)	0.015(2)	0.014(2)	0.016(2)	−0.0016(18)	−0.005(2)	0.0010(19)
O(1)	0.024(2)	0.021(2)	0.018(2)	0.0010(16)	−0.0085(18)	−0.0052(17)

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

Table S6. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(NO)] at 33 K, crystal 1[a]

atom	x	y	z	U(eq)
H(b1)	0.4997	0.8851	0.1184	0.023
H(b2)	0.3190	1.0213	0.3427	0.021
H(b3	0.1283	0.8885	0.8816	0.021
H(b4)	0.1714	0.6614	1.0155	0.022
H(11)	0.9037	0.6342	−0.0148	0.023
H(12)	0.9997	0.6947	−0.2537	0.024
H(13)	0.8481	0.7203	−0.3866	0.023
H(14)	0.5962	0.6951	−0.2783	0.027
H(15)	0.4993	0.6364	−0.0397	0.024
H(21)	−0.0250	0.9899	0.6442	0.026
H(22)	−0.1789	1.2298	0.7043	0.028
H(23)	−0.0649	1.3957	0.7234	0.025
H(24)	0.2032	1.3198	0.6845	0.033
H(25)	0.3577	1.0807	0.6217	0.030

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

Table S7. Complete Crystallographic Details for [Fe(TPP)(NO)] at 90 K, crystal 1

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	9.754(2)
b, Å	9.943(2)
c, Å	10.394(3)
α, deg	82.25(2)
β, deg	65.78(2)
γ, deg	69.44(2)
V, Å^3	860.7(4)
space group	$P\bar{1}$
Z	1
D_c, g/cm^3	1.348
F(000)	361
μ, mm^{-1}	0.481
crystal dimensions, mm	0.21 × 0.17 × 0.08
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	90(2)
diffractometer	Bruker SMART Apex II
θ range for collected data, deg	3.05–27.71
index range	$-11 \leq h \leq 12$
	$-12 \leq k \leq 12$
	$0 \leq l \leq 13$
total data collected	4337
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9625 and 0.9057
unique data	4337 (R_{int} = 0.0649)
unique observed data [I > 2σ(I)]	2843
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	4337/0/247
goodness-of-fit (pased on F^2)	0.949
final R indices [I > 2σ(I)]	R_1 = 0.0476, wR_2 = 0.1084
final R indices (all data)	R_1 = 0.0792, wR_2 = 0.1174

Table S8. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 90 K, crystal 1[a]

atom	x	y	z	U(eq)
Fe(1)	0.4801(5)	0.4983(7)	0.4996(7)	0.0196(5)
N(1)	0.4632(2)	0.68161(18)	0.39282(19)	0.0200(4)
N(2)	0.3569(2)	0.60885(18)	0.67908(19)	0.0200(4)
C(m1)	0.6311(3)	0.5886(2)	0.1495(2)	0.0207(5)
C(m2)	0.2809(3)	0.8545(2)	0.5876(2)	0.0204(5)
C(a1)	0.5269(3)	0.6981(2)	0.2478(2)	0.0216(5)
C(a2)	0.3685(3)	0.8177(2)	0.4459(2)	0.0214(5)
C(a3)	0.2780(3)	0.7553(2)	0.6961(2)	0.0223(5)
C(a4)	0.3168(3)	0.5555(2)	0.8143(2)	0.0220(5)
C(b1)	0.4713(3)	0.8458(2)	0.2116(2)	0.0255(5)
C(b2)	0.3731(3)	0.9198(2)	0.3333(2)	0.0239(5)
C(b3)	0.1902(3)	0.7928(2)	0.8432(2)	0.0270(6)
C(b4)	0.2127(3)	0.6696(2)	0.9164(2)	0.0253(5)
C(10)	0.6911(3)	0.6278(2)	−0.0037(2)	0.0212(5)
C(11)	0.8386(3)	0.6462(3)	−0.0685(3)	0.0283(6)
C(12)	0.8962(3)	0.6813(2)	−0.2102(3)	0.0296(6)
C(13)	0.8053(3)	0.6981(2)	−0.2885(2)	0.0273(6)
C(14)	0.6577(3)	0.6817(3)	−0.2243(3)	0.0334(6)
C(15)	0.6005(3)	0.6464(3)	−0.0822(3)	0.0311(6)
C(20)	0.1829(3)	1.0092(2)	0.6270(2)	0.0205(5)
C(21)	0.0226(3)	1.0579(2)	0.6517(3)	0.0303(6)
C(22)	−0.0682(3)	1.2007(3)	0.6866(3)	0.0338(6)
C(23)	0.0000(3)	1.2964(2)	0.6988(2)	0.0283(6)
C(24)	0.1592(3)	1.2479(3)	0.6761(3)	0.0369(7)
C(25)	0.2502(3)	1.1054(3)	0.6397(3)	0.0340(6)
N(3)	0.3085(5)	0.4907(4)	0.4910(4)	0.0198(8)
O(1)	0.1798(4)	0.5546(4)	0.5029(4)	0.0336(8)

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

Table S9. Bond Lengths for [Fe(TPP)(NO)] at 90 K, crystal 1[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.406(5)	C(b3)–H(b3)	0.9500
Fe(1)–N(3)	1.740(5)	C(b4)–H(b4)	0.9500
Fe(1)–N(2)	1.980(7)	C(10)–C(11)	1.383(3)
Fe(1)–N(1)	1.994(7)	C(10)–C(15)	1.385(3)
Fe(1)–N(1)#1)	2.007(7)	C(11)–C(12)	1.389(3)
Fe(1)–N(2)#1)	2.008(7)	C(11)–H(11)	0.9500
Fe(1)–N(3)#1)	2.146(5)	C(12)–C(13)	1.388(3)
N(1)–C(a2)	1.376(3)	C(12)–H(12)	0.9500
N(1)–C(a1)	1.387(3)	C(13)–C(14)	1.376(4)
N(1)–Fe(1)#1)	2.007(7)	C(13)–H(13)	0.9500
N(2)–C(a4)	1.380(3)	C(14)–C(15)	1.392(3)
N(2)–C(a3)	1.384(3)	C(14)–H(14)	0.9500
N(2)–Fe(1)#1)	2.008(7)	C(15)–H(15)	0.9500
C(m1)–C(a1)	1.390(3)	C(20)–C(25)	1.383(3)
C(m1)–C(a4#1)	1.397(3)	C(20)–C(21)	1.384(3)
C(m1)–C(10)	1.503(3)	C(21)–C(22)	1.386(3)
C(m2)–C(a2)	1.388(3)	C(21)–H(21)	0.9500
C(m2)–C(a3)	1.393(3)	C(22)–C(23)	1.383(4)
C(m2)–C(20)	1.504(3)	C(22)–H(22)	0.9500
C(a1)–C(b1)	1.433(3)	C(23)–C(24)	1.379(4)
C(a2)–C(b2)	1.439(3)	C(23)–H(23)	0.9500
C(a3)–C(b3)	1.437(3)	C(24)–C(25)	1.387(3)
C(a4)–C(m1#1)	1.397(3)	C(24)–H(24a)	0.9500
C(a4)–C(b4)	1.441(3)	C(25)–H(25a)	0.9500
C(b1)–C(b2)	1.349(3)	N(3)–O(1)	1.153(4)
C(b1)–H(b1)	0.9500	N(3)–Fe(1)#1)	2.146(5)
C(b2)–H(b2)	0.9500		
C(b3)–C(b4)	1.351(3)		

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

Table S10. Bond Angles for [Fe(TPP)(NO)] at 90 K, crystal 1[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(3)	177(2)	C(b2)–C(b1)–H(b1)	126.4
Fe(1)#1–Fe(1)–N(2)	88.1(19)	C(a1)–C(b1)–H(b1)	126.4
N(3)–Fe(1)–N(2)	92.0(3)	C(b1)–C(b2)–C(a2)	106.99(19)
Fe(1)#1–Fe(1)–N(1)	86.1(18)	C(b1)–C(b2)–H(b2)	126.5
N(3)–Fe(1)–N(1)	91.2(3)	C(a2)–C(b2)–H(b2)	126.5
N(2)–Fe(1)–N(1)	89.8(3)	C(b4)–C(b3)–C(a3)	107.1(2)
Fe(1)#1–Fe(1)–N(1)#1	82.3(18)	C(b4)–C(b3)–H(b3)	126.5
N(3)–Fe(1)–N(1)#1	100.5(3)	C(a3)–C(b3)–H(b2)	126.5
N(2)–Fe(1)–N(1)#1	89.8(3)	C(b3)–C(b4)–C(a4)	106.8(2)
N(1)–Fe(1)–N(1)#1	168.35(16)	C(b3)–C(b4)–H(b4)	126.6
Fe(1)#1–Fe(1)–N(2)#1	80.2(18)	C(a4)–C(b4)–H(b4)	126.6
N(3)–Fe(1)–N(2)#1	99.6(3)	C(11)–C(10)–C(15)	118.9(2)
N(2)–Fe(1)–N(2)#1	168.33(16)	C(11)–C(10)–C(m1)	120.2(2)
N(1)–Fe(1)–N(2)#1	89.4(3)	C(15)–C(10)–C(m1)	120.9(2)
N(1)#1–Fe(1)–N(2)#1	88.6(3)	C(10)–C(11)–C(12)	120.8(2)
Fe(1)#1–Fe(1)–N(3)#1	2.2(17)	C(10)–C(11)–H(11)	119.6
N(3)–Fe(1)–N(3)#1	179.5(4)	C(12)–C(11)–H(11)	119.6
N(2)–Fe(1)–N(3)#1	88.0(2)	C(13)–C(12)–C(11)	119.9(2)
N(1)–Fe(1)–N(3)#1	88.3(2)	C(13)–C(12)–H(12)	120.1
N(1)#1–Fe(1)–N(3)#1	80.1(2)	C(11)–C(12)–H(12)	120.1
N(2)#1–Fe(1)–N(3)#1	80.3(2)	C(14)–C(13)–C(12)	119.6(2)
C(a2)–N(1)–C(a1)	104.98(17)	C(14)–C(13)–H(13)	120.2
C(a2)–N(1)–Fe(1)	127.1(2)	C(12)–C(13)–H(13)	120.2
C(a1)–N(1)–Fe(1)	127.5(2)	C(13)–C(14)–C(15)	120.3(2)
C(a2)–N(1)–Fe(1)#1	127.9(2)	C(13)–C(14)–H(14a)	119.8
C(a1)–N(1)–Fe(1)#1	126.7(2)	C(15)–C(14)–H(14a)	119.8
C(a4)–N(2)–C(a3)	104.82(17)	C(10)–C(15)–C(14)	120.5(2)
C(a4)–N(2)–Fe(1)	127.5(2)	C(10)–C(15)–H(15)	119.8
C(a3)–N(2)–Fe(1)	127.3(2)	C(14)–C(15)–H(15)	119.8
C(a4)–N(2)–Fe(1)#1	127.1(2)	C(25)–C(20)–C(21)	118.6(2)
C(a3)–N(2)–Fe(1)#1	127.5(2)	C(25)–C(20)–C(m2)	120.9(2)
C(a1)–C(m1)–C(a4#1	123.5(2)	C(21)–C(20)–C(m2)	120.4(2)
C(a1)–C(m1)–C(10)	118.05(18)	C(20)–C(21)–C(22)	120.8(2)
C(a4#1–C(m1)–C(10)	118.42(19)	C(20)–C(21)–H(21)	119.6

Table S10. Continued

angle	degree	angle	degree
C(a2)–C(m2)–C(a3)	123.4(2)	C(22)–C(21)–H(21)	119.6
C(a2)–C(m2)–C(20)	118.72(18)	C(23)–C(22)–C(21)	120.3(2)
C(a3)–C(m2)–C(20)	117.90(19)	C(23)–C(22)–H(22)	119.8
N(1)–C(a1)–C(m1)	125.66(19)	C(21)–C(22)–H(22)	119.8
N(1)–C(a1)–C(b1)	110.39(18)	C(24)–C(23)–C(22)	119.1(2)
C(m1)–C(a1)–C(b1)	123.9(2)	C(24)–C(23)–H(2a)	120.4
N(1)–C(a2)–C(m2)	125.8(2)	C(22)–C(23)–H(23)	120.4
N(1)–C(a2)–C(b2)	110.51(19)	C(23)–C(24)–C(25)	120.5(2)
C(m2)–C(a2)–C(b2)	123.7(2)	C(23)–C(24)–H(24)	119.7
N(2)–C(a3)–C(m2)	125.7(2)	C(25)–C(24)–H(24)	119.7
N(2)–C(a3)–C(b3)	110.57(18)	C(20)–C(25)–C(24)	120.7(2)
C(m2)–C(a3)–C(b3)	123.8(2)	C(20)–C(25)–H(25)	119.7
N(2)–C(a4)–C(m1#1	125.74(19)	C(24)–C(25)–H(25)	119.7
N(2)–C(a4)–C(b4)	110.72(18)	O(1)–N(3)–Fe(1)	145.6(4)
C(m1#1–C(a4)–C(b4)	123.5(2)	O(1)–N(3)–Fe(1)#1	145.2(4)
C(b2)–C(b1)–C(a1)	107.13(19)		

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

Table S11. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 90 K, crystal 1[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0213(19)	0.0187(4)	0.0143(3)	0.0007(2)	−0.0038(13)	−0.0052(12)
N(1)	0.0198(11)	0.0192(9)	0.0158(10)	−0.0001(7)	−0.0051(8)	−0.0027(8)
N(2)	0.0189(11)	0.0185(9)	0.0167(10)	0.0013(7)	−0.0056(9)	−0.0016(8)
C(m1)	0.0214(13)	0.0236(11)	0.0150(11)	0.0030(8)	−0.0069(10)	−0.0061(10)
C(m2)	0.0186(13)	0.0208(11)	0.0191(12)	−0.0030(9)	−0.0066(10)	−0.0033(9)
C(a1)	0.0234(14)	0.0255(12)	0.0144(11)	0.0034(9)	−0.0070(10)	−0.0078(10)
C(a2)	0.0188(13)	0.0214(11)	0.0208(12)	−0.0007(8)	−0.0062(10)	−0.0045(10)
C(a3)	0.0212(14)	0.0224(12)	0.0196(12)	−0.0014(9)	−0.0074(10)	−0.0029(10)
C(a4)	0.0213(14)	0.0248(12)	0.0171(11)	0.0005(9)	−0.0069(10)	−0.0052(10)
C(b1)	0.0288(15)	0.0244(12)	0.0171(12)	0.0037(9)	−0.0067(11)	−0.0054(10)
C(b2)	0.0261(14)	0.0204(11)	0.0208(12)	0.0016(9)	−0.0085(11)	−0.0040(10)
C(b3)	0.0289(15)	0.0241(12)	0.0191(12)	−0.0029(9)	−0.0063(11)	−0.0009(10)
C(b4)	0.0262(15)	0.0271(13)	0.0140(11)	−0.0007(9)	−0.0049(10)	−0.0021(11)
C(10)	0.0261(14)	0.0157(11)	0.0165(11)	0.0001(8)	−0.0062(10)	−0.0032(10)
C(11)	0.0256(15)	0.0341(14)	0.0229(13)	0.0019(10)	−0.0098(11)	−0.0076(11)
C(12)	0.0288(15)	0.0298(13)	0.0236(13)	0.0023(10)	−0.0043(11)	−0.0097(11)
C(13)	0.0400(17)	0.0184(11)	0.0151(11)	0.0032(9)	−0.0064(11)	−0.0063(11)
C(14)	0.0448(18)	0.0363(15)	0.0238(14)	0.0067(11)	−0.0201(13)	−0.0130(13)
C(15)	0.0312(15)	0.0402(15)	0.0240(14)	0.0057(11)	−0.0112(12)	−0.0157(12)
C(20)	0.0256(14)	0.0187(11)	0.0133(11)	0.0002(8)	−0.0062(10)	−0.0045(10)
C(21)	0.0247(15)	0.0241(13)	0.0450(16)	−0.0056(11)	−0.0159(13)	−0.0063(11)
C(22)	0.0249(15)	0.0285(14)	0.0452(17)	−0.0070(11)	−0.0153(13)	−0.0009(11)
C(23)	0.0367(17)	0.0202(11)	0.0182(12)	−0.0030(9)	−0.0055(11)	−0.0032(11)
C(24)	0.0444(19)	0.0263(14)	0.0446(17)	−0.0064(11)	−0.0173(14)	−0.0145(12)
C(25)	0.0266(15)	0.0303(14)	0.0478(17)	−0.0057(12)	−0.0147(13)	−0.0100(11)
N(3)	0.020(2)	0.0179(19)	0.0145(19)	0.0027(14)	−0.0048(17)	−0.0018(16)
O(1)	0.023(2)	0.043(2)	0.031(2)	0.0001(16)	−0.0105(17)	−0.0073(17)

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

Table S12. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 90 K, crystal 1[a]

atom	x	y	z	U(eq)
H(b1)	0.4984	0.8845	0.1192	0.031
H(b2)	0.3177	1.0202	0.3428	0.029
H(b3)	0.1281	0.8867	0.8818	0.032
H(b4)	0.1683	0.6600	1.0160	0.030
H(11)	0.9013	0.6346	−0.0153	0.034
H(12)	0.9976	0.6938	−0.2536	0.036
H(13)	0.8448	0.7207	−0.3858	0.033
H(14)	0.5945	0.6946	−0.2772	0.040
H(15)	0.4985	0.6350	−0.0387	0.037
H(21)	−0.0258	0.9928	0.6447	0.036
H(22)	−0.1777	1.2328	0.7021	0.041
H(23)	−0.0619	1.3943	0.7226	0.034
H(24)	0.2068	1.3126	0.6853	0.044
H(25)	0.3600	1.0736	0.6234	0.041

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

Table S13. Complete Crystallographic Details for [Fe(TPP)(NO)] at 100 K, crystal 2

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	9.7310(8)
b, Å	9.9238(8)
c, Å	10.3902(6)
α, deg	82.1950(10)
β, deg	65.693(4)
γ, deg	69.384(5)
V, Å^3	855.81(11)
space group	$P\bar{1}$
Z	1
D_c, g/cm^3	1.355
F(000)	361
μ, mm^{-1}	0.484
crystal dimensions, mm	0.21 × 0.20 × 0.05
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.15–31.22
index range	$-12 \leq h \leq 14$
	$-14 \leq k \leq 14$
	$0 \leq l \leq 15$
total data collected	6497
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9785 and 0.9064
unique data	6497 (R_{int} = 0.0646)
unique observed data [I > 2σ(I)]	4766
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	6497/0/247
goodness-of-fit (pased on F^2)	0.994
final R indices [I > 2σ(I)]	R_1 = 0.0449, wR_2 = 0.1213
final R indices (all data)	R_1 = 0.0660, wR_2 = 0.1309

Table S14. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 100 K, crystal 2[a]

atom	x	y	z	U(eq)
Fe(1)	0.4807(3)	0.4983(4)	0.4986(4)	0.0166(3)
N(1)	0.46321(16)	0.68120(13)	0.39278(13)	0.0174(3)
N(2)	0.35704(16)	0.60896(14)	0.67936(13)	0.0179(3)
C(m1)	0.6314(2)	0.58824(17)	0.14934(15)	0.0180(3)
C(m2)	0.28062(19)	0.85505(16)	0.58793(16)	0.0169(3)
C(a1)	0.52685(19)	0.69787(16)	0.24781(15)	0.0183(3)
C(a2)	0.3682(2)	0.81761(16)	0.44628(15)	0.0173(3)
C(a3)	0.2786(2)	0.75531(16)	0.69620(16)	0.0179(3)
C(a4)	0.31648(19)	0.55493(16)	0.81498(15)	0.0185(3)
C(b1)	0.4710(2)	0.84603(16)	0.21156(16)	0.0217(3)
C(b2)	0.3725(2)	0.92018(16)	0.33371(16)	0.0207(3)
C(b3)	0.1905(2)	0.79302(17)	0.84369(16)	0.0217(3)
C(b4)	0.2132(2)	0.66964(17)	0.91643(16)	0.0223(3)
C(10)	0.6918(2)	0.62742(16)	−0.00410(15)	0.0188(3)
C(11)	0.8390(2)	0.64617(19)	−0.06820(17)	0.0255(4)
C(12)	0.8963(2)	0.68176(19)	−0.21056(17)	0.0268(4)
C(13)	0.8059(2)	0.69778(16)	−0.28827(16)	0.0249(4)
C(14)	0.6569(2)	0.6822(2)	−0.22403(18)	0.0301(4)
C(15)	0.5997(2)	0.64677(19)	−0.08165(18)	0.0270(4)
C(20)	0.1832(2)	1.00909(16)	0.62716(15)	0.0176(3)
C(21)	0.0225(2)	1.05790(19)	0.6516(2)	0.0276(4)
C(22)	−0.0683(2)	1.20081(19)	0.6872(2)	0.0312(4)
C(23)	−0.0002(2)	1.29624(17)	0.69867(16)	0.0246(4)
C(24)	0.1591(2)	1.2478(2)	0.6765(2)	0.0334(4)
C(25)	0.2498(2)	1.1053(2)	0.6402(2)	0.0313(4)
N(3)	0.3097(3)	0.4904(3)	0.4908(3)	0.0165(5)
O(1)	0.1797(3)	0.5554(3)	0.5026(3)	0.0287(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 S15. Bond Lengths for [Fe(TPP)(NO)] at 100 K, crystal 2[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.402(3)	C(b3)–H(b3)	0.9500
Fe(1)–N(3)	1.728(3)	C(b4)–H(b4)	0.9500
Fe(1)–N(1)	1.981(4)	C(10)–C(11)	1.378(2)
Fe(1)–N(2)	1.988(4)	C(10)–C(15)	1.386(2)
Fe(1)–N(2)#1)	1.998(4)	C(11)–C(12)	1.393(2)
Fe(1)–N(1)#1)	2.006(4)	C(11)–H(11)	0.9500
Fe(1)–N(3)#1)	2.129(3)	C(12)–C(13)	1.379(3)
N(1)–C(a2)	1.3772(19)	C(12)–H(12)	0.9500
N(1)–C(a1)	1.3843(18)	C(13)–C(14)	1.380(3)
N(1)–Fe(1)#1)	2.006(4)	C(13)–H(13)	0.9500
N(2)–C(a3)	1.3787(19)	C(14)–C(15)	1.393(2)
N(2)–C(a4)	1.3838(18)	C(14)–H(14)	0.9500
N(2)–Fe(1)#1)	1.998(4)	C(15)–H(15)	0.9500
C(m1)–C(a4#1)	1.385(2)	C(20)–C(25)	1.376(2)
C(m1)–C(a1)	1.390(2)	C(20)–C(21)	1.385(2)
C(m1)–C(10)	1.503(2)	C(21)–C(22)	1.386(2)
C(m2)–C(a2)	1.387(2)	C(21)–H(21)	0.9500
C(m2)–C(a3)	1.392(2)	C(22)–C(23)	1.374(3)
C(m2)–C(20)	1.494(2)	C(22)–H(22)	0.9500
C(a1)–C(b1)	1.433(2)	C(23)–C(24)	1.378(3)
C(a2)–C(b2)	1.439(2)	C(23)–H(23)	0.9500
C(a3)–C(b3)	1.439(2)	C(24)–C(25)	1.383(3)
C(a4)–C(m1#1)	1.385(2)	C(24)–H(24)	0.9500
C(a4)–C(b4)	1.437(2)	C(25)–H(25)	0.9500
C(b1)–C(b2)	1.351(2)	N(3)–O(1)	1.163(3)
C(b1)–H(ba)	0.9500	N(3)–Fe(1)#1)	2.129(3)
C(b2)–H(bb)	0.9500		
C(b3)–C(b4)	1.347(2)		

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

Table S16. Bond Angles for [Fe(TPP)(NO)] at 100 K, crystal 2[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(3)	177.6(12)	C(b2)–C(b1)–H(b1)	126.5
Fe(1)#1–Fe(1)–N(1)	87.7(11)	C(a1)–C(b1)–H(b1)	126.5
N(3)–Fe(1)–N(1)	91.34(16)	C(b1)–C(b2)–C(a2)	106.93(13)
Fe(1)#1–Fe(1)–N(2)	85.7(11)	C(b1)–C(b2)–H(b2)	126.5
N(3)–Fe(1)–N(2)	92.10(16)	C(a2)–C(b2)–H(b2)	126.5
N(1)–Fe(1)–N(2)	89.86(16)	C(b4)–C(b3)–C(a3)	106.96(13)
Fe(1)#1–Fe(1)–N(2)#1	82.7(11)	C(b4)–C(b3)–H(b3)	126.5
N(3)–Fe(1)–N(2)#1	99.48(17)	C(a3)–C(b3)–H(b3)	126.5
N(1)–Fe(1)–N(2)#1	89.67(17)	C(b3)–C(b4)–C(a4)	107.20(13)
N(2)–Fe(1)–N(2)#1	168.42(8)	C(b3)–C(b4)–H(b4)	126.4
Fe(1)#1–Fe(1)–N(1)#1	80.8(11)	C(a4)–C(b4)–H(b4)	126.4
N(3)–Fe(1)–N(1)#1	100.21(17)	C(11)–C(10)–C(15)	119.51(14)
N(1)–Fe(1)–N(1)#1	168.44(8)	C(11)–C(10)–C(m1)	119.94(15)
N(2)–Fe(1)–N(1)#1	89.28(16)	C(15)–C(10)–C(m1)	120.54(15)
N(2)#1–Fe(1)–N(1)#1	88.87(15)	C(10)–C(11)–C(12)	120.32(16)
Fe(1)#1–Fe(1)–N(3)#1	1.9(10)	C(10)–C(11)–H(11)	119.8
N(3)–Fe(1)–N(3)#1	179.5(2)	C(12)–C(11)–H(11)	119.8
N(1)–Fe(1)–N(3)#1	88.48(13)	C(13)–C(12)–C(11)	120.05(17)
N(2)–Fe(1)–N(3)#1	87.49(13)	C(13)–C(12)–H(12)	120.0
N(2)#1–Fe(1)–N(3)#1	80.93(12)	C(11)–C(12)–H(12)	120.0
N(1)#1–Fe(1)–N(3)#1	79.98(12)	C(12)–C(13)–C(14)	119.93(15)
C(a2)–N(1)–C(a1)	105.02(12)	C(12)–C(13)–H(13)	120.0
C(a2)–N(1)–Fe(1)	127.09(15)	C(14)–C(13)–H(13)	120.0
C(a1)–N(1)–Fe(1)	127.40(15)	C(13)–C(14)–C(15)	119.98(17)
C(a2)–N(1)–Fe(1)#1	127.48(15)	C(13)–C(14)–H(14)	120.0
C(a1)–N(1)–Fe(1)#1	127.09(15)	C(15)–C(14)–H(14)	120.0
Fe(1)–N(1)–Fe(1)#1	11.56(8)	C(10)–C(15)–C(14)	120.17(17)
C(a3)–N(2)–C(a4)	105.02(12)	C(10)–C(15)–H(15)	119.9
C(a3)–N(2)–Fe(1)	127.05(15)	C(14)–C(15)–H(15)	119.9
C(a4)–N(2)–Fe(1)	127.59(15)	C(25)–C(20)–C(21)	118.51(15)
C(a3)–N(2)–Fe(1)#1	127.49(15)	C(25)–C(20)–C(m2)	121.29(15)
C(a4)–N(2)–Fe(1)#1	126.91(15)	C(21)–C(20)–C(m2)	120.21(15)
Fe(1)–N(2)–Fe(1)#1	11.58(8)	C(20)–C(21)–C(22)	120.50(16)
C(a4#1–C(m1)–C(a1)	123.55(14)	C(20)–C(21)–H(21)	119.8

Table S16. Continued

angle	degree	angle	degree
C(a4#1–C(m1)–C(10)	118.27(13)	C(22)–C(21)–H(21a)	119.8
C(a1)–C(m1)–C(10)	118.18(13)	C(23)–C(22)–C(21)	120.51(17)
C(a2)–C(m2)–C(a3)	122.99(14)	C(23)–C(22)–H(22a)	119.7
C(a2)–C(m2)–C(20)	118.91(13)	C(21)–C(22)–H(22a)	119.7
C(a3)–C(m2)–C(20)	118.10(14)	C(22)–C(23)–C(24)	119.24(15)
N(1)–C(a1)–C(m1)	125.65(14)	C(22)–C(23)–H(23a)	120.4
N(1)–C(a1)–C(b1)	110.49(13)	C(24)–C(23)–H(23a)	120.4
C(m1)–C(a1)–C(b1)	123.86(14)	C(23)–C(24)–C(25)	120.20(17)
N(1)–C(a2)–C(m2)	126.10(13)	C(23)–C(24)–H(24a)	119.9
N(1)–C(a2)–C(b2)	110.50(13)	C(25)–C(24)–H(24a)	119.9
C(m2)–C(a2)–C(b2)	123.40(14)	C(20)–C(25)–C(24)	121.04(17)
N(2)–C(a3)–C(m2)	125.92(14)	C(20)–C(25)–H(25a)	119.5
N(2)–C(a3)–C(b3)	110.50(13)	C(24)–C(25)–H(25a)	119.5
C(m2)–C(a3)–C(b3)	123.57(14)	O(1)–N(3)–Fe(1)	145.3(3)
N(2)–C(a4)–C(m1#1	125.79(14)	O(1)–N(3)–Fe(1)#1	144.9(2)
N(2)–C(a4)–C(b4)	110.31(13)	Fe(1)–N(3)–Fe(1)#1	0.5(2)
C(m1#1–C(a4)–C(b4)	123.89(14)		
C(b2)–C(b1)–C(a1)	107.06(13)		

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

Table S17. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 100 K, crystal 2[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0188(10)	0.0152(2)	0.0106(2)	0.0013(2)	−0.0028(7)	−0.0038(7)
N(1)	0.0180(7)	0.0159(6)	0.0124(6)	−0.0006(5)	−0.0027(5)	−0.0024(5)
N(2)	0.0174(7)	0.0181(6)	0.0132(6)	0.0021(5)	−0.0042(5)	−0.0030(5)
C(m1)	0.0170(8)	0.0223(8)	0.0133(7)	0.0031(6)	−0.0054(6)	−0.0067(6)
C(m2)	0.0144(8)	0.0172(7)	0.0182(7)	0.0013(6)	−0.0066(6)	−0.0042(6)
C(a1)	0.0200(8)	0.0178(7)	0.0143(7)	0.0025(5)	−0.0056(7)	−0.0052(6)
C(a2)	0.0166(8)	0.0160(7)	0.0168(7)	0.0025(5)	−0.0061(6)	−0.0038(6)
C(a3)	0.0167(8)	0.0176(7)	0.0147(7)	−0.0009(5)	−0.0044(6)	−0.0022(6)
C(a4)	0.0196(8)	0.0198(7)	0.0111(7)	−0.0009(5)	−0.0036(6)	−0.0034(6)
C(b1)	0.0256(9)	0.0192(7)	0.0154(7)	0.0051(6)	−0.0066(7)	−0.0053(7)
C(b2)	0.0221(8)	0.0165(7)	0.0173(7)	0.0021(6)	−0.0053(7)	−0.0030(6)
C(b3)	0.0234(9)	0.0206(8)	0.0138(7)	−0.0009(6)	−0.0034(7)	−0.0031(7)
C(b4)	0.0252(9)	0.0215(8)	0.0119(7)	−0.0008(6)	−0.0037(7)	−0.0021(7)
C(10)	0.0221(8)	0.0146(7)	0.0128(7)	0.0015(5)	−0.0038(6)	−0.0025(6)
C(11)	0.0238(9)	0.0320(9)	0.0175(8)	0.0031(7)	−0.0075(7)	−0.0071(7)
C(12)	0.0257(9)	0.0274(9)	0.0188(8)	0.0029(7)	−0.0014(7)	−0.0087(7)
C(13)	0.0357(10)	0.0150(7)	0.0137(7)	0.0020(6)	−0.0039(7)	−0.0041(7)
C(14)	0.0422(11)	0.0315(10)	0.0215(9)	0.0059(7)	−0.0184(8)	−0.0130(8)
C(15)	0.0293(10)	0.0349(10)	0.0209(8)	0.0070(7)	−0.0108(8)	−0.0164(8)
C(20)	0.0207(8)	0.0177(7)	0.0128(7)	0.0000(5)	−0.0054(6)	−0.0056(6)
C(21)	0.0229(9)	0.0205(8)	0.0412(11)	−0.0052(7)	−0.0140(8)	−0.0056(7)
C(22)	0.0235(10)	0.0238(9)	0.0415(11)	−0.0075(8)	−0.0126(8)	0.0004(7)
C(23)	0.0334(10)	0.0173(7)	0.0155(7)	−0.0033(6)	−0.0052(7)	−0.0037(7)
C(24)	0.0394(12)	0.0237(9)	0.0402(11)	−0.0066(8)	−0.0131(9)	−0.0147(8)
C(25)	0.0213(9)	0.0283(10)	0.0450(11)	−0.0052(8)	−0.0111(9)	−0.0091(8)
N(3)	0.0207(13)	0.0162(12)	0.0084(11)	0.0013(9)	−0.0030(11)	−0.0047(10)
O(1)	0.0218(13)	0.0335(14)	0.0276(13)	0.0021(11)	−0.0111(11)	−0.0043(10)

[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 S18. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 100 K, crystal 2[a]

atom	x	y	z	U(eq)
H(BA	0.4980	0.8848	0.1191	0.026
H(BB	0.3168	1.0208	0.3434	0.025
H(BC	0.1281	0.8870	0.8824	0.026
H(BD	0.1693	0.6602	1.0162	0.027
H(11A)	0.9018	0.6348	−0.0151	0.031
H(12A)	0.9976	0.6950	−0.2541	0.032
H(13A)	0.8462	0.7195	−0.3859	0.030
H(14A)	0.5934	0.6957	−0.2769	0.036
H(15A)	0.4972	0.6358	−0.0376	0.032
H(21A)	−0.0258	0.9929	0.6438	0.033
H(22A)	−0.1784	1.2330	0.7038	0.037
H(23A)	−0.0623	1.3945	0.7216	0.030
H(24A)	0.2068	1.3125	0.6861	0.040
H(25A)	0.3599	1.0734	0.6240	0.038

[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 S19. Complete Crystallographic Details for [Fe(TPP)(NO)] at 100 K, crystal 3

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	9.734(3)
b, Å	9.960(3)
c, Å	10.391(3)
α, deg	82.100(3)
β, deg	65.63(2)
γ, deg	69.249(19)
V, Å^3	858.0(4)
space group	$P\bar{1}$
Z	1
D_c, g/cm^3	1.352
F(000)	361
μ, mm^{-1}	0.483
crystal dimensions, mm	0.48 × 0.26 × 0.25
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.15–26.00
index range	$-10 \leq h \leq 11$
	$-11 \leq k \leq 12$
	$0 \leq l \leq 12$
total data collected	5092
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.8888 and 0.8013
unique data	5092 (R_{int} = 0.0615)
unique observed data [I > 2σ(I)]	4085
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	5092/0/247
goodness-of-fit (pased on F^2)	1.035
final R indices [I > 2σ(I)]	R_1 = 0.0788, wR_2 = 0.1979
final R indices (all data)	R_1 = 0.0999, wR_2 = 0.2225

Table S20. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 100 K, crystal 3[a]

atom	x	y	z	U(eq)
Fe(1)	0.4836(12)	0.4969(15)	0.4979(15)	0.0219(11)
N(1)	0.4626(3)	0.6827(3)	0.3929(3)	0.0178(6)
N(2)	0.3564(3)	0.6086(3)	0.6810(3)	0.0185(6)
C(m1)	0.6315(4)	0.5878(3)	0.1505(3)	0.0189(7)
C(m2)	0.2818(4)	0.8529(3)	0.5878(3)	0.0180(6)
C(a1)	0.5263(4)	0.6986(3)	0.2480(3)	0.0189(7)
C(a2)	0.3691(4)	0.8172(3)	0.4461(3)	0.0199(7)
C(a3)	0.2775(4)	0.7554(3)	0.6976(3)	0.0190(7)
C(a4)	0.3168(4)	0.5560(3)	0.8149(3)	0.0195(7)
C(b1)	0.4715(4)	0.8448(3)	0.2121(3)	0.0232(7)
C(b2)	0.3742(4)	0.9190(3)	0.3329(3)	0.0215(7)
C(b3)	0.1901(4)	0.7931(3)	0.8433(3)	0.0237(7)
C(b4)	0.2123(4)	0.6698(3)	0.9160(3)	0.0207(7)
C(10)	0.6911(4)	0.6275(3)	−0.0034(3)	0.0191(7)
C(11)	0.8373(4)	0.6468(4)	−0.0676(4)	0.0301(9)
C(12)	0.8941(5)	0.6824(4)	−0.2102(4)	0.0302(9)
C(13)	0.8047(5)	0.6977(3)	−0.2883(3)	0.0267(8)
C(14)	0.6562(5)	0.6809(4)	−0.2231(4)	0.0336(9)
C(15)	0.6001(5)	0.6454(4)	−0.0809(4)	0.0310(9)
C(20)	0.1830(4)	1.0077(3)	0.6274(3)	0.0196(7)
C(21)	0.0221(5)	1.0590(4)	0.6511(4)	0.0327(9)
C(22)	−0.0680(5)	1.2014(4)	0.6862(4)	0.0349(9)
C(23)	0.0000(5)	1.2953(3)	0.6990(3)	0.0279(8)
C(24)	0.1591(5)	1.2452(4)	0.6777(4)	0.0374(10)
C(25)	0.2505(5)	1.1025(4)	0.6417(4)	0.0349(9)
N(3)	0.3115(6)	0.4892(6)	0.4913(6)	0.0186(11)
O(1)	0.1803(6)	0.5545(6)	0.5033(6)	0.0338(12)

[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 S21. Bond Lengths for [Fe(TPP)(NO)] at 100 K, crystal 3[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.365(13)	C(b3)–H(b3)	0.9500
Fe(1)–N(3)	1.734(8)	C(b4)–H(b4)	0.9500
Fe(1)–N(2)#1)	1.994(14)	C(10)–C(11)	1.372(5)
Fe(1)–N(1)	2.004(14)	C(10)–C(15)	1.379(5)
Fe(1)–N(1)#1)	2.008(14)	C(11)–C(12)	1.394(5)
Fe(1)–N(2)	2.013(14)	C(11)–H(11)	0.9500
Fe(1)–N(3)#1)	2.096(9)	C(12)–C(13)	1.376(5)
N(1)–C(a2)	1.361(4)	C(12)–H(12)	0.9500
N(1)–C(a1)	1.382(4)	C(13)–C(14)	1.382(6)
N(1)–Fe(1)#1)	2.008(14)	C(13)–H(13)	0.9500
N(2)–C(a4)	1.363(4)	C(14)–C(15)	1.390(5)
N(2)–C(a3)	1.386(4)	C(14)–H(14a)	0.9500
N(2)–Fe(1)#1)	1.993(14)	C(15)–H(15)	0.9500
C(m1)–C(a4#1)	1.390(4)	C(20)–C(25)	1.380(5)
C(m1)–C(a1)	1.394(4)	C(20)–C(21)	1.387(5)
C(m1)–C(10)	1.508(4)	C(21)–C(22)	1.382(5)
C(m2)–C(a2)	1.383(5)	C(21)–H(21)	0.9500
C(m2)–C(a3)	1.390(4)	C(22)–C(23)	1.370(6)
C(m2)–C(20)	1.506(5)	C(22)–H(22)	0.9500
C(a1)–C(b1)	1.417(4)	C(23)–C(24)	1.377(6)
C(a2)–C(b2)	1.440(4)	C(23)–H(23)	0.9500
C(a3)–C(b3)	1.423(4)	C(24)–C(25)	1.388(6)
C(a4)–C(m1#1)	1.390(4)	C(24)–H(24)	0.9500
C(a4)–C(b4)	1.432(4)	C(25)–H(25)	0.9500
C(b1)–C(b2)	1.341(4)	N(3)–O(1)	1.171(7)
C(b1)–H(ba)	0.9500	N(3)–Fe(1)#1)	2.096(9)
C(b2)–H(bb)	0.9500		
C(b3)–C(b4)	1.348(5)		

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

Table S22. Bond Angles for [Fe(TPP)(NO)] at 100 K, crystal 3[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(3)	172(5)	C(a1)–C(b1)–H(b1)	126.3
Fe(1)#1–Fe(1)–N(2)#1	88(4)	C(b1)–C(b2)–C(a2)	106.9(3)
N(3)–Fe(1)–N(2)#1	99.1(6)	C(b1)–C(b2)–H(b2)	126.6
Fe(1)#1–Fe(1)–N(1)	85(4)	C(a2)–C(b2)–H(b2)	126.6
N(3)–Fe(1)–N(1)	91.0(6)	C(b4)–C(b3)–C(a3)	106.7(3)
N(2)#1–Fe(1)–N(1)	90.0(6)	C(b4)–C(b3)–H(b3)	126.7
Fe(1)#1–Fe(1)–N(1)#1	84(4)	C(a3)–C(b3)–H(b3)	126.7
N(3)–Fe(1)–N(1)#1	99.3(6)	C(b3)–C(b4)–C(a4)	107.3(3)
N(2)#1–Fe(1)–N(1)#1	89.6(6)	C(b3)–C(b4)–H(b4)	126.4
N(1)–Fe(1)–N(1)#1	169.6(4)	C(a4)–C(b4)–H(b4)	126.4
Fe(1)#1–Fe(1)–N(2)	82(4)	C(11)–C(10)–C(15)	119.3(3)
N(3)–Fe(1)–N(2)	91.3(6)	C(11)–C(10)–C(m1)	119.9(3)
N(2)#1–Fe(1)–N(2)	169.6(4)	C(15)–C(10)–C(m1)	120.8(3)
N(1)–Fe(1)–N(2)	89.2(6)	C(10)–C(11)–C(12)	120.3(3)
N(1)#1–Fe(1)–N(2)	89.3(6)	C(10)–C(11)–H(11)	119.8
N(3)–Fe(1)–N(3)#1	178.6(9)	C(12)–C(11)–H(11)	119.8
N(2)#1–Fe(1)–N(3)#1	82.1(4)	C(13)–C(12)–C(11)	120.4(3)
N(1)–Fe(1)–N(3)#1	88.3(4)	C(13)–C(12)–H(12)	119.8
N(1)#1–Fe(1)–N(3)#1	81.3(4)	C(11)–C(12)–H(12)	119.8
N(2)–Fe(1)–N(3)#1	87.5(4)	C(12)–C(13)–C(14)	119.3(3)
C(a2)–N(1)–C(a1)	105.4(2)	C(12)–C(13)–H(13)	120.4
C(a2)–N(1)–Fe(1)	127.7(5)	C(14)–C(13)–H(13)	120.4
C(a1)–N(1)–Fe(1)	126.4(4)	C(13)–C(14)–C(15)	120.1(4)
C(a2)–N(1)–Fe(1)#1	127.2(5)	C(13)–C(14)–H(14)	120.0
C(a1)–N(1)–Fe(1)#1	127.0(5)	C(15)–C(14)–H(14)	120.0
C(a4)–N(2)–C(a3)	105.0(2)	C(10)–C(15)–C(14)	120.6(4)
C(a4)–N(2)–Fe(1)#1	127.6(4)	C(10)–C(15)–H(15)	119.7
C(a3)–N(2)–Fe(1)#1	126.9(5)	C(14)–C(15)–H(15)	119.7
C(a4)–N(2)–Fe(1)	127.8(5)	C(25)–C(20)–C(21)	118.1(3)
C(a3)–N(2)–Fe(1)	127.0(4)	C(25)–C(20)–C(m2)	120.6(3)
C(a4#1–C(m1)–C(a1)	124.7(3)	C(21)–C(20)–C(m2)	121.3(3)
C(a4#1–C(m1)–C(10)	118.0(3)	C(22)–C(21)–C(20)	121.2(3)
C(a1)–C(m1)–C(10)	117.3(3)	C(22)–C(21)–H(21)	119.4
C(a2)–C(m2)–C(a3)	124.5(3)	C(20)–C(21)–H(21)	119.4

Table S22. Continued

angle	degree	angle	degree
C(a2)–C(m2)–C(20)	118.4(3)	C(23)–C(22)–C(21)	120.5(4)
C(a3)–C(m2)–C(20)	117.1(3)	C(23)–C(22)–H(22)	119.8
N(1)–C(a1)–C(m1)	125.2(3)	C(21)–C(22)–H(22)	119.8
N(1)–C(a1)–C(b1)	110.3(3)	C(22)–C(23)–C(24)	118.9(3)
C(m1)–C(a1)–C(b1)	124.5(3)	C(22)–C(23)–H(23)	120.5
N(1)–C(a2)–C(m2)	125.7(3)	C(24)–C(23)–H(23)	120.5
N(1)–C(a2)–C(b2)	110.1(3)	C(23)–C(24)–C(25)	120.9(4)
C(m2)–C(a2)–C(b2)	124.2(3)	C(23)–C(24)–H(24)	119.5
N(2)–C(a3)–C(m2)	125.1(3)	C(25)–C(24)–H(24)	119.5
N(2)–C(a3)–C(b3)	110.6(3)	C(20)–C(25)–C(24)	120.4(4)
C(m2)–C(a3)–C(b3)	124.4(3)	C(20)–C(25)–H(25)	119.8
N(2)–C(a4)–C(m1#1	125.1(3)	C(24)–C(25)–H(25)	119.8
N(2)–C(a4)–C(b4)	110.5(3)	O(1)–N(3)–Fe(1)	145.4(7)
C(m1#1–C(a4)–C(b4)	124.4(3)	O(1)–N(3)–Fe(1)#1	144.1(6)
C(b2)–C(b1)–C(a1)	107.4(3)		
C(b2)–C(b1)–H(ba)	126.3		

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

Table S23. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 100 K, crystal 3[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.029(3)	0.0168(10)	0.0125(7)	0.0027(6)	−0.005(2)	−0.004(2)
N(1)	0.0186(15)	0.0208(14)	0.0120(12)	0.0039(10)	−0.0053(11)	−0.0063(12)
N(2)	0.0164(15)	0.0178(13)	0.0173(13)	0.0024(10)	−0.0060(12)	−0.0025(11)
C(m1)	0.0159(17)	0.0253(17)	0.0134(15)	0.0014(12)	−0.0055(13)	−0.0051(14)
C(m2)	0.0202(18)	0.0175(15)	0.0201(16)	0.0047(12)	−0.0105(14)	−0.0091(13)
C(a1)	0.0189(18)	0.0212(16)	0.0133(15)	0.0011(12)	−0.0054(14)	−0.0042(14)
C(a2)	0.0188(18)	0.0173(16)	0.0230(17)	0.0070(12)	−0.0092(14)	−0.0068(14)
C(a3)	0.0186(18)	0.0189(16)	0.0205(16)	0.0063(12)	−0.0103(14)	−0.0064(14)
C(a4)	0.0177(17)	0.0259(17)	0.0103(14)	−0.0037(12)	−0.0011(13)	−0.0058(14)
C(b1)	0.028(2)	0.0207(16)	0.0153(15)	0.0050(12)	−0.0070(15)	−0.0051(15)
C(b2)	0.029(2)	0.0153(15)	0.0173(16)	0.0056(12)	−0.0089(15)	−0.0061(14)
C(b3)	0.0252(19)	0.0218(17)	0.0195(16)	0.0002(13)	−0.0066(15)	−0.0051(15)
C(b4)	0.0235(18)	0.0220(16)	0.0089(14)	−0.0020(12)	−0.0040(13)	−0.0011(14)
C(10)	0.0231(18)	0.0136(15)	0.0162(15)	0.0009(11)	−0.0066(14)	−0.0027(13)
C(11)	0.028(2)	0.040(2)	0.0216(19)	0.0030(16)	−0.0097(16)	−0.0115(17)
C(12)	0.028(2)	0.034(2)	0.0220(19)	0.0037(16)	−0.0011(15)	−0.0140(16)
C(13)	0.039(2)	0.0154(16)	0.0155(16)	−0.0016(12)	−0.0042(16)	−0.0043(15)
C(14)	0.046(2)	0.035(2)	0.026(2)	0.0081(17)	−0.0210(19)	−0.0149(19)
C(15)	0.034(2)	0.041(2)	0.023(2)	0.0091(16)	−0.0135(17)	−0.0191(18)
C(20)	0.0228(19)	0.0233(16)	0.0103(14)	0.0036(12)	−0.0047(14)	−0.0083(14)
C(21)	0.027(2)	0.0252(19)	0.049(2)	−0.0033(17)	−0.0192(19)	−0.0060(16)
C(22)	0.026(2)	0.030(2)	0.044(2)	−0.0053(18)	−0.0145(19)	−0.0008(17)
C(23)	0.041(2)	0.0190(16)	0.0133(16)	0.0027(13)	−0.0061(16)	−0.0047(16)
C(24)	0.043(3)	0.028(2)	0.043(2)	−0.0045(18)	−0.014(2)	−0.0155(18)
C(25)	0.026(2)	0.030(2)	0.049(3)	−0.0026(18)	−0.0137(19)	−0.0094(17)
N(3)	0.018(3)	0.023(3)	0.010(2)	0.006(2)	−0.004(2)	−0.006(2)
O(1)	0.026(3)	0.039(3)	0.035(3)	0.004(2)	−0.015(2)	−0.007(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 S24. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(NO)] at 100 K, crystal 3[a]

atom	x	y	z	U(eq)
H(b1)	0.4986	0.8831	0.1195	0.028
H(b2)	0.3192	1.0195	0.3421	0.026
H(b3)	0.1281	0.8869	0.8819	0.028
H(b4)	0.1671	0.6601	1.0157	0.025
H(11)	0.9001	0.6360	−0.0147	0.036
H(12)	0.9952	0.6961	−0.2537	0.036
H(13)	0.8447	0.7196	−0.3860	0.032
H(14)	0.5923	0.6937	−0.2754	0.040
H(15)	0.4982	0.6333	−0.0368	0.037
H(21)	−0.0270	0.9952	0.6431	0.039
H(22)	−0.1780	1.2344	0.7016	0.042
H(23)	−0.0616	1.3934	0.7222	0.033
H(24)	0.2069	1.3091	0.6878	0.045
H(25)	0.3603	1.0699	0.6268	0.042

[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 S25. Complete Crystallographic Details for [Fe(TPP)(NO)] at 100 K, crystal 4

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	9.7201(7)
b, Å	9.9105(6)
c, Å	10.3715(6)
α, deg	82.304(4)
β, deg	65.802(4)
γ, deg	69.546(4)
V, Å^3	853.81(9)
space group	$P\bar{1}$
Z	1
D_c, g/cm^3	1.359
F(000)	361
μ, mm^{-1}	0.485
crystal dimensions, mm	0.28 × 0.28 × 0.28
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.15–34.57
index range	$-13 \leq h \leq 15$
	$-15 \leq k \leq 15$
	$0 \leq l \leq 16$
total data collected	6741
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.90 and 0.86
unique data	6741 (R_{int} = 0.0854)
unique observed data [I > 2σ(I)]	4480
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	6741/0/247
goodness-of-fit (pased on F^2)	1.050
final R indices [I > 2σ(I)]	R_1 = 0.0638, wR_2 = 0.1543
final R indices (all data)	R_1 = 0.1118, wR_2 = 0.1806

Table S26. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 100 K, crystal 4[a]

atom	x	y	z	U(eq)
Fe(1)	−0.0205(2)	0.4985(3)	0.9982(3)	0.0166(2)
N(1)	0.0362(3)	0.3189(2)	1.10761(19)	0.0176(3)
N(2)	0.1431(2)	0.3907(2)	0.82052(19)	0.0186(4)
N(3)	−0.1906(4)	0.4897(4)	0.9906(4)	0.0208(7)
O(1)	−0.3201(4)	0.5556(5)	1.0025(5)	0.0332(9)
C(a1)	−0.0271(3)	0.3022(2)	1.2526(2)	0.0191(4)
C(b1)	0.0289(3)	0.1535(2)	1.2885(2)	0.0232(4)
C(b2)	0.1267(3)	0.0802(3)	1.1669(2)	0.0224(4)
C(a2)	0.1307(3)	0.1824(2)	1.0541(2)	0.0183(4)
C(m1)	0.2192(3)	0.1448(2)	0.9121(2)	0.0188(4)
C(a3)	0.2215(3)	0.2451(3)	0.8039(2)	0.0198(4)
C(b3)	0.3103(3)	0.2059(3)	0.6561(2)	0.0227(4)
C(b4)	0.2872(3)	0.3305(3)	0.5833(2)	0.0235(5)
C(a4)	0.1841(3)	0.4445(2)	0.6848(2)	0.0193(4)
C(m2)	0.1308(3)	0.5888(2)	0.6495(2)	0.0186(4)
C(10)	0.3166(3)	−0.0085(2)	0.8726(2)	0.0187(4)
C(11)	0.4770(3)	−0.0572(3)	0.8489(3)	0.0297(6)
C(12)	0.5680(3)	−0.2003(3)	0.8133(3)	0.0325(6)
C(13)	0.5005(4)	−0.2961(2)	0.8005(2)	0.0259(5)
C(14)	0.3407(4)	−0.2480(3)	0.8234(4)	0.0360(6)
C(15)	0.2493(4)	−0.1054(3)	0.8601(4)	0.0335(6)
C(20)	0.1917(3)	0.6275(2)	0.4957(2)	0.0199(4)
C(21)	0.3392(3)	0.6466(3)	0.4317(3)	0.0276(5)
C(22)	0.3961(3)	0.6821(3)	0.2892(3)	0.0294(6)
C(23)	0.3062(3)	0.6979(3)	0.2114(2)	0.0264(5)
C(24)	0.1577(4)	0.6816(3)	0.2752(3)	0.0330(6)
C(25)	0.1006(3)	0.6461(3)	0.4176(3)	0.0295(6)

[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 S27. Bond Lengths for [Fe(TPP)(NO)] at 100 K, crystal 4[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.4272(16)	C(b4)–H(b4)	0.9500
Fe(1)–N(3)	1.720(4)	C(a4)–C(m2)	1.394(3)
Fe(1)–N(1)#1)	1.979(3)	C(m2)–C(a1#1)	1.381(3)
Fe(1)–N(2)#1)	1.990(3)	C(m2)–C(20)	1.504(3)
Fe(1)–N(2)	2.001(3)	C(10)–C(15)	1.381(4)
Fe(1)–N(1)	2.011(3)	C(10)–C(11)	1.383(4)
Fe(1)–N(3)#1)	2.146(4)	C(11)–C(12)	1.388(4)
N(1)–C(a2)	1.377(3)	C(11)–H(11)	0.9500
N(1)–C(a1)	1.384(3)	C(12)–C(13)	1.376(4)
N(1)–Fe(1)#1)	1.979(3)	C(12)–H(12)	0.9500
N(2)–C(a3)	1.372(3)	C(13)–C(14)	1.381(4)
N(2)–C(a4)	1.383(3)	C(13)–H(13)	0.9500
N(2)–Fe(1)#1)	1.990(3)	C(14)–C(15)	1.386(4)
N(3)–O(1)	1.160(5)	C(14)–H(14)	0.9500
N(3)–Fe(1)#1)	2.146(4)	C(15)–H(15)	0.9500
C(a1)–C(m2#1)	1.381(3)	C(20)–C(25)	1.381(4)
C(a1)–C(b1)	1.437(3)	C(20)–C(21)	1.382(4)
C(b1)–C(b2)	1.343(3)	C(21)–C(22)	1.393(4)
C(b1)–H(b1)	0.9500	C(21)–H(21)	0.9500
C(b2)–C(a2)	1.439(3)	C(22)–C(23)	1.373(4)
C(b2)–H(b2)	0.9500	C(22)–H(22)	0.9500
C(a2)–C(m1)	1.389(3)	C(23)–C(24)	1.379(4)
C(m1)–C(a3)	1.395(3)	C(23)–H(23)	0.9500
C(m1)–C(10)	1.489(3)	C(24)–C(25)	1.393(4)
C(a3)–C(b3)	1.444(3)	C(24)–H(24)	0.9500
C(b3)–C(b4)	1.357(3)	C(25)–H(25)	0.9500
C(b3)–H(b3)	0.9500		
C(b4)–C(a4)	1.433(3)		

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

Table S28. Bond Angles for [Fe(TPP)(NO)] at 100 K, crystal 4[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(3)	177.7(9)	N(2)–C(a3)–C(b3)	110.95(18)
Fe(1)#1–Fe(1)–N(1)#1	88.2(8)	C(m1)–C(a3)–C(b3)	122.9(2)
N(3)–Fe(1)–N(1)#1	91.98(18)	C(b4)–C(b3)–C(a3)	106.2(2)
Fe(1)#1–Fe(1)–N(2)#1	85.3(8)	C(b4)–C(b3)–H(b3)	126.9
N(3)–Fe(1)–N(2)#1	92.37(19)	C(a3)–C(b3)–H(b3)	126.9
N(1)#1–Fe(1)–N(2)#1	89.91(15)	C(b3)–C(b4)–C(a4)	107.2(2)
Fe(1)#1–Fe(1)–N(2)	82.4(7)	C(b3)–C(b4)–H(b4)	126.4
N(3)–Fe(1)–N(2)	99.92(19)	C(a4)–C(b4)–H(b4)	126.4
N(1)#1–Fe(1)–N(2)	89.70(15)	N(2)–C(a4)–C(m2)	125.4(2)
N(2)#1–Fe(1)–N(2)	167.72(5)	N(2)–C(a4)–C(b4)	110.55(19)
Fe(1)#1–Fe(1)–N(1)	79.6(8)	C(m2)–C(a4)–C(b4)	124.0(2)
N(3)–Fe(1)–N(1)	100.27(19)	C(a1#1–C(m2)–C(a4)	123.9(2)
N(1)#1–Fe(1)–N(1)	167.74(5)	C(a1#1–C(m2)–C(20)	118.3(2)
N(2)#1–Fe(1)–N(1)	89.10(14)	C(a4)–C(m2)–C(20)	117.8(2)
N(2)–Fe(1)–N(1)	88.69(14)	C(15)–C(10)–C(11)	118.6(2)
Fe(1)#1–Fe(1)–N(3)#1	1.9(7)	C(15)–C(10)–C(m1)	121.0(2)
N(3)–Fe(1)–N(3)#1	179.54(18)	C(11)–C(10)–C(m1)	120.4(2)
N(1)#1–Fe(1)–N(3)#1	88.05(15)	C(10)–C(11)–C(12)	120.6(2)
N(2)#1–Fe(1)–N(3)#1	87.17(15)	C(10)–C(11)–H(11)	119.7
N(2)–Fe(1)–N(3)#1	80.55(14)	C(12)–C(11)–H(11)	119.7
N(1)–Fe(1)–N(3)#1	79.70(14)	C(13)–C(12)–C(11)	120.5(3)
C(a2)–N(1)–C(a1)	104.99(18)	C(13)–C(12)–H(12)	119.7
C(a2)–N(1)–Fe(1)#1	126.99(17)	C(11)–C(12)–H(12)	119.7
C(a1)–N(1)–Fe(1)#1	127.47(18)	C(12)–C(13)–C(14)	119.1(2)
C(a2)–N(1)–Fe(1)	127.35(17)	C(12)–C(13)–H(13)	120.5
C(a1)–N(1)–Fe(1)	127.21(17)	C(14)–C(13)–H(13)	120.5
Fe(1)#1–N(1)–Fe(1)	12.26(5)	C(13)–C(14)–C(15)	120.4(3)
C(a3)–N(2)–C(a4)	105.00(18)	C(13)–C(14)–H(14)	119.8
C(a3)–N(2)–Fe(1)#1	126.90(16)	C(15)–C(14)–H(14)	119.8
C(a4)–N(2)–Fe(1)#1	127.68(18)	C(10)–C(15)–C(14)	120.7(3)
C(a3)–N(2)–Fe(1)	127.63(16)	C(10)–C(15)–H(15)	119.6
C(a4)–N(2)–Fe(1)	126.79(18)	C(14)–C(15)–H(15)	119.6
Fe(1)#1–N(2)–Fe(1)	12.28(5)	C(25)–C(20)–C(21)	119.3(2)
O(1)–N(3)–Fe(1)	144.5(4)	C(25)–C(20)–C(m2)	120.7(2)

Table S28. Continued

angle	degree	angle	degree
O(1)–N(3)–Fe(1)#1	144.2(4)	C(21)–C(20)–C(m2)	120.0(2)
Fe(1)–N(3)–Fe(1)#1	0.46(18)	C(20)–C(21)–C(22)	120.1(3)
C(m2#1–C(a1)–N(1)	125.6(2)	C(20)–C(21)–H(21)	119.9
C(m2#1–C(a1)–C(b1)	124.1(2)	C(22)–C(21)–H(21)	119.9
N(1)–C(a1)–C(b1)	110.3(2)	C(23)–C(22)–C(21)	120.3(3)
C(b2)–C(b1)–C(a1)	107.09(19)	C(23)–C(22)–H(22)	119.9
C(b2)–C(b1)–H(b1)	126.5	C(21)–C(22)–H(22)	119.9
C(a1)–C(b1)–H(b1)	126.5	C(22)–C(23)–C(24)	119.9(2)
C(b1)–C(b2)–C(a2)	107.2(2)	C(22)–C(23)–H(23)	120.0
C(b1)–C(b2)–H(b2)	126.4	C(24)–C(23)–H(23)	120.0
C(a2)–C(b2)–H(b2)	126.4	C(23)–C(24)–C(25)	119.9(3)
N(1)–C(a2)–C(m1)	126.2(2)	C(23)–C(24)–H(24)	120.1
N(1)–C(a2)–C(b2)	110.40(19)	C(25)–C(24)–H(24)	120.1
C(m1)–C(a2)–C(b2)	123.4(2)	C(20)–C(25)–C(24)	120.4(3)
C(a2)–C(m1)–C(a3)	122.7(2)	C(20)–C(25)–H(25)	119.8
C(a2)–C(m1)–C(10)	119.18(19)	C(24)–C(25)–H(25)	119.8
C(a3)–C(m1)–C(10)	118.1(2)		
N(2)–C(a3)–C(m1)	126.2(2)		

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

Table S29. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 100 K, crystal 4[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0193(9)	0.0174(3)	0.0122(3)	0.0030(2)	−0.0065(6)	−0.0054(7)
N(1)	0.0192(9)	0.0171(8)	0.0128(7)	0.0025(6)	−0.0053(7)	−0.0036(7)
N(2)	0.0201(10)	0.0194(8)	0.0123(8)	0.0040(6)	−0.0051(7)	−0.0046(8)
N(3)	0.0226(17)	0.024(2)	0.0151(16)	0.0040(14)	−0.0070(15)	−0.0086(15)
O(1)	0.0235(18)	0.039(2)	0.035(2)	0.0023(17)	−0.0148(17)	−0.0041(16)
C(a1)	0.0220(11)	0.0197(10)	0.0143(9)	0.0042(7)	−0.0071(9)	−0.0067(9)
C(b1)	0.0263(12)	0.0198(10)	0.0179(10)	0.0050(8)	−0.0073(9)	−0.0045(9)
C(b2)	0.0249(12)	0.0197(10)	0.0180(10)	0.0029(8)	−0.0077(9)	−0.0038(9)
C(a2)	0.0189(11)	0.0178(9)	0.0151(9)	0.0028(7)	−0.0065(8)	−0.0034(8)
C(m1)	0.0187(10)	0.0189(9)	0.0181(9)	0.0035(7)	−0.0088(9)	−0.0047(8)
C(a3)	0.0201(11)	0.0206(10)	0.0170(9)	0.0018(8)	−0.0075(9)	−0.0050(9)
C(b3)	0.0257(12)	0.0202(10)	0.0170(9)	0.0018(8)	−0.0063(9)	−0.0044(9)
C(b4)	0.0258(12)	0.0234(11)	0.0146(9)	0.0007(8)	−0.0062(9)	−0.0025(10)
C(a4)	0.0213(11)	0.0222(10)	0.0130(9)	0.0023(7)	−0.0067(8)	−0.0063(9)
C(m2)	0.0193(10)	0.0216(10)	0.0133(8)	0.0045(7)	−0.0068(8)	−0.0059(8)
C(10)	0.0207(11)	0.0171(9)	0.0167(9)	0.0012(7)	−0.0065(8)	−0.0056(8)
C(11)	0.0249(12)	0.0195(11)	0.0469(16)	−0.0062(11)	−0.0165(12)	−0.0043(10)
C(12)	0.0257(13)	0.0228(12)	0.0456(17)	−0.0056(11)	−0.0152(12)	−0.0003(10)
C(13)	0.0361(14)	0.0175(9)	0.0176(9)	−0.0022(7)	−0.0068(10)	−0.0049(10)
C(14)	0.0407(16)	0.0270(14)	0.0459(17)	−0.0054(12)	−0.0170(14)	−0.0154(12)
C(15)	0.0231(12)	0.0305(14)	0.0485(17)	−0.0055(12)	−0.0125(12)	−0.0103(11)
C(20)	0.0258(12)	0.0179(9)	0.0131(8)	0.0023(7)	−0.0070(8)	−0.0054(9)
C(21)	0.0245(12)	0.0397(15)	0.0186(11)	0.0054(10)	−0.0084(9)	−0.0124(11)
C(22)	0.0282(12)	0.0347(14)	0.0208(11)	0.0046(10)	−0.0043(10)	−0.0130(11)
C(23)	0.0387(14)	0.0190(10)	0.0134(9)	0.0043(7)	−0.0054(10)	−0.0073(10)
C(24)	0.0445(16)	0.0391(15)	0.0231(12)	0.0084(11)	−0.0210(12)	−0.0161(13)
C(25)	0.0316(13)	0.0408(15)	0.0238(12)	0.0106(11)	−0.0154(11)	−0.0190(12)

[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 S30. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(NO)] at 100 K, crystal 4[a]

atom	x	y	z	U(eq)
H(b1)	0.0019	0.1144	1.3809	0.028
H(b2)	0.1828	−0.0203	1.1571	0.027
H(b3)	0.3723	0.1118	0.6177	0.027
H(b4)	0.3312	0.3402	0.4835	0.028
H(11)	0.5252	0.0079	0.8569	0.036
H(12)	0.6779	−0.2324	0.7978	0.039
H(13)	0.5629	−0.3941	0.7762	0.031
H(14)	0.2931	−0.3131	0.8139	0.043
H(15)	0.1392	−0.0739	0.8768	0.040
H(21)	0.4019	0.6356	0.4849	0.033
H(22)	0.4975	0.6953	0.2456	0.035
H(23)	0.3464	0.7202	0.1138	0.032
H(24)	0.0944	0.6945	0.2220	0.040
H(25)	−0.0017	0.6345	0.4614	0.035

[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 S31. Complete Crystallographic Details for [Fe(TPP)(NO)] at 130 K, crystal 4

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	9.7394(10)
b, Å	9.9634(10)
c, Å	10.3998(10)
α, deg	82.078(4)
β, deg	65.661(4)
γ, deg	69.225(4)
V, Å^3	859.65(15)
space group	$P\bar{1}$
Z	1
D_c, g/cm^3	1.349
F(000)	361
μ, mm^{-1}	0.482
crystal dimensions, mm	0.28 × 0.28 × 0.28
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	128(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.15–28.22
index range	$-11 \leq h \leq 12$
	$-12 \leq k \leq 13$
	$0 \leq l \leq 13$
total data collected	4103
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.90 and 0.86
unique data	4103 (R_{int} = 0.0749)
unique observed data [I > 2σ(I)]	3204
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	4103/0/247
goodness-of-fit (pased on F^2)	1.053
final R indices [I > 2σ(I)]	R_1 = 0.0537, wR_2 = 0.1354
final R indices (all data)	R_1 = 0.0757, wR_2 = 0.1517

Table S32. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 130 K, crystal 4[a]

atom	x	y	z	U(eq)
Fe(1)	−0.0198(4)	0.4980(5)	0.9983(6)	0.0221(4)
N(1)	0.0363(3)	0.3191(2)	1.1076(2)	0.0222(5)
N(2)	0.1434(3)	0.3910(3)	0.8208(2)	0.0237(5)
N(3)	−0.1910(5)	0.4905(5)	0.9910(5)	0.0237(9)
O(1)	−0.3205(5)	0.5546(5)	1.0025(6)	0.0425(11)
C(a1)	−0.0268(3)	0.3024(3)	1.2526(3)	0.0235(6)
C(b1)	0.0296(4)	0.1543(3)	1.2878(3)	0.0282(6)
C(b2)	0.1271(4)	0.0804(3)	1.1666(3)	0.0280(6)
C(a2)	0.1315(4)	0.1830(3)	1.0536(3)	0.0239(6)
C(m1)	0.2198(3)	0.1448(3)	0.9122(3)	0.0233(5)
C(a3)	0.2214(4)	0.2459(3)	0.8038(3)	0.0244(6)
C(b3)	0.3108(4)	0.2071(3)	0.6561(3)	0.0280(6)
C(b4)	0.2874(4)	0.3310(3)	0.5836(3)	0.0289(6)
C(a4)	0.1836(3)	0.4448(3)	0.6849(3)	0.0236(5)
C(m2)	0.1306(3)	0.5885(3)	0.6504(3)	0.0228(5)
C(10)	0.3165(3)	−0.0083(3)	0.8728(3)	0.0236(5)
C(11)	0.4771(4)	−0.0585(4)	0.8487(4)	0.0360(7)
C(12)	0.5668(4)	−0.2008(4)	0.8138(4)	0.0394(8)
C(13)	0.4986(4)	−0.2948(3)	0.8004(3)	0.0326(6)
C(14)	0.3393(4)	−0.2451(4)	0.8232(4)	0.0411(8)
C(15)	0.2490(4)	−0.1031(4)	0.8592(4)	0.0397(8)
C(20)	0.1908(4)	0.6278(3)	0.4964(3)	0.0242(5)
C(21)	0.3376(4)	0.6468(4)	0.4317(3)	0.0337(7)
C(22)	0.3948(4)	0.6820(4)	0.2893(3)	0.0366(7)
C(23)	0.3042(4)	0.6985(3)	0.2121(3)	0.0323(6)
C(24)	0.1569(4)	0.6816(4)	0.2760(3)	0.0396(8)
C(25)	0.0995(4)	0.6464(4)	0.4189(3)	0.0360(7)

[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 S33. Bond Lengths for [Fe(TPP)(NO)] at 130 K, crystal 4[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.418(4)	C(b4)–H(b4)	0.9500
Fe(1)–N(3)	1.728(5)	C(a4)–C(m2)	1.390(4)
Fe(1)–N(1)#1)	1.986(6)	C(m2)–C(a1#1)	1.379(4)
Fe(1)–N(2)#1)	1.993(6)	C(m2)–C(20)	1.510(3)
Fe(1)–N(2)	1.999(6)	C(10)–C(15)	1.378(5)
Fe(1)–N(1)	2.008(6)	C(10)–C(11)	1.384(4)
Fe(1)–N(3)#1)	2.145(5)	C(11)–C(12)	1.380(4)
N(1)–C(a2)	1.379(4)	C(11)–H(11)	0.9500
N(1)–C(a1)	1.385(3)	C(12)–C(13)	1.376(5)
N(1)–Fe(1)#1)	1.986(6)	C(12)–H(12)	0.9500
N(2)–C(a3)	1.371(4)	C(13)–C(14)	1.376(5)
N(2)–C(a4)	1.386(3)	C(13)–H(13)	0.9500
N(2)–Fe(1)#1)	1.993(6)	C(14)–C(15)	1.381(5)
N(3)–O(1)	1.156(6)	C(14)–H(14)	0.9500
N(3)–Fe(1)#1)	2.145(5)	C(15)–H(15)	0.9500
C(a1)–C(m2#1)	1.379(4)	C(20)–C(21)	1.377(4)
C(a1)–C(b1)	1.434(4)	C(20)–C(25)	1.382(4)
C(b1)–C(b2)	1.344(4)	C(21)–C(22)	1.394(4)
C(b1)–H(b1)	0.9500	C(21)–H(21)	0.9500
C(b2)–C(a2)	1.445(4)	C(22)–C(23)	1.376(5)
C(b2)–H(b2)	0.9500	C(22)–H(22)	0.9500
C(a2)–C(m1)	1.388(4)	C(23)–C(24)	1.372(5)
C(m1)–C(a3)	1.403(4)	C(23)–H(23)	0.9500
C(m1)–C(10)	1.488(4)	C(24)–C(25)	1.398(4)
C(a3)–C(b3)	1.445(4)	C(24)–H(24)	0.9500
C(b3)–C(b4)	1.353(4)	C(25)–H(25)	0.9500
C(b3)–H(b3)	0.9500		
C(b4)–C(a4)	1.434(4)		

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

Table S34. Bond Angles for [Fe(TPP)(NO)] at 130 K, crystal 4[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(3)	176.6(16)	N(2)–C(a3)–C(b3)	111.1(2)
Fe(1)#1–Fe(1)–N(1)#1	86.9(15)	C(m1)–C(a3)–C(b3)	122.7(3)
N(3)–Fe(1)–N(1)#1	91.7(3)	C(b4)–C(b3)–C(a3)	106.3(2)
Fe(1)#1–Fe(1)–N(2)#1	84.7(14)	C(b4)–C(b3)–H(b3)	126.9
N(3)–Fe(1)–N(2)#1	92.1(3)	C(a3)–C(b3)–H(b3)	126.9
N(1)#1–Fe(1)–N(2)#1	89.7(2)	C(b3)–C(b4)–C(a4)	107.3(2)
Fe(1)#1–Fe(1)–N(2)	83.3(14)	C(b3)–C(b4)–H(b4)	126.3
N(3)–Fe(1)–N(2)	99.9(3)	C(a4)–C(b4)–H(b4)	126.3
N(1)#1–Fe(1)–N(2)	89.6(2)	N(2)–C(a4)–C(m2)	125.2(2)
N(2)#1–Fe(1)–N(2)	167.99(10)	N(2)–C(a4)–C(b4)	110.5(2)
Fe(1)#1–Fe(1)–N(1)	81.1(15)	C(m2)–C(a4)–C(b4)	124.3(2)
N(3)–Fe(1)–N(1)	100.2(3)	C(a1#1–C(m2)–C(a4)	124.4(2)
N(1)#1–Fe(1)–N(1)	168.01(10)	C(a1#1–C(m2)–C(20)	117.8(2)
N(2)#1–Fe(1)–N(1)	89.2(2)	C(a4)–C(m2)–C(20)	117.7(2)
N(2)–Fe(1)–N(1)	88.9(2)	C(15)–C(10)–C(11)	118.4(3)
Fe(1)#1–Fe(1)–N(3)#1	2.8(13)	C(15)–C(10)–C(m1)	121.1(3)
N(3)–Fe(1)–N(3)#1	179.3(3)	C(11)–C(10)–C(m1)	120.5(3)
N(1)#1–Fe(1)–N(3)#1	88.0(2)	C(12)–C(11)–C(10)	120.7(3)
N(2)#1–Fe(1)–N(3)#1	87.3(2)	C(12)–C(11)–H(11)	119.6
N(2)–Fe(1)–N(3)#1	80.73(19)	C(10)–C(11)–H(11)	119.6
N(1)–Fe(1)–N(3)#1	80.0(2)	C(13)–C(12)–C(11)	120.5(3)
C(a2)–N(1)–C(a1)	105.2(2)	C(13)–C(12)–H(12)	119.7
C(a2)–N(1)–Fe(1)#1	126.8(2)	C(11)–C(12)–H(12)	119.7
C(a1)–N(1)–Fe(1)#1	127.4(2)	C(14)–C(13)–C(12)	118.9(3)
C(a2)–N(1)–Fe(1)	127.1(2)	C(14)–C(13)–H(13)	120.5
C(a1)–N(1)–Fe(1)	127.3(2)	C(12)–C(13)–H(13)	120.5
Fe(1)#1–N(1)–Fe(1)	11.99(10)	C(13)–C(14)–C(15)	120.7(3)
C(a3)–N(2)–C(a4)	104.9(2)	C(13)–C(14)–H(14)	119.7
C(a3)–N(2)–Fe(1)#1	127.3(2)	C(15)–C(14)–H(14)	119.7
C(a4)–N(2)–Fe(1)#1	127.6(3)	C(10)–C(15)–C(14)	120.7(3)
C(a3)–N(2)–Fe(1)	127.6(2)	C(10)–C(15)–H(15)	119.6
C(a4)–N(2)–Fe(1)	126.9(2)	C(14)–C(15)–H(15)	119.6
Fe(1)#1–N(2)–Fe(1)	12.01(10)	C(21)–C(20)–C(25)	119.2(2)
O(1)–N(3)–Fe(1)	145.7(5)	C(21)–C(20)–C(m2)	120.1(3)

Table S34. Continued

angle	degree	angle	degree
O(1)–N(3)–Fe(1)#1	145.1(4)	C(25)–C(20)–C(m2)	120.7(3)
Fe(1)–N(3)–Fe(1)#1	0.7(3)	C(20)–C(21)–C(22)	120.5(3)
C(m2#1–C(a1)–N(1)	125.3(3)	C(20)–C(21)–H(21)	119.7
C(m2#1–C(a1)–C(b1)	124.6(2)	C(22)–C(21)–H(21)	119.7
N(1)–C(a1)–C(b1)	110.1(2)	C(23)–C(22)–C(21)	120.0(3)
C(b2)–C(b1)–C(a1)	107.6(2)	C(23)–C(22)–H(22)	120.0
C(b2)–C(b1)–H(b1)	126.2	C(21)–C(22)–H(22)	120.0
C(a1)–C(b1)–H(b1)	126.2	C(24)–C(23)–C(22)	119.8(3)
C(b1)–C(b2)–C(a2)	106.8(2)	C(24)–C(23)–H(23)	120.1
C(b1)–C(b2)–H(b2)	126.6	C(22)–C(23)–H(23)	120.1
C(a2)–C(b2)–H(b2)	126.6	C(23)–C(24)–C(25)	120.2(3)
N(1)–C(a2)–C(m1)	126.7(2)	C(23)–C(24)–H(24)	119.9
N(1)–C(a2)–C(b2)	110.2(2)	C(25)–C(24)–H(24)	119.9
C(m1)–C(a2)–C(b2)	123.0(2)	C(20)–C(25)–C(24)	120.2(3)
C(a2)–C(m1)–C(a3)	122.2(2)	C(20)–C(25)–H(25)	119.9
C(a2)–C(m1)–C(10)	119.4(2)	C(24)–C(25)–H(25)	119.9
C(a3)–C(m1)–C(10)	118.4(2)		
N(2)–C(a3)–C(m1)	126.2(3)		

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

Table S35. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 130 K, crystal 4[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0255(15)	0.0228(4)	0.0155(4)	0.0036(3)	−0.0069(11)	−0.0077(11)
N(1)	0.0218(12)	0.0232(12)	0.0147(10)	0.0021(8)	−0.0042(9)	−0.0037(9)
N(2)	0.0245(12)	0.0275(13)	0.0168(10)	0.0038(9)	−0.0082(10)	−0.0073(10)
N(3)	0.027(2)	0.025(2)	0.017(2)	0.0034(17)	−0.0082(19)	−0.0080(18)
O(1)	0.028(2)	0.051(3)	0.047(3)	0.001(2)	−0.019(2)	−0.006(2)
C(a1)	0.0241(14)	0.0262(14)	0.0181(13)	0.0046(10)	−0.0081(11)	−0.0077(11)
C(b1)	0.0301(15)	0.0254(14)	0.0222(13)	0.0064(11)	−0.0075(12)	−0.0071(12)
C(b2)	0.0311(15)	0.0243(14)	0.0225(13)	0.0046(11)	−0.0084(12)	−0.0063(12)
C(a2)	0.0238(14)	0.0255(14)	0.0208(13)	0.0076(10)	−0.0098(11)	−0.0077(11)
C(m1)	0.0215(13)	0.0261(14)	0.0221(13)	0.0047(10)	−0.0099(11)	−0.0078(11)
C(a3)	0.0254(14)	0.0274(15)	0.0203(12)	0.0031(11)	−0.0109(12)	−0.0073(12)
C(b3)	0.0302(15)	0.0266(14)	0.0218(13)	0.0004(11)	−0.0090(12)	−0.0048(12)
C(b4)	0.0307(16)	0.0322(16)	0.0172(12)	0.0008(11)	−0.0076(12)	−0.0051(13)
C(a4)	0.0257(14)	0.0263(14)	0.0162(12)	0.0038(10)	−0.0082(11)	−0.0071(11)
C(m2)	0.0224(13)	0.0282(14)	0.0154(11)	0.0070(10)	−0.0068(10)	−0.0089(11)
C(10)	0.0254(14)	0.0236(13)	0.0183(12)	0.0027(10)	−0.0071(11)	−0.0066(11)
C(11)	0.0299(16)	0.0300(16)	0.052(2)	−0.0038(14)	−0.0191(15)	−0.0085(13)
C(12)	0.0303(17)	0.0345(18)	0.051(2)	−0.0050(15)	−0.0177(15)	−0.0035(14)
C(13)	0.0448(19)	0.0243(14)	0.0189(12)	−0.0018(10)	−0.0064(13)	−0.0068(13)
C(14)	0.0444(19)	0.0336(18)	0.049(2)	−0.0068(15)	−0.0159(16)	−0.0168(15)
C(15)	0.0290(16)	0.0401(19)	0.055(2)	−0.0035(16)	−0.0169(15)	−0.0148(14)
C(20)	0.0289(14)	0.0239(13)	0.0151(11)	0.0028(9)	−0.0071(11)	−0.0064(11)
C(21)	0.0313(15)	0.0468(19)	0.0230(14)	0.0075(13)	−0.0106(12)	−0.0154(14)
C(22)	0.0358(16)	0.0429(19)	0.0246(14)	0.0067(13)	−0.0049(13)	−0.0161(14)
C(23)	0.0451(18)	0.0255(14)	0.0179(12)	0.0060(10)	−0.0072(13)	−0.0106(13)
C(24)	0.053(2)	0.047(2)	0.0253(15)	0.0075(14)	−0.0234(15)	−0.0158(16)
C(25)	0.0372(17)	0.050(2)	0.0280(16)	0.0108(14)	−0.0159(14)	−0.0226(15)

[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 S36. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 130 K, crystal 4[a]

atom	x	y	z	U(eq)
H(b1)	0.0030	0.1155	1.3801	0.034
H(b2)	0.1824	−0.0201	1.1570	0.034
H(b3)	0.3734	0.1133	0.6177	0.034
H(b4)	0.3316	0.3408	0.4840	0.035
H(11)	0.5261	0.0056	0.8563	0.043
H(12)	0.6766	−0.2340	0.7989	0.047
H(13)	0.5606	−0.3926	0.7757	0.039
H(14)	0.2909	−0.3090	0.8142	0.049
H(15)	0.1391	−0.0705	0.8747	0.048
H(21)	0.4004	0.6359	0.4847	0.040
H(22)	0.4964	0.6945	0.2455	0.044
H(23)	0.3436	0.7216	0.1148	0.039
H(24)	0.0939	0.6938	0.2231	0.047
H(25)	−0.0028	0.6352	0.4628	0.043

[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 S37. Complete Crystallographic Details for [Fe(TPP)(NO)] at 180 K, crystal 1

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	9.765(2)
b, Å	10.120(2)
c, Å	10.466(2)
α, deg	81.35(2)
β, deg	65.23(2)
γ, deg	68.12(2)
V, Å^3	871.4(4)
space group	$P\bar{1}$
Z	1
D_c, g/cm^3	1.331
F(000)	361
μ, mm^{-1}	0.476
crystal dimensions, mm	0.21 × 0.17 × 0.08
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	180(2)
diffractometer	Bruker SMART Apex II
θ range for collected data, deg	3.04–28.37
index range	$-11 \leq h \leq 13$
	$-13 \leq k \leq 13$
	$0 \leq l \leq 13$
total data collected	4628
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9629 and 0.9067
unique data	4628 ($R_{\rm int}$ = 0.0764)
unique observed data [I > 2σ(I)]	2579
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	4628/0/247
goodness-of-fit (pased on F^2)	0.893
final R indices [I > 2σ(I)]	R_1 = 0.0481, wR_2 = 0.0981
final R indices (all data)	R_1 = 0.1034, wR_2 = 0.1102

Table S38. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 180 K, crystal 1[a]

atom	x	y	z	U(eq)
Fe(1)	0.4794(5)	0.4972(7)	0.5008(8)	0.0274(6)
N(1)	0.4619(2)	0.68075(18)	0.39300(19)	0.0291(5)
N(2)	0.3566(2)	0.60801(19)	0.67935(18)	0.0286(5)
C(m1)	0.6301(3)	0.5889(2)	0.1504(2)	0.0296(5)
C(m2)	0.2801(3)	0.8529(2)	0.5884(2)	0.0282(5)
C(a1)	0.5255(3)	0.6974(2)	0.2482(2)	0.0300(6)
C(a2)	0.3673(3)	0.8151(2)	0.4472(2)	0.0287(5)
C(a3)	0.2773(3)	0.7531(2)	0.6972(2)	0.0310(6)
C(a4)	0.3170(3)	0.5539(2)	0.8147(2)	0.0315(6)
C(b1)	0.4694(3)	0.8445(2)	0.2135(2)	0.0370(6)
C(b2)	0.3717(3)	0.9179(2)	0.3350(2)	0.0346(6)
C(b3)	0.1897(3)	0.7896(2)	0.8428(2)	0.0381(6)
C(b4)	0.2138(3)	0.6672(2)	0.9150(2)	0.0369(6)
C(10)	0.6892(3)	0.6280(2)	−0.0032(2)	0.0311(6)
C(11)	0.8357(3)	0.6466(3)	−0.0691(3)	0.0430(7)
C(12)	0.8920(3)	0.6813(3)	−0.2102(3)	0.0457(7)
C(13)	0.8018(3)	0.6979(2)	−0.2867(3)	0.0427(7)
C(14)	0.6541(4)	0.6817(3)	−0.2212(3)	0.0521(8)
C(15)	0.5982(3)	0.6473(3)	−0.0792(3)	0.0460(7)
C(20)	0.1843(3)	1.0063(2)	0.6278(2)	0.0291(5)
C(21)	0.0231(3)	1.0604(3)	0.6514(3)	0.0436(7)
C(22)	−0.0651(3)	1.2025(3)	0.6861(3)	0.0514(8)
C(23)	0.0043(4)	1.2918(3)	0.6988(2)	0.0427(7)
C(24)	0.1638(4)	1.2381(3)	0.6768(3)	0.0510(8)
C(25)	0.2525(3)	1.0969(3)	0.6411(3)	0.0470(7)
N(3)	0.3085(4)	0.4909(4)	0.4914(4)	0.0293(9)
O(1)	0.1806(4)	0.5506(4)	0.5019(4)	0.0590(11)

[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 S39. Bond Lengths for [Fe(TPP)(NO)] at 180 K, crystal 1[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.421(6)	C(b3)–H(b3)	0.9500
Fe(1)–N(3)	1.736(5)	C(b4)–H(b4)	0.9500
Fe(1)–N(2)	1.984(7)	C(10)–C(15)	1.370(3)
Fe(1)–N(1)#1)	1.993(7)	C(10)–C(11)	1.376(3)
Fe(1)–N(1)	2.012(7)	C(11)–C(12)	1.384(3)
Fe(1)–N(2)#1)	2.014(7)	C(11)–H(11)	0.9500
Fe(1)–N(3)#1)	2.154(5)	C(12)–C(13)	1.372(4)
N(1)–C(a2)	1.371(3)	C(12)–H(12)	0.9500
N(1)–C(a1)	1.387(3)	C(13)–C(14)	1.376(4)
N(1)–Fe(1)#1)	1.993(7)	C(13)–H(13)	0.9500
N(2)–C(a3)	1.380(3)	C(14)–C(15)	1.390(3)
N(2)–C(a4)	1.386(3)	C(14)–H(14)	0.9500
N(2)–Fe(1)#1)	2.014(7)	C(15)–H(15)	0.9500
C(m1)–C(a1)	1.386(3)	C(20)–C(25)	1.369(4)
C(m1)–C(a4#1)	1.390(3)	C(20)–C(21)	1.383(4)
C(m1)–C(10)	1.508(3)	C(21)–C(22)	1.384(3)
C(m2)–C(a2)	1.389(3)	C(21)–H(21)	0.9500
C(m2)–C(a3)	1.402(3)	C(22)–C(23)	1.364(4)
C(m2)–C(20)	1.497(3)	C(22)–H(22)	0.9500
C(a1)–C(b1)	1.431(3)	C(23)–C(24)	1.371(4)
C(a2)–C(b2)	1.444(3)	C(23)–H(23)	0.9500
C(a3)–C(b3)	1.426(3)	C(24)–C(25)	1.378(3)
C(a4)–C(m1#1)	1.390(3)	C(24)–H(24)	0.9500
C(a4)–C(b4)	1.431(3)	C(25)–H(25)	0.9500
C(b1)–C(b2)	1.348(3)	N(3)–O(1)	1.131(4)
C(b1)–H(b1)	0.9500	N(3)–Fe(1)#1)	2.154(5)
C(b2)–H(b2)	0.9500		
C(b3)–C(b4)	1.345(3)		

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

Table S40. Bond Angles for [Fe(TPP)(NO)] at 180 K, crystal 1[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(3)	173(2)	C(b2)–C(b1)–H(b1)	126.2
Fe(1)#1–Fe(1)–N(2)	88(2)	C(a1)–C(b1)–H(b1)	126.2
N(3)–Fe(1)–N(2)	93.6(3)	C(b1)–C(b2)–C(a2)	106.71(19)
Fe(1)#1–Fe(1)–N(1)#1	87(2)	C(b1)–C(b2)–H(b2)	126.6
N(3)–Fe(1)–N(1)#1	100.5(3)	C(a2)–C(b2)–H(b2)	126.6
N(2)–Fe(1)–N(1)#1	90.2(3)	C(b4)–C(b3)–C(a3)	106.9(2)
Fe(1)#1–Fe(1)–N(1)	81.4(19)	C(b4)–C(b3)–H(b3)	126.5
N(3)–Fe(1)–N(1)	91.5(3)	C(a3)–C(b3)–H(b3)	126.5
N(2)–Fe(1)–N(1)	89.4(3)	C(b3)–C(b4)–C(a4)	107.5(2)
N(1)#1–Fe(1)–N(1)	167.95(17)	C(b3)–C(b4)–H(b4)	126.2
Fe(1)#1–Fe(1)–N(2)#1	79.9(19)	C(a4)–C(b4)–H(b4)	126.2
N(3)–Fe(1)–N(2)#1	98.4(3)	C(15)–C(10)–C(11)	118.8(2)
N(2)–Fe(1)–N(2)#1	167.96(18)	C(15)–C(10)–C(m1)	121.1(2)
N(1)#1–Fe(1)–N(2)#1	89.1(3)	C(11)–C(10)–C(m1)	120.2(2)
N(1)–Fe(1)–N(2)#1	88.8(3)	C(10)–C(11)–C(12)	120.8(3)
Fe(1)#1–Fe(1)–N(3)#1	5.8(18)	C(10)–C(11)–H(11)	119.6
N(3)–Fe(1)–N(3)#1	178.6(4)	C(12)–C(11)–H(11)	119.6
N(2)–Fe(1)–N(3)#1	86.7(2)	C(13)–C(12)–C(11)	120.3(3)
N(1)#1–Fe(1)–N(3)#1	80.9(2)	C(13)–C(12)–H(12)	119.9
N(1)–Fe(1)–N(3)#1	87.1(2)	C(11)–C(12)–H(12)	119.9
N(2)#1–Fe(1)–N(3)#1	81.3(2)	C(12)–C(13)–C(14)	119.4(2)
C(a2)–N(1)–C(a1)	105.52(18)	C(12)–C(13)–H(13)	120.3
C(a2)–N(1)–Fe(1)#1	127.4(3)	C(14)–C(13)–H(13)	120.3
C(a1)–N(1)–Fe(1)#1	126.6(2)	C(13)–C(14)–C(15)	119.9(3)
C(a2)–N(1)–Fe(1)	126.5(3)	C(13)–C(14)–H(14)	120.0
C(a1)–N(1)–Fe(1)	127.5(3)	C(15)–C(14)–H(14)	120.0
C(a3)–N(2)–C(a4)	104.73(18)	C(10)–C(15)–C(14)	120.9(3)
C(a3)–N(2)–Fe(1)	128.1(3)	C(10)–C(15)–H(15)	119.6
C(a4)–N(2)–Fe(1)	126.9(3)	C(14)–C(15)–H(15)	119.6
C(a3)–N(2)–Fe(1)#1	127.2(2)	C(25)–C(20)–C(21)	118.1(2)
C(a4)–N(2)–Fe(1)#1	127.4(3)	C(25)–C(20)–C(m2)	121.5(2)
C(a1)–C(m1)–C(a4#1	123.9(2)	C(21)–C(20)–C(m2)	120.3(2)
C(a1)–C(m1)–C(10)	118.13(19)	C(20)–C(21)–C(22)	120.4(3)
C(a4#1–C(m1)–C(10)	117.97(19)	C(20)–C(21)–H(21)	119.8

Table S40. Continued

angle	degree	angle	degree
C(a2)–C(m2)–C(a3)	122.8(2)	C(22)–C(21)–H(21)	119.8
C(a2)–C(m2)–C(20)	119.25(19)	C(23)–C(22)–C(21)	121.0(3)
C(a3)–C(m2)–C(20)	118.0(2)	C(23)–C(22)–H(22)	119.5
C(m1)–C(a1)–N(1)	125.7(2)	C(21)–C(22)–H(22)	119.5
C(m1)–C(a1)–C(b1)	124.4(2)	C(22)–C(23)–C(24)	118.8(2)
N(1)–C(a1)–C(b1)	109.93(18)	C(22)–C(23)–H(23)	120.6
N(1)–C(a2)–C(m2)	126.8(2)	C(24)–C(23)–H(23)	120.6
N(1)–C(a2)–C(b2)	110.3(2)	C(23)–C(24)–C(25)	120.5(3)
C(m2)–C(a2)–C(b2)	122.9(2)	C(23)–C(24)–H(24)	119.7
N(2)–C(a3)–C(m2)	125.4(2)	C(25)–C(24)–H(24)	119.7
N(2)–C(a3)–C(b3)	110.81(19)	C(20)–C(25)–C(24)	121.3(2)
C(m2)–C(a3)–C(b3)	123.8(2)	C(20)–C(25)–H(25)	119.4
N(2)–C(a4)–C(m1#1	125.6(2)	C(24)–C(25)–H(25)	119.4
N(2)–C(a4)–C(b4)	110.01(19)	O(1)–N(3)–Fe(1)	147.3(4)
C(m1#1–C(a4)–C(b4)	124.4(2)	O(1)–N(3)–Fe(1)#1	146.5(4)
C(b2)–C(b1)–C(a1)	107.6(2)		

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

Table S41. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 180 K, crystal 1[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0263(19)	0.0261(5)	0.0208(3)	0.0031(3)	−0.0021(15)	−0.0088(13)
N(1)	0.0277(11)	0.0279(10)	0.0237(11)	0.0030(8)	−0.0083(9)	−0.0045(9)
N(2)	0.0291(11)	0.0276(10)	0.0229(10)	0.0035(8)	−0.0089(9)	−0.0062(9)
C(m1)	0.0278(13)	0.0349(13)	0.0223(12)	0.0056(9)	−0.0090(10)	−0.0097(11)
C(m2)	0.0264(13)	0.0261(12)	0.0285(13)	0.0005(9)	−0.0102(11)	−0.0060(10)
C(a1)	0.0292(13)	0.0325(13)	0.0252(13)	0.0045(10)	−0.0099(11)	−0.0098(11)
C(a2)	0.0265(13)	0.0297(12)	0.0279(13)	0.0034(9)	−0.0107(11)	−0.0088(11)
C(a3)	0.0280(14)	0.0308(13)	0.0282(13)	−0.0008(10)	−0.0091(11)	−0.0058(11)
C(a4)	0.0292(14)	0.0342(13)	0.0251(13)	0.0032(10)	−0.0096(11)	−0.0071(11)
C(b1)	0.0395(15)	0.0307(13)	0.0327(14)	0.0078(10)	−0.0122(12)	−0.0088(11)
C(b2)	0.0388(15)	0.0263(12)	0.0309(14)	0.0035(10)	−0.0117(12)	−0.0065(11)
C(b3)	0.0376(15)	0.0333(13)	0.0334(14)	−0.0025(10)	−0.0097(12)	−0.0056(12)
C(b4)	0.0417(15)	0.0378(14)	0.0202(12)	−0.0011(10)	−0.0063(11)	−0.0083(12)
C(10)	0.0367(15)	0.0263(12)	0.0230(12)	0.0041(9)	−0.0092(11)	−0.0075(11)
C(11)	0.0386(15)	0.0575(17)	0.0333(15)	0.0095(12)	−0.0145(13)	−0.0203(14)
C(12)	0.0446(17)	0.0527(17)	0.0338(16)	0.0052(12)	−0.0063(13)	−0.0230(14)
C(13)	0.0597(19)	0.0292(13)	0.0234(13)	0.0046(10)	−0.0073(13)	−0.0108(13)
C(14)	0.067(2)	0.0599(19)	0.0353(17)	0.0122(13)	−0.0296(15)	−0.0214(16)
C(15)	0.0430(16)	0.0623(18)	0.0386(17)	0.0121(13)	−0.0192(13)	−0.0254(14)
C(20)	0.0320(14)	0.0284(12)	0.0218(12)	0.0007(9)	−0.0072(11)	−0.0091(11)
C(21)	0.0335(15)	0.0347(15)	0.0643(19)	−0.0080(12)	−0.0199(14)	−0.0098(12)
C(22)	0.0367(17)	0.0414(17)	0.068(2)	−0.0085(14)	−0.0202(15)	−0.0016(14)
C(23)	0.059(2)	0.0263(13)	0.0293(14)	−0.0017(10)	−0.0107(13)	−0.0077(14)
C(24)	0.064(2)	0.0374(16)	0.060(2)	−0.0034(13)	−0.0260(16)	−0.0229(15)
C(25)	0.0378(16)	0.0440(17)	0.063(2)	−0.0056(13)	−0.0210(14)	−0.0144(14)
N(3)	0.028(2)	0.032(2)	0.022(2)	0.0044(16)	−0.0101(18)	−0.0070(18)
O(1)	0.040(2)	0.069(3)	0.071(3)	0.004(2)	−0.028(2)	−0.017(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 S42. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 180 K, crystal 1[a]

atom	x	y	z	U(eq)
H(b1)	0.4962	0.8835	0.1215	0.044
H(b2)	0.3165	1.0178	0.3449	0.042
H(b3)	0.1264	0.8825	0.8816	0.046
H(b4)	0.1702	0.6578	1.0144	0.044
H(11)	0.8990	0.6354	−0.0171	0.052
H(12)	0.9934	0.6938	−0.2544	0.055
H(13)	0.8411	0.7203	−0.3839	0.051
H(14)	0.5902	0.6940	−0.2730	0.063
H(15)	0.4957	0.6372	−0.0343	0.055
H(21)	−0.0274	0.9996	0.6437	0.052
H(22)	−0.1756	1.2385	0.7013	0.062
H(23)	−0.0567	1.3894	0.7224	0.051
H(24)	0.2135	1.2988	0.6862	0.061
H(25)	0.3631	1.0618	0.6254	0.056

[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 S43. Complete Crystallographic Details for [Fe(TPP)(NO)] at 273 K, crystal 4

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	13.4152(2)
b, Å	13.4152(2)
c, Å	9.7151(3)
β, deg	90
V, Å^3	1748.40(7)
space group	$I4/m$
Z	2
D_c, g/cm^3	1.327
F(000)	722
μ, mm^{-1}	0.474
crystal dimensions, mm	0.28 × 0.28 × 0.28
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	272(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.15–27.87
index range	$-17 \leq h \leq 17$
	$-17 \leq k \leq 17$
	$-12 \leq l \leq 12$
total data collected	11545
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.8783 and 0.8783
unique data	1101 (R_{int} = 0.0238)
unique observed data [I > 2σ(I)]	918
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	1101/0/82
goodness-of-fit (pased on F^2)	1.087
final R indices [I > 2σ(I)]	R_1 = 0.0391, wR_2 = 0.1132
final R indices (all data)	R_1 = 0.0486, wR_2 = 0.1239

Table S44. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 273 K, crystal 4[a]

atom	x	y	z	U(eq)
Fe(1)	0.5000	0.5000	0.02458(14)	0.0458(5)
N(1)	0.35686(13)	0.53668(13)	0.0000	0.0489(4)
N(2)	0.5000	0.5000	0.1998(6)	0.0494(11)
O(1)	0.516(6)	0.4625(10)	0.2967(10)	0.095(15)
C(a1)	0.27652(16)	0.47339(17)	0.0000	0.0513(5)
C(b1)	0.18567(18)	0.52908(18)	0.0000	0.0617(6)
C(b2)	0.21027(17)	0.62567(19)	0.0000	0.0610(6)
C(a2)	0.31728(16)	0.63098(17)	0.0000	0.0520(5)
C(m1)	0.37002(17)	0.71920(16)	0.0000	0.0511(5)
C(10)	0.31341(16)	0.81527(16)	0.0000	0.0535(5)
C(11)	0.28725(18)	0.86012(15)	0.1208(2)	0.0770(6)
C(12)	0.2335(2)	0.94844(16)	0.1204(3)	0.0857(7)
C(13)	0.2066(2)	0.99164(18)	0.0000	0.0730(7)

[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 S45. Bond Lengths for [Fe(TPP)(NO)] at 273 K, crystal 4[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.478(3)	C(a1)–C(m1#3)	1.388(3)
Fe(1)–N(2)	1.702(5)	C(a1)–C(b1)	1.430(3)
Fe(1)–N(1)#2)	1.9966(18)	C(b1)–C(b2)	1.337(4)
Fe(1)–N(1)	1.9966(18)	C(b1)–H(b1)	0.9300
Fe(1)–N(1)#1)	1.9966(18)	C(b2)–C(a2)	1.437(3)
Fe(1)–N(1)#3)	1.9966(18)	C(b2)–H(b2)	0.9300
Fe(1)–N(2)#1)	2.180(6)	C(a2)–C(m1)	1.379(3)
N(1)–C(a2)	1.372(3)	C(m1)–C(a1#2)	1.388(3)
N(1)–C(a1)	1.372(3)	C(m1)–C(10)	1.496(3)
N(1)–Fe(1)#1)	1.9966(18)	C(10)–C(11)#6)	1.364(2)
N(2)–O(1)#3)	1.088(18)	C(10)–C(11)	1.364(2)
N(2)–O(1)#4)	1.088(18)	C(11)–C(12)	1.387(3)
N(2)–O(1)	1.088(18)	C(11)–H(11)	0.9300
N(2)–O(1)#5)	1.088(18)	C(12)–C(13)	1.354(3)
N(2)–Fe(1)#1)	2.180(6)	C(12)–H(12)	0.9300
O(1)–O(1)#3)	0.77(4)	C(13)–C(12)#6)	1.354(3)
O(1)–O(1)#5)	0.77(4)	C(13)–H(13)	0.9300
O(1)–O(1)#4)	1.09(6)		

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

Table S46. Bond Angles for [Fe(TPP)(NO)] at 273 K, crystal 4[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(2)	180.000(2)	O(1)#4–N(2)–Fe(1)#1	149.9(13)
Fe(1)#1–Fe(1)–N(1)#2	83.13(4)	O(1)–N(2)–Fe(1)#1	149.9(13)
N(2)–Fe(1)–N(1)#2	96.87(4)	O(1)#5–N(2)–Fe(1)#1	149.9(13)
Fe(1)#1–Fe(1)–N(1)	83.13(4)	Fe(1)–N(2)–Fe(1)#1	0.0
N(2)–Fe(1)–N(1)	96.87(4)	O(1)#3–O(1)–O(1)#5	90.00(3)
N(1)#2–Fe(1)–N(1)	89.180(10)	O(1)#3–O(1)–N(2)	69.3(9)
Fe(1)#1–Fe(1)–N(1)#1	83.13(4)	O(1)#5–O(1)–N(2)	69.3(8)
N(2)–Fe(1)–N(1)#1	96.87(4)	O(1)#3–O(1)–O(1)#4	45.00(3)
N(1)#2–Fe(1)–N(1)#1	89.180(10)	O(1)#5–O(1)–O(1)#4	45.000(12)
N(1)–Fe(1)–N(1)#1	166.26(8)	N(2)–O(1)–O(1)#4	59.9(13)
Fe(1)#1–Fe(1)–N(1)#3	83.13(4)	N(1)–C(a1)–C(m1#3	125.86(19)
N(2)–Fe(1)–N(1)#3	96.87(4)	N(1)–C(a1)–C(b1)	110.3(2)
N(1)#2–Fe(1)–N(1)#3	166.26(8)	C(m1#3–C(a1)–C(b1)	123.9(2)
N(1)–Fe(1)–N(1)#3	89.180(10)	C(b2)–C(b1)–C(a1)	107.2(2)
N(1)#1–Fe(1)–N(1)#3	89.180(10)	C(b2)–C(b1)–H(b1)	126.4
Fe(1)#1–Fe(1)–N(2)#1	0.000(1)	C(a1)–C(b1)–H(b1)	126.4
N(2)–Fe(1)–N(2)#1	180.000(1)	C(b1)–C(b2)–C(a2)	107.1(2)
N(1)#2–Fe(1)–N(2)#1	83.13(4)	C(b1)–C(b2)–H(b2)	126.4
N(1)–Fe(1)–N(2)#1	83.13(4)	C(a2)–C(b2)–H(b2)	126.4
N(1)#1–Fe(1)–N(2)#1	83.13(4)	N(1)–C(a2)–C(m1)	126.4(2)
N(1)#3–Fe(1)–N(2)#1	83.13(4)	N(1)–C(a2)–C(b2)	109.9(2)
C(a2)–N(1)–C(a1)	105.46(17)	C(m1)–C(a2)–C(b2)	123.7(2)
C(a2)–N(1)–Fe(1)	126.83(14)	C(a2)–C(m1)–C(a1#2	123.2(2)
C(a1)–N(1)–Fe(1)	127.08(14)	C(a2)–C(m1)–C(10)	118.6(2)
C(a2)–N(1)–Fe(1)#1	126.83(14)	C(a1#2–C(m1)–C(10)	118.13(19)
C(a1)–N(1)–Fe(1)#1	127.08(14)	C(11)#6–C(10)–C(11)	118.6(2)
Fe(1)–N(1)–Fe(1)#1	13.74(8)	C(11)#6–C(10)–C(m1)	120.70(11)
O(1)#3–N(2)–O(1)#4	41.5(17)	C(11)–C(10)–C(m1)	120.70(11)
O(1)#3–N(2)–O(1)	41.5(17)	C(10)–C(11)–C(12)	120.53(19)
O(1)#4–N(2)–O(1)	60(3)	C(10)–C(11)–H(11)	119.7
O(1)#3–N(2)–O(1)#5	60(3)	C(12)–C(11)–H(11)	119.7
O(1)#4–N(2)–O(1)#5	41.5(17)	C(13)–C(12)–C(11)	120.4(2)
O(1)–N(2)–O(1)#5	41.5(17)	C(13)–C(12)–H(12)	119.8
O(1)#3–N(2)–Fe(1)	149.9(13)	C(11)–C(12)–H(12)	119.8

Table S46. Continued

angle	degree	angle	degree
O(1)#4–N(2)–Fe(1)	149.9(13)	C(12)#6–C(13)–C(12)	119.4(2)
O(1)–N(2)–Fe(1)	149.9(13)	C(12)#6–C(13)–H(13)	120.3
O(1)#5–N(2)–Fe(1)	149.9(13)	C(12)–C(13)–H(13)	120.3
O(1)#3–N(2)–Fe(1)#1	149.9(13)		

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

Table S47. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 273 K, crystal 4[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0429(3)	0.0429(3)	0.0515(13)	0.000	0.000	0.000
N(1)	0.0471(9)	0.0464(9)	0.0532(9)	0.000	0.000	0.0005(6)
N(2)	0.0456(15)	0.0456(15)	0.057(3)	0.000	0.000	0.000
O(1)	0.15(4)	0.077(7)	0.061(4)	0.025(8)	−0.036(17)	−0.023(18)
C(a1)	0.0461(10)	0.0535(11)	0.0544(11)	0.000	0.000	−0.0002(8)
C(b1)	0.0462(11)	0.0591(13)	0.0799(15)	0.000	0.000	0.0009(9)
C(b2)	0.0476(11)	0.0556(12)	0.0798(15)	0.000	0.000	0.0054(9)
C(a2)	0.0479(11)	0.0524(11)	0.0557(11)	0.000	0.000	0.0040(9)
C(m1)	0.0532(11)	0.0486(11)	0.0515(10)	0.000	0.000	0.0058(9)
C(10)	0.0500(11)	0.0455(10)	0.0649(12)	0.000	0.000	0.0025(8)
C(11)	0.0974(15)	0.0696(11)	0.0640(10)	−0.0043(9)	−0.0019(10)	0.0239(10)
C(12)	0.0977(16)	0.0686(12)	0.0909(15)	−0.0196(10)	0.0041(12)	0.0212(11)
C(13)	0.0612(14)	0.0450(12)	0.113(2)	0.000	0.000	0.0051(10)

[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 S48. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(NO)] at 273 K, crystal 4[a]

atom	x	y	z	U(eq)
H(b1)	0.1214	0.5030	0.0000	0.074
H(b2)	0.1664	0.6793	0.0000	0.073
H(11)	0.3056	0.8312	0.2040	0.092
H(12)	0.2158	0.9782	0.2033	0.103
H(13)	0.1699	1.0505	0.0000	0.088

[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 S49. Complete Crystallographic Details for [Fe(TPP)(NO)] at 290 K, crystal 2

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	13.4466(3)
b, Å	13.4466(3)
c, Å	9.7498(5)
β, deg	90
V, Å^3	1762.87(11)
space group	$I4/m$
Z	2
D_c, g/cm^3	1.316
F(000)	722.
μ, mm^{-1}	0.470
crystal dimensions, mm	0.21 × 0.20 × 0.05
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.14–28.23
index range	$-17 \leq h \leq 17$
	$-17 \leq k \leq 17$
	$-12 \leq l \leq 12$
total data collected	33834
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9792 and 0.9090
unique data	1155 (R_{int} = 0.0310)
unique observed data [I > 2σ(I)]	973
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	1155/0/83
goodness-of-fit (pased on F^2)	1.077
final R indices [I > 2σ(I)]	R_1 = 0.0340, wR_2 = 0.0996
final R indices (all data)	R_1 = 0.0419, wR_2 = 0.1077

Table S50. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 290 K, crystal 2[a]

atom	x	y	z	U(eq)
Fe(1)	0.5000	0.5000	0.02351(16)	0.0457(5)
N(1)	0.46314(11)	0.35716(12)	0.0000	0.0499(4)
C(m1)	0.28062(14)	0.37030(15)	0.0000	0.0522(4)
C(a1)	0.52642(15)	0.27656(14)	0.0000	0.0524(4)
C(a2)	0.36874(14)	0.31738(14)	0.0000	0.0527(4)
C(b1)	0.47062(16)	0.18593(15)	0.0000	0.0632(5)
C(b2)	0.37407(16)	0.21065(15)	0.0000	0.0625(5)
C(10)	0.18473(14)	0.31364(14)	0.0000	0.0547(5)
C(11)	0.13974(14)	0.28742(16)	−0.12077(19)	0.0791(5)
C(12)	0.05158(14)	0.23357(17)	−0.1201(2)	0.0877(6)
C(13)	0.00852(16)	0.20639(18)	0.0000	0.0755(7)
N(2)	0.5000	0.5000	0.2004(5)	0.0470(9)
O(1)	0.512(9)	0.4626(13)	0.2978(9)	0.10(2)

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

Table S51. Bond Lengths for [Fe(TPP)(NO)] at 290 K, crystal 2[a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(2)	1.725(5)	C(b1)–H(b1)	0.9300
Fe(1)–N(1)	1.9968(16)	C(b2)–H(b2)	0.9300
Fe(1)–N(2)#1)	2.183(5)	C(10)–C(11)	1.370(2)
N(1)–C(a2)	1.378(2)	C(10)–C(11)#4)	1.370(2)
N(1)–C(a1)	1.378(2)	C(11)–C(12)	1.389(2)
N(1)–Fe(1)#1)	1.9969(16)	C(11)–H(11)	0.9300
C(m1)–C(a2)	1.382(3)	C(12)–C(13)	1.356(3)
C(m1)–C(a1#2)	1.390(3)	C(12)–H(12)	0.9300
C(m1)–C(10)	1.498(3)	C(13)–C(12)#4)	1.356(3)
C(a1)–C(m1#3)	1.390(3)	C(13)–H(13)	0.9300
C(a1)–C(b1)	1.431(3)	N(2)–O(1)	1.09(3)
C(a2)–C(b2)	1.437(3)	N(2)–Fe(1)#1)	2.183(5)
C(b1)–C(b2)	1.340(3)		

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

Table S52. Bond Angles for [Fe(TPP)(NO)] at 290 K, crystal 2[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(2)	179.997(1)	C(m1)–C(a2)–C(b2)	123.85(19)
Fe(1)#1–Fe(1)–N(1)#2	83.41(5)	C(b2)–C(b1)–C(a1)	107.26(18)
N(2)–Fe(1)–N(1)#2	96.59(4)	C(b2)–C(b1)–H(b1)	126.4
Fe(1)#1–Fe(1)–N(1)#3	83.41(4)	C(a1)–C(b1)–H(b1)	126.4
N(2)–Fe(1)–N(1)#3	96.59(4)	C(b1)–C(b2)–C(a2)	107.22(18)
N(1)#2–Fe(1)–N(1)#3	166.82(9)	C(b1)–C(b2)–H(b2)	126.4
Fe(1)#1–Fe(1)–N(1)#1	83.41(4)	C(a2)–C(b2)–H(b2)	126.4
N(2)–Fe(1)–N(1)#1	96.59(4)	C(11)–C(10)–C(11)#4	118.5(2)
N(1)#2–Fe(1)–N(1)#1	89.244(10)	C(11)–C(10)–C(m1)	120.74(10)
N(1)#3–Fe(1)–N(1)#1	89.244(10)	C(11)#4–C(10)–C(m1)	120.74(10)
Fe(1)#1–Fe(1)–N(1)	83.41(4)	C(10)–C(11)–C(12)	120.45(18)
N(2)–Fe(1)–N(1)	96.59(4)	C(10)–C(11)–H(11)	119.8
N(1)#2–Fe(1)–N(1)	89.246(10)	C(12)–C(11)–H(11)	119.8
N(1)#3–Fe(1)–N(1)	89.245(10)	C(13)–C(12)–C(11)	120.60(19)
N(1)#1–Fe(1)–N(1)	166.82(9)	C(13)–C(12)–H(12)	119.7
N(2)–Fe(1)–N(2)#1	180.0	C(11)–C(12)–H(12)	119.7
N(1)#2–Fe(1)–N(2)#1	83.41(4)	C(12)#4–C(13)–C(12)	119.4(2)
N(1)#3–Fe(1)–N(2)#1	83.41(4)	C(12)#4–C(13)–H(13)	120.3
N(1)#1–Fe(1)–N(2)#1	83.41(4)	C(12)–C(13)–H(13)	120.3
N(1)–Fe(1)–N(2)#1	83.41(4)	O(1)#5–N(2)–O(1)#3	58(4)
C(a2)–N(1)–C(a1)	105.29(15)	O(1)–N(2)–O(1)#6	58(4)
C(a2)–N(1)–Fe(1)	127.03(13)	O(1)–N(2)–Fe(1)	151(2)
C(a1)–N(1)–Fe(1)	127.11(13)	O(1)#5–N(2)–Fe(1)	151(2)
C(a2)–N(1)–Fe(1)#1	127.03(13)	O(1)#3–N(2)–Fe(1)	151(2)
C(a1)–N(1)–Fe(1)#1	127.11(13)	O(1)#6–N(2)–Fe(1)	151(2)
C(a2)–C(m1)–C(a1#2	123.24(18)	O(1)–N(2)–Fe(1)#1	151(2)
C(a2)–C(m1)–C(10)	118.43(17)	O(1)#5–N(2)–Fe(1)#1	151(2)
C(a1#2–C(m1)–C(10)	118.33(17)	O(1)#3–N(2)–Fe(1)#1	151(2)
N(1)–C(a1)–C(m1#3	125.88(17)	O(1)#6–N(2)–Fe(1)#1	151(2)
N(1)–C(a1)–C(b1)	110.24(18)	O(1)#5–O(1)–N(2)	69.9(15)
C(m1#3–C(a1)–C(b1)	123.87(18)	O(1)#3–O(1)–N(2)	69.9(14)
N(1)–C(a2)–C(m1)	126.17(17)	O(1)#6–O(1)–N(2)	61(2)
N(1)–C(a2)–C(b2)	109.98(18)		

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

Table S53. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 290 K, crystal 2[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0421(2)	0.0421(2)	0.0530(13)	0.000	0.000	0.000
N(1)	0.0457(8)	0.0464(8)	0.0575(9)	0.000	0.000	−0.0007(6)
C(m1)	0.0473(9)	0.0529(10)	0.0564(10)	0.000	0.000	−0.0048(7)
C(a1)	0.0531(10)	0.0449(9)	0.0592(10)	0.000	0.000	0.0009(7)
C(a2)	0.0503(10)	0.0478(9)	0.0599(11)	0.000	0.000	−0.0050(7)
C(b1)	0.0591(11)	0.0448(10)	0.0858(14)	0.000	0.000	−0.0006(8)
C(b2)	0.0555(11)	0.0473(10)	0.0847(14)	0.000	0.000	−0.0059(8)
C(10)	0.0448(9)	0.0505(10)	0.0688(12)	0.000	0.000	−0.0018(7)
C(11)	0.0688(10)	0.0979(13)	0.0706(10)	0.0022(9)	−0.0051(8)	−0.0238(9)
C(12)	0.0678(10)	0.0978(14)	0.0975(14)	−0.0039(11)	−0.0207(10)	−0.0216(9)
C(13)	0.0447(10)	0.0603(12)	0.121(2)	0.000	0.000	−0.0060(9)
N(2)	0.0422(12)	0.0422(12)	0.057(3)	0.000	0.000	0.000
O(1)	0.17(6)	0.071(6)	0.062(4)	0.022(9)	−0.031(17)	−0.03(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 S54. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(NO)] at 290 K, crystal 2[a]

atom	x	y	z	U(eq)
H(b1)	0.4965	0.1218	0.0000	0.076
H(b2)	0.3205	0.1669	0.0000	0.075
H(11)	0.1684	0.3058	−0.2038	0.095
H(12)	0.0218	0.2160	−0.2027	0.105
H(13)	−0.0500	0.1695	0.0000	0.091

[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 S55. Complete Crystallographic Details for [Fe(TPP)(NO)] at 293 K, crystal 1

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	13.4748(12)
b, Å	13.4748(12)
c, Å	9.7686(18)
β, deg	90
V, Å^3	1773.7(4)
space group	$I4/m$
Z	2
D_c, g/cm^3	1.308
F(000)	722.
μ, mm^{-1}	0.467
crystal dimensions, mm	0.21 × 0.17 × 0.08
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	293(2)
diffractometer	Bruker SMART Apex II
θ range for collected data, deg	3.02–27.48
index range	$-17 \leq h \leq 17$
	$-17 \leq k \leq 17$
	$-12 \leq l \leq 12$
total data collected	9839
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9636 and 0.9082
unique data	1081 (R_{int} = 0.0308)
unique observed data [I > 2σ(I)]	842
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	1081/0/82
goodness-of-fit (pased on F^2)	1.071
final R indices [I > 2σ(I)]	R_1 = 0.0351, wR_2 = 0.0989
final R indices (all data)	R_1 = 0.0477, wR_2 = 0.1069

Table S56. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 293 K, crystal 1[a]

atom	x	y	z	U(eq)
Fe(1)	0.5000	0.5000	0.0235(3)	0.0542(7)
N(1)	0.35716(13)	0.46326(12)	0.0000	0.0573(4)
C(m1)	0.37029(16)	0.28062(15)	0.0000	0.0596(5)
C(a1)	0.27646(15)	0.52653(16)	0.0000	0.0609(5)
C(a2)	0.31742(15)	0.36876(16)	0.0000	0.0603(5)
C(b1)	0.18617(17)	0.47046(18)	0.0000	0.0716(6)
C(b2)	0.21081(17)	0.37432(18)	0.0000	0.0711(6)
C(10)	0.31374(16)	0.18469(16)	0.0000	0.0627(5)
C(11)	0.28741(17)	0.13999(15)	0.1203(2)	0.0872(6)
C(12)	0.23382(18)	0.05178(15)	0.1197(3)	0.0956(7)
C(13)	0.2067(2)	0.00887(18)	0.0000	0.0845(8)
N(2)	0.5000	0.5000	0.1995(6)	0.0568(11)
O(1)	0.472(4)	0.469(4)	0.2972(10)	0.090(7)

[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 S57. Bond Lengths for [Fe(TPP)(NO)] at 293 K, crystal 1[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.459(5)	C(b1)–H(b1)	0.9300
Fe(1)–N(2)	1.720(6)	C(b2)–H(b2)	0.9300
Fe(1)–N(1)#1)	2.0005(17)	C(10)–C(11)#4)	1.367(2)
Fe(1)–N(2)#1)	2.179(7)	C(10)–C(11)	1.367(2)
N(1)–C(a2)	1.381(3)	C(11)–C(12)	1.391(3)
N(1)–C(a1)	1.382(3)	C(11)–H(11)	0.9300
N(1)–Fe(1)#1)	2.0005(17)	C(12)–C(13)	1.355(3)
C(m1)–C(a2)	1.385(3)	C(12)–H(12)	0.9300
C(m1)–C(a1#2)	1.391(3)	C(13)–C(12)#4)	1.355(3)
C(m1)–C(10)	1.500(3)	C(13)–H(13)	0.9300
C(a1)–C(m1#3)	1.391(3)	N(2)–O(1)	1.107(11)
C(a1)–C(b1)	1.432(3)	N(2)–Fe(1)#1)	2.179(7)
C(a2)–C(b2)	1.438(3)	O(1)–O(1)#5)	0.795(19)
C(b1)–C(b2)	1.337(3)		

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

Table S58. Bond Angles for [Fe(TPP)(NO)] at 293 K, crystal 1[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(2)	179.999(2)	C(b2)–C(b1)–C(a1)	107.46(19)
Fe(1)#1–Fe(1)–N(1)	83.42(8)	C(b2)–C(b1)–H(b1)	126.3
N(2)–Fe(1)–N(1)	96.58(8)	C(a1)–C(b1)–H(b1)	126.3
Fe(1)#1–Fe(1)–N(1)#2	83.42(8)	C(b1)–C(b2)–C(a2)	107.36(19)
N(2)–Fe(1)–N(1)#2	96.58(8)	C(b1)–C(b2)–H(b2)	126.3
N(1)–Fe(1)–N(1)#2	89.247(18)	C(a2)–C(b2)–H(b2)	126.3
Fe(1)#1–Fe(1)–N(1)#3	83.42(8)	C(11)#4–C(10)–C(11)	118.5(2)
N(2)–Fe(1)–N(1)#3	96.58(8)	C(11)#4–C(10)–C(m1)	120.76(11)
N(1)–Fe(1)–N(1)#3	89.248(18)	C(11)–C(10)–C(m1)	120.76(11)
N(1)#2–Fe(1)–N(1)#3	166.84(16)	C(10)–C(11)–C(12)	120.5(2)
Fe(1)#1–Fe(1)–N(1)#1	83.42(8)	C(10)–C(11)–H(11)	119.7
N(2)–Fe(1)–N(1)#1	96.58(8)	C(12)–C(11)–H(11)	119.7
N(1)–Fe(1)–N(1)#1	166.84(16)	C(13)–C(12)–C(11)	120.6(2)
N(1)#2–Fe(1)–N(1)#1	89.247(18)	C(13)–C(12)–H(12)	119.7
N(1)#3–Fe(1)–N(1)#1	89.247(18)	C(11)–C(12)–H(12)	119.7
Fe(1)#1–Fe(1)–N(2)#1	0.001(1)	C(12)–C(13)–C(12)#4	119.3(2)
N(2)–Fe(1)–N(2)#1	180.0	C(12)–C(13)–H(13)	120.3
N(1)–Fe(1)–N(2)#1	83.42(8)	C(12)#4–C(13)–H(13)	120.3
N(1)#2–Fe(1)–N(2)#1	83.42(8)	O(1)#5–N(2)–O(1)#2	61.0(14)
N(1)#3–Fe(1)–N(2)#1	83.42(8)	O(1)–N(2)–O(1)#6	61.0(14)
N(1)#1–Fe(1)–N(2)#1	83.42(8)	O(1)–N(2)–Fe(1)	149.5(7)
C(a2)–N(1)–C(a1)	105.29(17)	O(1)#5–N(2)–Fe(1)	149.5(7)
C(a2)–N(1)–Fe(1)	126.95(14)	O(1)#2–N(2)–Fe(1)	149.5(7)
C(a1)–N(1)–Fe(1)	127.19(14)	O(1)#6–N(2)–Fe(1)	149.5(7)
C(a2)–N(1)–Fe(1)#1	126.95(14)	O(1)–N(2)–Fe(1)#1	149.5(7)
C(a1)–N(1)–Fe(1)#1	127.19(14)	O(1)#5–N(2)–Fe(1)#1	149.5(7)
C(a2)–C(m1)–C(a1#2	123.3(2)	O(1)#2–N(2)–Fe(1)#1	149.5(7)
C(a2)–C(m1)–C(10)	118.53(19)	O(1)#6–N(2)–Fe(1)#1	149.5(7)
C(a1#2–C(m1)–C(10)	118.21(19)	O(1)#5–O(1)–O(1)#2	90.01(2)
N(1)–C(a1)–C(m1#3	125.79(19)	O(1)#5–O(1)–N(2)	69.0(4)
N(1)–C(a1)–C(b1)	110.07(19)	O(1)#2–O(1)–N(2)	69.0(5)
C(m1#3–C(a1)–C(b1)	124.1(2)	O(1)#5–O(1)–O(1)#6	45.003(8)
N(1)–C(a2)–C(m1)	126.24(19)	O(1)#2–O(1)–O(1)#6	45.003(14)
N(1)–C(a2)–C(b2)	109.83(19)	N(2)–O(1)–O(1)#6	59.5(7)

Table S58. Continued

angle	degree	angle	degree
C(m1)–C(a2)–C(b2)	123.9(2)		

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

Table S59. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 293 K, crystal 1[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0475(3)	0.0475(3)	0.068(2)	0.000	0.000	0.000
N(1)	0.0521(9)	0.0511(9)	0.0688(11)	0.000	0.000	−0.0002(7)
C(m1)	0.0586(11)	0.0541(11)	0.0661(12)	0.000	0.000	−0.0053(9)
C(a1)	0.0497(11)	0.0601(12)	0.0728(14)	0.000	0.000	0.0017(8)
C(a2)	0.0538(11)	0.0555(11)	0.0717(13)	0.000	0.000	−0.0049(9)
C(b1)	0.0508(11)	0.0660(13)	0.0978(17)	0.000	0.000	−0.0006(9)
C(b2)	0.0529(11)	0.0614(13)	0.0991(17)	0.000	0.000	−0.0067(9)
C(10)	0.0569(11)	0.0509(11)	0.0803(15)	0.000	0.000	−0.0015(8)
C(11)	0.1044(14)	0.0754(11)	0.0818(12)	0.0060(10)	−0.0015(11)	−0.0238(10)
C(12)	0.1048(15)	0.0740(12)	0.1081(17)	0.0216(11)	0.0035(12)	−0.0227(10)
C(13)	0.0670(14)	0.0514(12)	0.135(3)	0.000	0.000	−0.0063(10)
N(2)	0.0496(15)	0.0496(15)	0.071(3)	0.000	0.000	0.000
O(1)	0.080(17)	0.11(3)	0.080(5)	0.025(12)	0.003(9)	0.000(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 S60. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(NO)] at 293 K, crystal 1[a]

atom	x	y	z	U(eq)
H(b1)	0.1221	0.4962	0.0000	0.086
H(b2)	0.1671	0.3209	0.0000	0.085
H(11)	0.3055	0.1688	0.2031	0.105
H(12)	0.2165	0.0220	0.2022	0.115
H(13)	0.1697	−0.0495	0.0000	0.101

[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 S61. Complete Crystallographic Details for [Fe(TPP)(NO)] at 293 K, crystal 2

formula	$C_{44}H_{28}FeN_5O$
FW, amu	698.56
a, Å	13.4502(3)
b, Å	13.4502(3)
c, Å	9.7533(4)
β, deg	90
V, Å^3	1764.45(9)
space group	$I4/m$
Z	2
D_c, g/cm^3	1.315
F(000)	722.
μ, mm^{-1}	0.470
crystal dimensions, mm	0.36 × 0.25 × 0.15
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	293(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	2.14–27.85
index range	$-17 \leq h \leq 17$
	$-17 \leq k \leq 17$
	$-12 \leq l \leq 12$
total data collected	9687
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9320 and 0.8491
unique data	1108 (R_{int} = 0.0318)
unique observed data [I > 2σ(I)]	881
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	1108/0/83
goodness-of-fit (pased on F^2)	1.064
final R indices [I > 2σ(I)]	R_1 = 0.0372, wR_2 = 0.1024
final R indices (all data)	R_1 = 0.0497, wR_2 = 0.1115

Table S62. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 293 K, crystal 2[a]

atom	x	y	z	U(eq)
Fe(1)	0.5000	0.5000	0.0231(3)	0.0481(7)
N(1)	0.35723(13)	0.46306(13)	0.0000	0.0510(4)
C(m1)	0.37032(16)	0.28065(15)	0.0000	0.0532(5)
C(a1)	0.27654(15)	0.52632(17)	0.0000	0.0540(5)
C(a2)	0.31748(15)	0.36872(16)	0.0000	0.0538(5)
C(b1)	0.18608(17)	0.47042(18)	0.0000	0.0648(6)
C(b2)	0.21075(17)	0.37414(18)	0.0000	0.0640(6)
C(10)	0.31372(16)	0.18460(16)	0.0000	0.0559(5)
C(11)	0.28751(17)	0.13973(15)	0.1203(2)	0.0802(6)
C(12)	0.23390(19)	0.05176(16)	0.1200(3)	0.0894(7)
C(13)	0.2065(2)	0.00859(18)	0.0000	0.0778(8)
N(2)	0.5000	0.5000	0.1998(6)	0.0481(11)
O(1)	0.478(5)	0.464(3)	0.2972(10)	0.084(6)

[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 S63. Bond Lengths for [Fe(TPP)(NO)] at 293 K, crystal 2[a]

bond	length (Å)	bond	length (Å)
Fe(1)–Fe(1)#1)	0.450(5)	C(b1)–H(b1)	0.9300
Fe(1)–N(2)	1.724(6)	C(b2)–H(b2)	0.9300
Fe(1)–N(1)#2)	1.9962(17)	C(10)–C(11)#4)	1.366(2)
Fe(1)–N(1)#3)	1.9962(17)	C(10)–C(11)	1.366(2)
Fe(1)–N(1)	1.9963(17)	C(11)–C(12)	1.386(3)
Fe(1)–N(1)#1)	1.9963(17)	C(11)–H(11)	0.9300
Fe(1)–N(2)#1)	2.174(6)	C(12)–C(13)	1.357(3)
N(1)–C(a2)	1.377(3)	C(12)–H(12)	0.9300
N(1)–C(a1)	1.379(3)	C(13)–C(12)#4)	1.357(3)
N(1)–Fe(1)#1)	1.9963(17)	C(13)–H(13)	0.9300
C(m1)–C(a2)	1.381(3)	N(2)–O(1)#3)	1.108(11)
C(m1)–C(a1#3)	1.391(3)	N(2)–O(1)#5)	1.108(11)
C(m1)–C(10)	1.499(3)	N(2)–O(1)#6)	1.108(11)
C(a1)–C(m1#2)	1.391(3)	N(2)–O(1)	1.108(11)
C(a1)–C(b1)	1.430(3)	N(2)–Fe(1)#1)	2.174(6)
C(a2)–C(b2)	1.437(3)		
C(b1)–C(b2)	1.337(3)		

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

Table S64. Bond Angles for [Fe(TPP)(NO)] at 293 K, crystal 2[a]

angle	degree	angle	degree
Fe(1)#1–Fe(1)–N(2)	179.995(2)	C(m1)–C(a2)–C(b2)	123.9(2)
Fe(1)#1–Fe(1)–N(1)#2	83.53(7)	C(b2)–C(b1)–C(a1)	107.34(19)
N(2)–Fe(1)–N(1)#2	96.47(7)	C(b2)–C(b1)–H(b1)	126.3
Fe(1)#1–Fe(1)–N(1)#3	83.52(7)	C(a1)–C(b1)–H(b1)	126.3
N(2)–Fe(1)–N(1)#3	96.47(7)	C(b1)–C(b2)–C(a2)	107.3(2)
N(1)#2–Fe(1)–N(1)#3	167.05(15)	C(b1)–C(b2)–H(b2)	126.4
Fe(1)#1–Fe(1)–N(1)	83.53(8)	C(a2)–C(b2)–H(b2)	126.4
N(2)–Fe(1)–N(1)	96.47(7)	C(11)#4–C(10)–C(11)	118.5(2)
N(1)#2–Fe(1)–N(1)	89.272(17)	C(11)#4–C(10)–C(m1)	120.77(11)
N(1)#3–Fe(1)–N(1)	89.271(17)	C(11)–C(10)–C(m1)	120.77(11)
Fe(1)#1–Fe(1)–N(1)#1	83.52(7)	C(10)–C(11)–C(12)	120.6(2)
N(2)–Fe(1)–N(1)#1	96.47(7)	C(10)–C(11)–H(11)	119.7
N(1)#2–Fe(1)–N(1)#1	89.271(17)	C(12)–C(11)–H(11)	119.7
N(1)#3–Fe(1)–N(1)#1	89.273(17)	C(13)–C(12)–C(11)	120.6(2)
N(1)–Fe(1)–N(1)#1	167.05(15)	C(13)–C(12)–H(12)	119.7
Fe(1)#1–Fe(1)–N(2)#1	0.004(2)	C(11)–C(12)–H(12)	119.7
N(2)–Fe(1)–N(2)#1	180.0	C(12)–C(13)–C(12)#4	119.1(2)
N(1)#2–Fe(1)–N(2)#1	83.53(7)	C(12)–C(13)–H(13)	120.4
N(1)#3–Fe(1)–N(2)#1	83.53(7)	C(12)#4–C(13)–H(13)	120.4
N(1)–Fe(1)–N(2)#1	83.53(7)	O(1)#3–N(2)–O(1)#5	62.1(13)
N(1)#1–Fe(1)–N(2)#1	83.53(7)	O(1)#6–N(2)–O(1)	62.1(13)
C(a2)–N(1)–C(a1)	105.25(17)	O(1)#3–N(2)–Fe(1)	149.0(6)
C(a2)–N(1)–Fe(1)	127.08(14)	O(1)#5–N(2)–Fe(1)	149.0(6)
C(a1)–N(1)–Fe(1)	127.12(14)	O(1)#6–N(2)–Fe(1)	149.0(7)
C(a2)–N(1)–Fe(1)#1	127.08(14)	O(1)–N(2)–Fe(1)	149.0(6)
C(a1)–N(1)–Fe(1)#1	127.12(14)	O(1)#3–N(2)–Fe(1)#1	149.0(6)
C(a2)–C(m1)–C(a1#3	123.2(2)	O(1)#5–N(2)–Fe(1)#1	149.0(6)
C(a2)–C(m1)–C(10)	118.53(19)	O(1)#6–N(2)–Fe(1)#1	149.0(7)
C(a1#3–C(m1)–C(10)	118.23(19)	O(1)–N(2)–Fe(1)#1	149.0(6)
N(1)–C(a1)–C(m1#2	125.82(19)	O(1)#5–O(1)–O(1)#3	90.00(2)
N(1)–C(a1)–C(b1)	110.2(2)	O(1)#5–O(1)–N(2)	68.6(4)
C(m1#2–C(a1)–C(b1)	124.0(2)	O(1)#3–O(1)–N(2)	68.6(4)
N(1)–C(a2)–C(m1)	126.19(19)	N(2)–O(1)–O(1)#6	59.0(6)
N(1)–C(a2)–C(b2)	109.94(19)		

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

Table S65. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(NO)] at 293 K, crystal 2[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0433(3)	0.0433(3)	0.058(2)	0.000	0.000	0.000
N(1)	0.0473(9)	0.0467(9)	0.0591(11)	0.000	0.000	−0.0006(7)
C(m1)	0.0542(11)	0.0485(11)	0.0568(12)	0.000	0.000	−0.0053(9)
C(a1)	0.0465(10)	0.0550(11)	0.0604(13)	0.000	0.000	0.0007(9)
C(a2)	0.0475(10)	0.0515(11)	0.0624(13)	0.000	0.000	−0.0052(9)
C(b1)	0.0457(11)	0.0615(13)	0.0871(17)	0.000	0.000	−0.0006(9)
C(b2)	0.0486(11)	0.0563(12)	0.0872(17)	0.000	0.000	−0.0056(9)
C(10)	0.0512(11)	0.0464(10)	0.0700(14)	0.000	0.000	−0.0014(8)
C(11)	0.0982(14)	0.0701(11)	0.0722(12)	0.0051(9)	−0.0032(10)	−0.0238(10)
C(12)	0.1003(16)	0.0699(12)	0.0982(16)	0.0208(11)	0.0038(12)	−0.0216(11)
C(13)	0.0610(14)	0.0453(12)	0.127(3)	0.000	0.000	−0.0055(10)
N(2)	0.0427(14)	0.0427(14)	0.059(3)	0.000	0.000	0.000
O(1)	0.10(3)	0.079(16)	0.070(5)	0.015(7)	0.021(13)	0.005(11)

[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 S66. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(NO)] at 293 K, crystal 2[a]

atom	x	y	z	U(eq)
H(b1)	0.1219	0.4963	0.0000	0.078
H(b2)	0.1670	0.3206	0.0000	0.077
H(11)	0.3058	0.1685	0.2033	0.096
H(12)	0.2165	0.0220	0.2027	0.107
H(13)	0.1694	−0.0498	0.0000	0.093

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

Supporting Information

Figure 1. Simulated X-ray powder diffraction spectra of [Fe(TPP)(NO)] in the $I-1$ and $I4/m$ crystalline phases.

Figure 2. Plot of X-ray powder diffraction intensity vs. temperature for the 101, 121, and 231 reflections of [Fe(TPP)(NO)] ($I4/m$). A plot of the first-derivative is also given.

Figure 3.

Figure 4. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 33 K. Hydrogen atoms are omitted for clarity.

Figure 5. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 90 K. Hydrogen atoms are omitted for clarity.

Figure 6. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 100 K. Hydrogen atoms are omitted for clarity.

Figure 7. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 100 K. Hydrogen atoms are omitted for clarity.

Figure 8. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 100 K. Hydrogen atoms are omitted for clarity.

Figure 9. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 130 K. Hydrogen atoms are omitted for clarity.

Figure 10. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 180 K. Hydrogen atoms are omitted for clarity.

Figure 11. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 290 K. Hydrogen atoms are omitted for clarity.

Figure 12. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 293 K. Hydrogen atoms are omitted for clarity.

Figure 13. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 273 K. Hydrogen atoms are omitted for clarity.

Figure 14. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(NO)(1-MeIm)] at 293 K. Hydrogen atoms are omitted for clarity.

Figure 15. Formal diagram of the porphyrinato cores of [Fe(TPP)(NO)] at 33, 90, 100, 130, and 180 K displaying the perpendicular displacements (in units of 0.01 Å) of the core atoms from the 24-atom mean plane. Positive displacements are toward the nitrosyl-coordinated face. The location of the nitrosyl oxygen atom projection onto the porphyrin core is indicated by the small circle.

Figure 16. stero view

Table S1. Complete Crystallographic Details for [Fe(TPP)(NO)] at 33 K, crystal 1.

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for [Fe(TPP)(NO)] at 33 K, crystal 1.

Table S3. Bond Lengths for [Fe(TPP)(NO)] at 33 K, crystal 1.

Table S4. Bond Angles for [Fe(TPP)(NO)] at 33 K, crystal 1.

Table S5. Anisotropic Isotropic Displacement Parameters for [Fe(TPP)(NO)] at 33 K, crystal 1.