Supporting Information for

Heme Carbonyls: Bond Length Correlations and Environmental Effects on ν(CO) and Fe–C/C–O Bond Length Correlations

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Captions for Supporting Information Figures

Figure S1. Formal diagram of the porphyrinato core of [Fe(TPP)(CO)(1,2-Me_2Im)]·C_7H_8 and [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8 both 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 carbonyl-coordinated face, while the imidazole ligand is displaced on the negative side of the porphyrin core. The orientation of the imidazole ligand with respect to the porphyrin core is also illustrated. The location of the 2-methyl group is represented by the circle. Average bond distances (Å) and angles (degrees) are also displayed.

Figure S2. Formal diagram of the porphyrinato core of Fe(TPP)(CO)(1,2-Me_2Im)] 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 carbonyl-coordinated face, while the imidazole ligand is displaced on the negative side of the porphyrin core. The orientation of the imidazole ligand with respect to the porphyrin core is also illustrated. The location of the 2-methyl group is represented by the circle. Average bond distances (Å) and angles (degrees) are also displayed.

Figure S3. Formal diagram of the porphyrinato core of [Fe(TPP)(CO)(1-MeIm)]·C_6H_6 displays the perpendicular displacements (in units of 0.01 Å) of the core atoms from the 24-atom mean plane. Positive displacements are toward the carbonyl-coordinated face, while the imidazole ligand is displaced on the negative side of the porphyrin core. The orientation of the imidazole ligand with respect to the porphyrin core is also illustrated. The location of the 1-methyl group is represented by the circle. Average bond distances (Å) and angles (degrees) are also displayed.

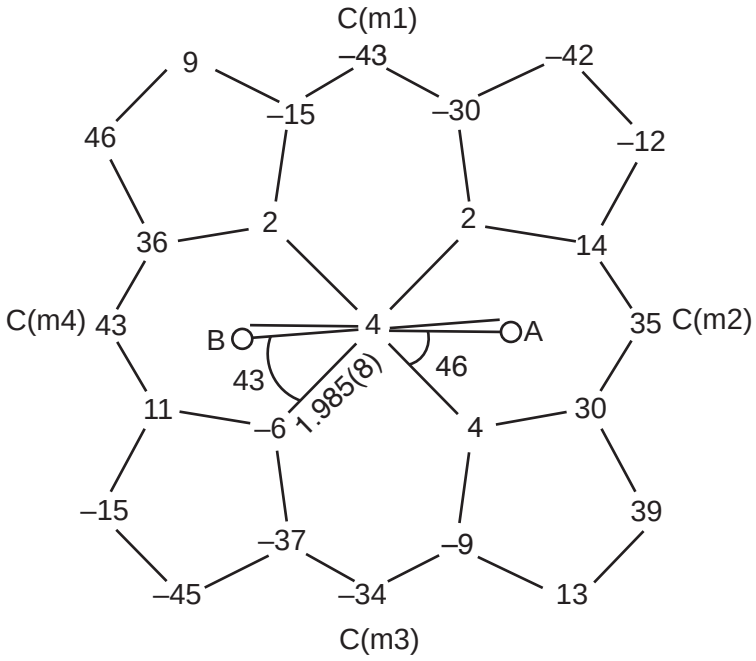
Figure S4. Diagrams illustrating the herringbone-like crystal packing pattern of a) [Fe(TPP)(CO)(1,2-Me_2Im)]·C_7H_8 (left) and b) [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8 (right) with solvent and phenyl groups omitted for clarity.

Figure S5. Plots showing the correlation and inverse correlation between C–O and Fe–C distances (Å) and ν(CO) (cm^{-1}). The figures include all carbonyl iron(II) imidazole structures. The points of the left panel are fit linearly with an R = 0.15.[1] The right panel is also fit linearly with an R = 0.14.

Figure S6. ORTEP diagram (50% probability ellipsoids) of [Fe(TPP)(CO)(1,2-Me_2Im)]·C_7H_8. Significant hydrogen atoms are displayed, all other hydrogen atoms are omitted for clarity. The tilt of the Fe-N_{Im} off of the heme normal may be observed.

Figure S7. Illustration showing the environment of the oxygen in the unsolvated form of [Fe(TPP)(CO)(1,2-Me_2Im)]. Imidazoles and peripheral substituents, with the exception of the hydrogens within 3.5 Å, are omitted for clarity.

24-Atom Diagram of [Fe(TPP)(1,2-DiMeIm)(CO)].C_7H_8



24-Atom Diagram of [Fe(TPP)(2-MeHIm)(CO)].C_7H_8

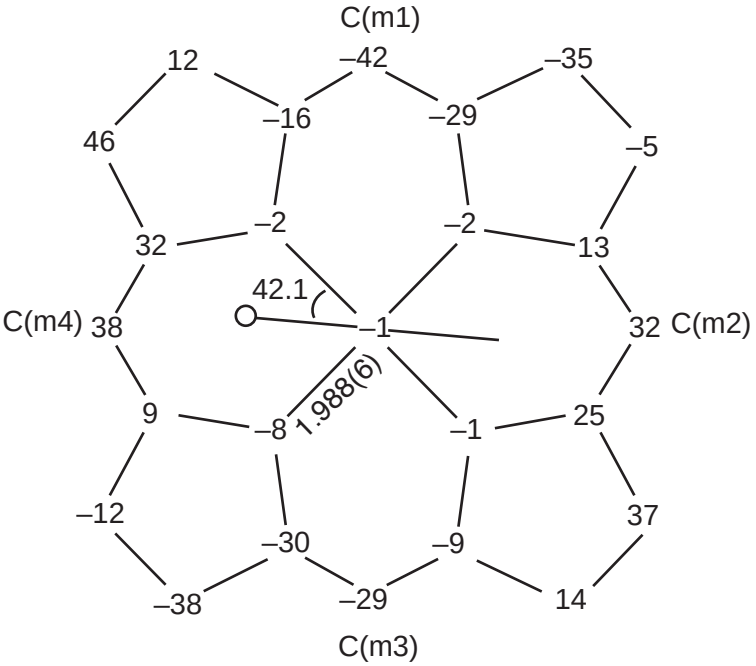


Figure S-1

24-Atom Diagram of [Fe(TPP)(1,2-DiMeIm)(CO)] (2-fold)

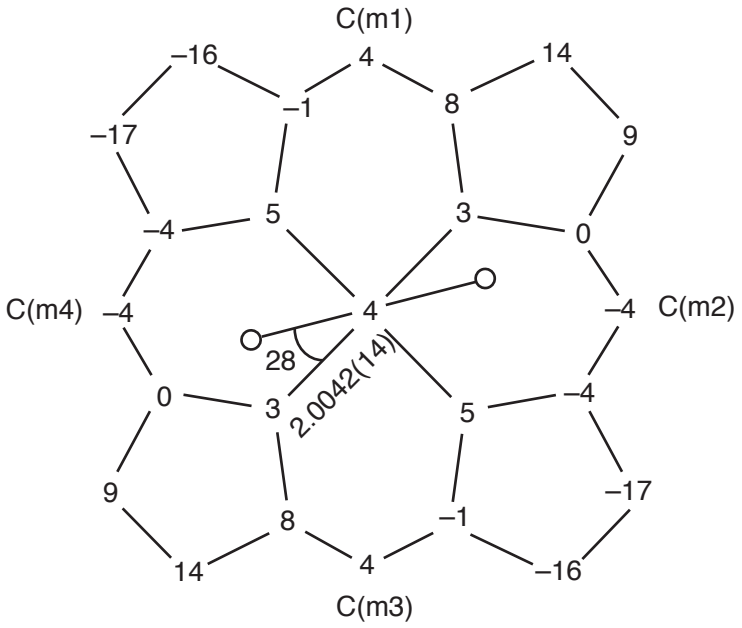


Figure S-2

24-Atom Diagram of [Fe(TPP)(1-MeIm)(CO)].C_6H_6

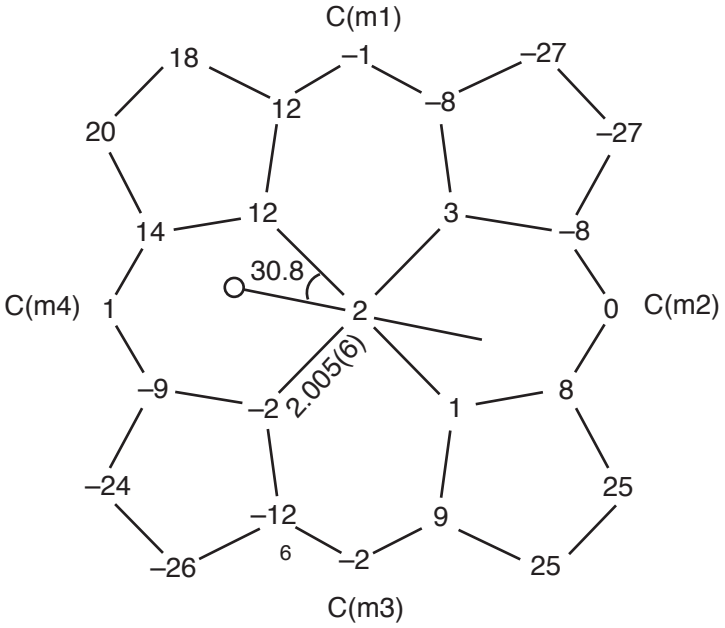


Figure S-3

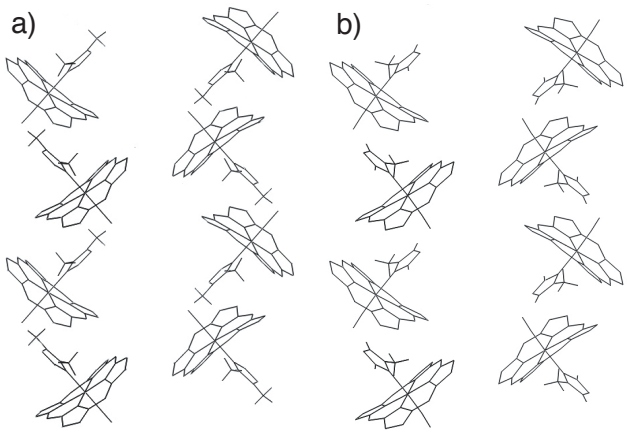


Figure S-4

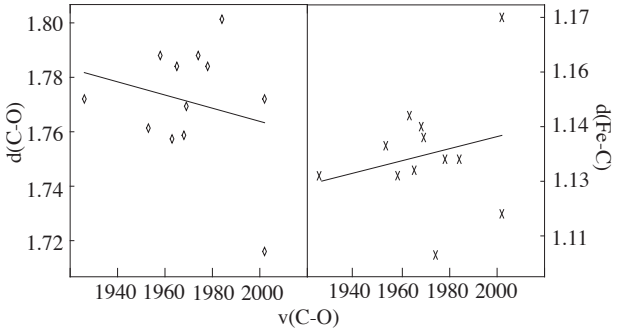


Figure S-5

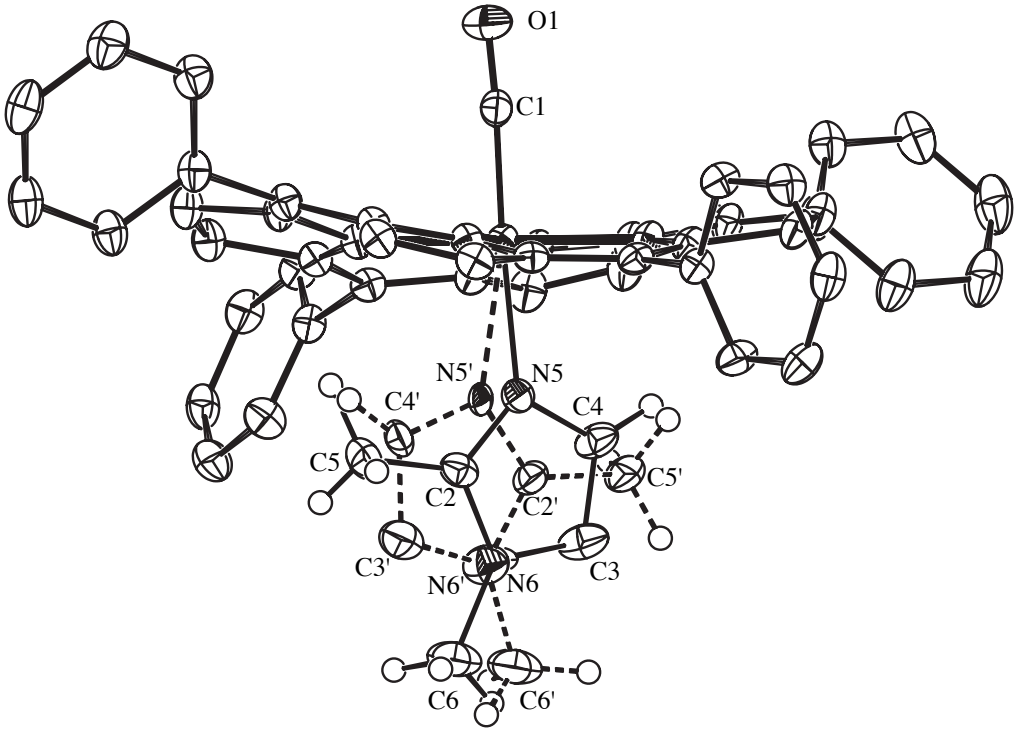


Figure S-6

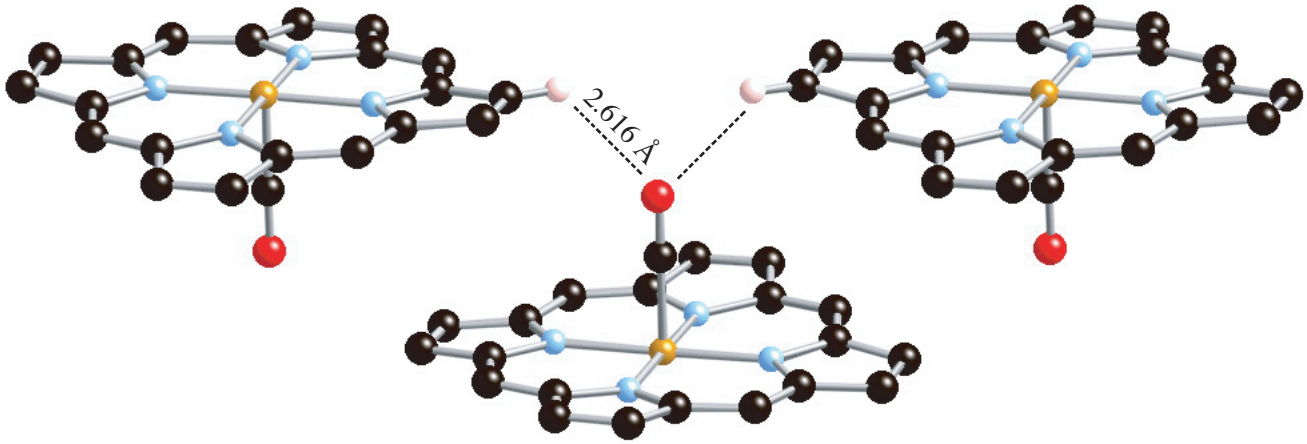


Figure S-7

Table S1. Crystallographic details for [Fe(TPP)(CO)(1,2-Me_2Im)]·C_7H_8, [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8, [Fe(TPP)(CO)(1,2-Me_2Im)] and [Fe(TPP)(CO)(1-MeIm)]·C_6H_6

	[Fe(TPP)(CO)-(1,2-Me_2Im)]·C_7H_8	[Fe(TPP)(CO)-(2-MeHIm)]·C_7H_8	[Fe(TPP)(CO)-(1,2-Me_2Im)]	[Fe(TPP)(CO)-(1-MeIm)]·C_6H_6
empirical formula	$C_{57.05}H_{36}FeN_6O$	$C_{56}H_{34}FeN_6O$	$C_{50}H_{36}FeN_6O$	$C_{55}H_{40}FeN_6O$
FW, amu	877.34	862.74	792.70	856.78
a, Å	13.1599(5)	13.1961(2)	15.0577(8)	9.6313(19)
b, Å	23.6195(9)	23.4514(3)	18.8294(10)	13.189(3)
c, Å	14.4695(6)	14.2630(2)	13.7197(7)	17.622(4)
α, deg				75.25(3)
β, deg	101.561(2)	105.198(1)	102.894(1)	88.95(3)
γ, deg				81.52(3)
V, Å^3	4406.3(3)	4259.6(1)	3791.8(3)	2140.6(7)
space group	$P2_1/n$	$P2_1/n$	$C2/c$	$P\bar{1}$
Z	4	4	4	2
crystal color	dark red	dark red	dark red	dark red
crystal dimensions, mm	0.58 × 0.20 × 0.13	0.66 × 0.39 × 0.27	0.40 × 0.30 × 0.20	0.29 × 0.26 × 0.10
temp, K	100	100	100	100
total data collected	72726	66278	20612	45838
unique data	15956 (R_{int} = 0.034)	15413 (R_{int} = 0.037)	4695 (R_{int} = 0.0376)	15633 (R_{int} = 0.035)
unique obsd data [I > 2σ(I)]	11874	12118	4169	11562
goodness-of-fit (based on F^2)	1.098	1.062	1.052	1.024
final R indices	R_1 = 0.0426	R_1 = 0.0446	R_1 = 0.0406	R_1 = 0.0459
[I > 2σ(I)]	wR_2 = 0.1203	wR_2 = 0.1173	wR_2 = 0.1073	wR_2 = 0.1155
final R indices	R_1 = 0.0614	R_1 = 0.0619	R_1 = 0.0453	R_1 = 0.0615
(all data)	wR_2 = 0.1271	wR_2 = 0.1286	wR_2 = 0.1115	wR_2 = 0.1259

Table S2. Complete Crystallographic Details for [Fe(TPP)(CO)(1,2-DiMeIm)]·C_7H_8

formula	$C_{56.77}H_{39.46}FeN_6O$
FW, amu	877.58
a, Å	13.1599(5)
b, Å	23.6195(9)
c, Å	14.4695(6)
β, deg	101.561(2)
V, Å^3	4406.3(3)
space group	P2(1)/n
Z	4
D_c, g/cm^3	1.323
F(000)	1824
μ, mm^{-1}	0.392
crystal dimensions, mm	0.58 × 0.20 × 0.13
radiation	MoKα, $\bar{\lambda} = 0.71073$ Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.68–32.50
index range	$-14 \leq h \leq 19$
	$-35 \leq k \leq 25$
	$-21 \leq l \leq 21$
total data collected	72726
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9493 and 0.8051
unique data	15956 ($R_{int} = 0.034$)
unique observed data [I > 2σ(I)]	11874
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	15956/0/611
goodness-of-fit (pased on F^2)	1.120
final R indices [I > 2σ(I)]	$R_1 = 0.0487$, $wR_2 = 0.1473$
final R indices (all data)	$R_1 = 0.0675$, $wR_2 = 0.1559$

Table S3. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1,2-DiMeIm)]·C_7H_8[a]

atom	x	y	z	U(eq)
Fe(1)	0.34684(2)	0.19502(1)	0.62892(1)	0.0163(1)
N(1)	0.23740(9)	0.21653(5)	0.69822(8)	0.0184(2)
N(2)	0.43569(9)	0.25891(5)	0.68878(9)	0.0201(2)
N(3)	0.45596(9)	0.17387(5)	0.55866(8)	0.0199(2)
N(4)	0.25458(9)	0.13469(5)	0.56410(8)	0.0180(2)
C(a1)	0.15621(11)	0.18332(6)	0.71336(10)	0.0200(3)
C(a2)	0.23492(11)	0.26457(6)	0.75111(10)	0.0193(3)
C(a3)	0.40253(12)	0.30449(6)	0.73415(10)	0.0209(3)
C(a4)	0.53642(12)	0.27058(6)	0.68175(11)	0.0231(3)
C(a5)	0.55781(12)	0.19192(6)	0.57566(11)	0.0222(3)
C(a6)	0.44792(12)	0.13306(6)	0.48959(10)	0.0204(3)
C(a7)	0.26782(11)	0.10414(6)	0.48630(9)	0.0184(2)
C(a8)	0.16360(11)	0.11556(6)	0.58606(10)	0.0193(3)
C(b1)	0.10483(11)	0.21028(7)	0.78087(11)	0.0242(3)
C(b2)	0.15082(11)	0.26141(7)	0.80131(11)	0.0238(3)
C(b3)	0.48382(12)	0.34643(6)	0.75436(11)	0.0260(3)
C(b4)	0.56701(13)	0.32513(7)	0.72442(12)	0.0277(3)
C(b5)	0.61504(12)	0.15993(6)	0.51767(11)	0.0247(3)
C(b6)	0.54697(12)	0.12471(6)	0.46350(11)	0.0231(3)
C(b7)	0.17875(11)	0.06839(6)	0.45426(10)	0.0219(3)
C(b8)	0.11572(11)	0.07463(6)	0.51695(11)	0.0225(3)
C(m1)	0.30705(11)	0.30878(6)	0.76148(10)	0.0197(3)
C(m2)	0.59699(11)	0.23784(6)	0.63318(11)	0.0233(3)
C(m3)	0.35857(11)	0.10248(6)	0.45104(10)	0.0197(3)
C(m4)	0.12096(11)	0.13460(6)	0.66165(10)	0.0207(3)
C(11)	0.27918(11)	0.36287(6)	0.80347(10)	0.0213(3)
C(12)	0.20072(13)	0.39599(7)	0.75123(12)	0.0277(3)
C(13)	0.17394(13)	0.44814(7)	0.78482(13)	0.0296(3)
C(14)	0.22555(12)	0.46691(7)	0.87228(12)	0.0266(3)
C(15)	0.30231(13)	0.43400(7)	0.92610(11)	0.0265(3)
C(16)	0.32958(12)	0.38215(6)	0.89169(11)	0.0241(3)
C(21)	0.70647(12)	0.25634(6)	0.63629(12)	0.0265(3)
C(22)	0.77671(12)	0.26081(7)	0.72124(13)	0.0291(3)
C(23)	0.87821(13)	0.27870(7)	0.72451(15)	0.0345(4)

Table S3. Continued

atom	x	y	z	U(eq)
C(24)	0.91056(14)	0.29202(8)	0.64179(17)	0.0416(5)
C(25)	0.84151(16)	0.28823(9)	0.55686(16)	0.0425(5)
C(26)	0.74008(14)	0.27082(8)	0.55329(14)	0.0352(4)
C(31)	0.36665(11)	0.06184(6)	0.37320(10)	0.0202(3)
C(32)	0.35083(13)	0.08028(7)	0.28007(11)	0.0266(3)
C(33)	0.36869(14)	0.04420(7)	0.20883(11)	0.0300(3)
C(34)	0.40334(12)	−0.01033(7)	0.23072(11)	0.0278(3)
C(35)	0.41630(12)	−0.02980(7)	0.32278(11)	0.0264(3)
C(36)	0.39699(12)	0.00615(6)	0.39342(10)	0.0233(3)
C(41)	0.03137(11)	0.10282(6)	0.68491(11)	0.0226(3)
C(42)	0.04738(13)	0.04875(7)	0.72354(13)	0.0302(3)
C(43)	−0.03469(14)	0.01873(7)	0.74795(13)	0.0342(4)
C(44)	−0.13308(14)	0.04212(8)	0.73275(13)	0.0338(4)
C(45)	−0.14985(13)	0.09537(8)	0.69279(13)	0.0323(4)
C(46)	−0.06847(12)	0.12587(7)	0.66923(12)	0.0278(3)
C(1)	0.39421(11)	0.14754(6)	0.72063(10)	0.0221(3)
N(5)	0.29926(11)	0.25201(6)	0.51939(11)	0.0209(5)
C(2)	0.20696(10)	0.26897(5)	0.47433(9)	0.0233(5)
N(6)	0.21452(11)	0.31261(6)	0.41643(10)	0.0287(11)
C(3)	0.31903(12)	0.32434(7)	0.42497(12)	0.0344(6)
C(4)	0.37061(10)	0.28701(8)	0.48860(12)	0.0280(6)
C(5)	0.10611(12)	0.24448(9)	0.48511(16)	0.0331(7)
C(6)	0.13101(15)	0.34090(10)	0.35197(16)	0.0445(7)
N(5')	0.25983(18)	0.24862(10)	0.52244(17)	0.0188(8)
C(2')	0.28591(14)	0.28972(9)	0.46985(15)	0.0240(8)
N(6')	0.20210(17)	0.31204(10)	0.41299(16)	0.033(2)
C(3')	0.11635(14)	0.28322(12)	0.4305(2)	0.0366(11)
C(4')	0.15257(18)	0.24429(11)	0.4975(2)	0.0233(9)
C(5')	0.39316(16)	0.30951(15)	0.4707(3)	0.0336(11)
C(6')	0.1985(3)	0.35978(15)	0.3488(3)	0.0445(7)
C(51)	0.2613(4)	0.07518(14)	−0.0534(3)	0.0651(17)
C(56)	0.3388(3)	0.03668(17)	−0.0618(3)	0.0608(16)
C(52)	0.3273(3)	−0.02018(16)	−0.0414(3)	0.0585(15)
C(54)	0.2382(4)	−0.03854(15)	−0.0126(4)	0.096(3)

Table S3. Continued

atom	x	y	z	U(eq)
C(53)	0.1607(3)	0.0000(2)	−0.0042(4)	0.089(2)
C(55)	0.1723(3)	0.05682(19)	−0.0246(4)	0.076(2)
C(57)	0.0865(8)	0.0965(4)	−0.0130(7)	0.096(3)
C(60)	0.4749(7)	0.0511(4)	−0.0104(6)	0.109(3)
C(61)	0.5787(6)	0.0374(4)	0.0210(9)	0.172(5)
C(62)	0.6078(9)	−0.0187(6)	0.0391(10)	0.185(6)
C(63)	0.5330(15)	−0.0611(4)	0.026(3)	0.200
C(64)	0.4291(13)	−0.0474(6)	−0.006(4)	0.200
C(65)	0.4000(7)	0.0088(7)	−0.024(3)	0.200
C(70)	0.0165(13)	0.0545(7)	0.0118(11)	0.115(5)
C(71)	0.0521(5)	0.0379(4)	0.0000(2)	0.100(5)
C(72)	0.0628(7)	−0.0182(4)	−0.0253(2)	0.102(4)
C(73)	0.1478(8)	−0.0347(3)	−0.0624(2)	0.117(5)
C(74)	0.2222(6)	0.0050(5)	−0.07418(19)	0.138(6)
C(75)	0.2115(7)	0.0612(4)	−0.04885(12)	0.132(6)
C(76)	0.1264(7)	0.0776(3)	−0.01176(15)	0.108(5)
O(1)	0.41914(12)	0.11559(6)	0.77996(10)	0.0475(4)

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

Table S4. Bond Lengths for [Fe(TPP)(CO)(1,2-DiMeIm)]·C_7H_8[a]

bond	length (Å)	bond	length (Å)
Fe(1)–C(1)	1.7537(15)	C(36)–H(36)	0.9500
Fe(1)–N(1)	1.9790(12)	C(41)–C(42)	1.393(2)
Fe(1)–N(4)	1.9819(12)	C(41)–C(46)	1.398(2)
Fe(1)–N(3)	1.9826(12)	C(42)–C(43)	1.395(2)
Fe(1)–N(2)	1.9972(12)	C(42)–H(42)	0.9500
Fe(1)–N(5)	2.0779(11)	C(43)–C(44)	1.384(3)
Fe(1)–N(5′)	2.1402(18)	C(43)–H(43)	0.9500
N(1)–C(a2)	1.3728(17)	C(44)–C(45)	1.383(3)
N(1)–C(a1)	1.3778(18)	C(44)–H(44)	0.9500
N(2)–C(a3)	1.3767(18)	C(45)–C(46)	1.389(2)
N(2)–C(a4)	1.3776(18)	C(45)–H(45)	0.9500
N(3)–C(a6)	1.3771(18)	C(46)–H(46)	0.9500
N(3)–C(a5)	1.3808(19)	C(1)–O(1)	1.1408(19)
N(4)–C(a8)	1.3752(17)	N(5)–C(2)	1.3204
N(4)–C(a7)	1.3774(17)	N(5)–C(4)	1.3898
C(a1)–C(m4)	1.400(2)	C(2)–N(6)	1.3446
C(a1)–C(b1)	1.443(2)	C(2)–C(5)	1.4845
C(a2)–C(m1)	1.3989(19)	N(6)–C(3)	1.3840
C(a2)–C(b2)	1.442(2)	N(6)–C(6)	1.4537
C(a3)–C(m1)	1.395(2)	C(3)–C(4)	1.3548
C(a3)–C(b3)	1.444(2)	C(3)–H(3a)	0.9500
C(a4)–C(m2)	1.397(2)	C(4)–H(4a)	0.9500
C(a4)–C(b4)	1.450(2)	C(5)–H(5a)	1.08(4)
C(a5)–C(m2)	1.401(2)	C(5)–H(5b)	0.85(4)
C(a5)–C(b5)	1.448(2)	C(5)–H(5C)	0.84(4)
C(a6)–C(m3)	1.397(2)	C(6)–H(6a)	1.09(4)
C(a6)–C(b6)	1.441(2)	C(6)–H(6b)	0.85(4)
C(a7)–C(m3)	1.3901(19)	C(6)–H(6C)	0.97(4)
C(a7)–C(b7)	1.444(2)	N(5′)–C(2′)	1.3206
C(a8)–C(m4)	1.400(2)	N(5′)–C(4′)	1.3889
C(a8)–C(b8)	1.4419(19)	C(2′)–N(6′)	1.3445
C(b1)–C(b2)	1.357(2)	C(2′)–C(5′)	1.4844
C(b1)–H(b1)	0.9500	N(6′)–C(3′)	1.3841
C(b2)–H(b2)	0.9500	N(6′)–C(6′)	1.4557

Table S4. Continued

bond	length (Å)	bond	length (Å)
C(b3)–C(b4)	1.353(2)	C(3ı)–C(4ı)	1.3516
C(b3)–H(b3)	0.9500	C(3ı)–H(5C)	1.20(4)
C(b4)–H(b4)	0.9500	C(3ı)–H(3ıa)	0.9500
C(b5)–C(b6)	1.352(2)	C(4ı)–H(5a)	1.16(4)
C(b5)–H(b5)	0.9500	C(4ı)–H(5b)	1.22(4)
C(b6)–H(b6)	0.9500	C(4ı)–H(4ıa)	0.9500
C(b7)–C(b8)	1.354(2)	C(5ı)–H(5ıa)	0.9800
C(b7)–H(b7)	0.9500	C(5ı)–H(5ıb)	0.9800
C(b8)–H(b8)	0.9500	C(5ı)–H(5ıC)	0.9800
C(m1)–C(11)	1.4917(19)	C(6ı)–H(6b)	0.62(4)
C(m2)–C(21)	1.498(2)	C(6ı)–H(6ıa)	0.9800
C(m3)–C(31)	1.4998(19)	C(6ı)–H(6ıb)	0.9800
C(m4)–C(41)	1.4919(19)	C(6ı)–H(6ıC)	0.9800
C(11)–C(12)	1.392(2)	C(51)–C(56)	1.3900
C(11)–C(16)	1.392(2)	C(51)–C(55)	1.3900
C(12)–C(13)	1.395(2)	C(51)–H(51a)	0.9500
C(12)–H(12)	0.9500	C(56)–C(52)	1.3900
C(13)–C(14)	1.384(2)	C(56)–H(56a)	0.9500
C(13)–H(13)	0.9500	C(52)–C(54)	1.3900
C(14)–C(15)	1.384(2)	C(52)–H(52a)	0.9500
C(14)–H(14)	0.9500	C(54)–C(53)	1.3900
C(15)–C(16)	1.396(2)	C(54)–H(54a)	0.9500
C(15)–H(15)	0.9500	C(53)–C(55)	1.3900
C(16)–H(16)	0.9500	C(53)–H(53a)	0.9500
C(21)–C(22)	1.386(2)	C(55)–C(57)	1.502(11)
C(21)–C(26)	1.403(2)	C(57)–H(57a)	0.9800
C(22)–C(23)	1.393(2)	C(57)–H(57b)	0.9800
C(22)–H(22)	0.9500	C(57)–H(57C)	0.9800
C(23)–C(24)	1.385(3)	C(60)–C(62)#1)	1.327(19)
C(23)–H(23)	0.9500	C(60)–C(61)	1.3900
C(24)–C(25)	1.377(3)	C(61)–C(62)	1.3900
C(24)–H(24)	0.9500	C(62)–C(60)#1)	1.327(14)
C(25)–C(26)	1.388(2)	C(70)–C(71)	0.660(18)
C(25)–H(25)	0.9500	C(70)–C(72)#2)	1.394(17)

Table S4. Continued

bond	length (Å)	bond	length (Å)
C(26)–H(26)	0.9500	C(70)–C(76)	1.64(2)
C(31)–C(36)	1.389(2)	C(71)–C(72)	1.3900
C(31)–C(32)	1.392(2)	C(71)–C(76)	1.3900
C(32)–C(33)	1.393(2)	C(71)–C(72)#2)	1.690(16)
C(32)–H(32)	0.9500	C(72)–C(73)	1.3900
C(33)–C(34)	1.382(2)	C(72)–C(70)#2)	1.393(16)
C(33)–H(33)	0.9500	C(72)–C(71)#2)	1.690(15)
C(34)–C(35)	1.387(2)	C(73)–C(74)	1.3900
C(34)–H(34)	0.9500	C(74)–C(75)	1.3900
C(35)–C(36)	1.391(2)	C(75)–C(76)	1.3900
C(35)–H(35)	0.9500		

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

Table S5. Bond Angles for [Fe(TPP)(CO)(1,2-DiMeIm)]·C_7H_8[a]

angle	degree	angle	degree
C(1)–Fe(1)–N(1)	88.00(6)	C(35)–C(36)–H(36)	119.6
C(1)–Fe(1)–N(4)	89.40(6)	C(42)–C(41)–C(46)	118.92(14)
N(1)–Fe(1)–N(4)	89.15(5)	C(42)–C(41)–C(m4)	119.28(13)
C(1)–Fe(1)–N(3)	92.45(6)	C(46)–C(41)–C(m4)	121.80(14)
N(1)–Fe(1)–N(3)	179.55(5)	C(41)–C(42)–C(43)	120.33(16)
N(4)–Fe(1)–N(3)	90.81(5)	C(41)–C(42)–H(42)	119.8
C(1)–Fe(1)–N(2)	93.81(6)	C(43)–C(42)–H(42)	119.8
N(1)–Fe(1)–N(2)	90.50(5)	C(44)–C(43)–C(42)	120.26(17)
N(4)–Fe(1)–N(2)	176.75(5)	C(44)–C(43)–H(43)	119.9
N(3)–Fe(1)–N(2)	89.51(5)	C(42)–C(43)–H(43)	119.9
C(1)–Fe(1)–N(5)	176.77(6)	C(45)–C(44)–C(43)	119.67(15)
N(1)–Fe(1)–N(5)	94.68(6)	C(45)–C(44)–H(44)	120.2
N(4)–Fe(1)–N(5)	92.43(6)	C(43)–C(44)–H(44)	120.2
N(3)–Fe(1)–N(5)	84.87(6)	C(44)–C(45)–C(46)	120.53(16)
N(2)–Fe(1)–N(5)	84.38(6)	C(44)–C(45)–H(45)	119.7
C(1)–Fe(1)–N(5′)	168.73(8)	C(46)–C(45)–H(45)	119.7
N(1)–Fe(1)–N(5′)	82.77(8)	C(45)–C(46)–C(41)	120.27(16)
N(4)–Fe(1)–N(5′)	84.03(8)	C(45)–C(46)–H(46)	119.9
N(3)–Fe(1)–N(5′)	96.77(8)	C(41)–C(46)–H(46)	119.9
N(2)–Fe(1)–N(5′)	92.73(8)	O(1)–C(1)–Fe(1)	175.95(14)
N(5)–Fe(1)–N(5′)	14.49(6)	C(2)–N(5)–C(4)	106.0
C(a2)–N(1)–C(a1)	106.03(11)	C(2)–N(5)–Fe(1)	132.84(8)
C(a2)–N(1)–Fe(1)	126.56(9)	C(4)–N(5)–Fe(1)	120.67(8)
C(a1)–N(1)–Fe(1)	126.92(10)	N(5)–C(2)–N(6)	111.4
C(a3)–N(2)–C(a4)	106.28(12)	N(5)–C(2)–C(5)	125.7
C(a3)–N(2)–Fe(1)	125.71(10)	N(6)–C(2)–C(5)	122.9
C(a4)–N(2)–Fe(1)	127.42(10)	C(2)–N(6)–C(3)	107.1
C(a6)–N(3)–C(a5)	106.03(12)	C(2)–N(6)–C(6)	127.7
C(a6)–N(3)–Fe(1)	126.18(10)	C(3)–N(6)–C(6)	125.1
C(a5)–N(3)–Fe(1)	127.43(10)	C(4)–C(3)–N(6)	106.5
C(a8)–N(4)–C(a7)	105.98(11)	C(4)–C(3)–H(3a)	126.7
C(a8)–N(4)–Fe(1)	127.31(9)	N(6)–C(3)–H(3a)	126.7
C(a7)–N(4)–Fe(1)	126.70(9)	C(3)–C(4)–N(5)	109.0
N(1)–C(a1)–C(m4)	124.57(13)	C(3)–C(4)–H(4a)	125.5

Table S5. Continued

angle	degree	angle	degree
N(1)–C(a1)–C(b1)	109.87(12)	N(5)–C(4)–H(4a)	125.5
C(m4)–C(a1)–C(b1)	125.07(13)	C(2)–C(5)–H(5a)	112(2)
N(1)–C(a2)–C(m1)	125.83(13)	C(2)–C(5)–H(5b)	108(3)
N(1)–C(a2)–C(b2)	110.14(12)	H(5a)–C(5)–H(5b)	113(3)
C(m1)–C(a2)–C(b2)	123.87(13)	C(2)–C(5)–H(5C)	115(3)
N(2)–C(a3)–C(m1)	125.58(13)	H(5a)–C(5)–H(5C)	109(3)
N(2)–C(a3)–C(b3)	109.89(13)	H(5b)–C(5)–H(5C)	100(3)
C(m1)–C(a3)–C(b3)	124.45(13)	N(6)–C(6)–H(6a)	112(2)
N(2)–C(a4)–C(m2)	125.51(13)	N(6)–C(6)–H(6b)	109(3)
N(2)–C(a4)–C(b4)	109.60(13)	H(6a)–C(6)–H(6b)	115(3)
C(m2)–C(a4)–C(b4)	124.63(13)	N(6)–C(6)–H(6C)	110(2)
N(3)–C(a5)–C(m2)	124.99(13)	H(6a)–C(6)–H(6C)	112(3)
N(3)–C(a5)–C(b5)	109.55(13)	H(6b)–C(6)–H(6C)	99(3)
C(m2)–C(a5)–C(b5)	125.19(14)	C(2′)–N(5′)–C(4′)	105.8
N(3)–C(a6)–C(m3)	125.99(13)	C(2′)–N(5′)–Fe(1)	133.34(12)
N(3)–C(a6)–C(b6)	110.11(13)	C(4′)–N(5′)–Fe(1)	120.85(12)
C(m3)–C(a6)–C(b6)	123.88(13)	N(5′)–C(2′)–N(6′)	111.4
N(4)–C(a7)–C(m3)	124.99(12)	N(5′)–C(2′)–C(5′)	125.7
N(4)–C(a7)–C(b7)	109.96(12)	N(6′)–C(2′)–C(5′)	122.9
C(m3)–C(a7)–C(b7)	124.59(13)	C(2′)–N(6′)–C(3′)	107.1
N(4)–C(a8)–C(m4)	125.37(12)	C(2′)–N(6′)–C(6′)	127.7
N(4)–C(a8)–C(b8)	109.86(12)	C(3′)–N(6′)–C(6′)	125.1
C(m4)–C(a8)–C(b8)	124.71(13)	C(4′)–C(3′)–N(6′)	106.4
C(b2)–C(b1)–C(a1)	106.94(13)	C(4′)–C(3′)–H(5b)	49.9(15)
C(b2)–C(b1)–H(b1)	126.5	N(6′)–C(3′)–H(5b)	136.8(16)
C(a1)–C(b1)–H(b1)	126.5	C(4′)–C(3′)–H(5C)	63.8(19)
C(b1)–C(b2)–C(a2)	106.86(13)	N(6′)–C(3′)–H(5C)	155.8(19)
C(b1)–C(b2)–H(b2)	126.6	H(5b)–C(3′)–H(5C)	55(2)
C(a2)–C(b2)–H(b2)	126.6	C(4′)–C(3′)–H(3′a)	126.8
C(b4)–C(b3)–C(a3)	107.10(13)	N(6′)–C(3′)–H(3′a)	126.8
C(b4)–C(b3)–H(b3)	126.4	H(5b)–C(3′)–H(3′a)	85.9
C(a3)–C(b3)–H(b3)	126.4	H(5C)–C(3′)–H(3′a)	66.9
C(b3)–C(b4)–C(a4)	107.07(13)	C(3′)–C(4′)–N(5′)	109.3
C(b3)–C(b4)–H(b4)	126.5	C(3′)–C(4′)–H(5a)	129.4(19)

Table S5. Continued

angle	degree	angle	degree
C(a4)–C(b4)–H(b4)	126.5	N(5′)–C(4′)–H(5a)	116.1(19)
C(b6)–C(b5)–C(a5)	107.23(13)	C(3′)–C(4′)–H(5b)	72.0(19)
C(b6)–C(b5)–H(b5)	126.4	N(5′)–C(4′)–H(5b)	141(2)
C(a5)–C(b5)–H(b5)	126.4	H(5a)–C(4′)–H(5b)	86(3)
C(b5)–C(b6)–C(a6)	107.03(13)	C(3′)–C(4′)–H(5C)	52.6(17)
C(b5)–C(b6)–H(b6)	126.5	N(5′)–C(4′)–H(5C)	152.2(17)
C(a6)–C(b6)–H(b6)	126.5	H(5a)–C(4′)–H(5C)	77(2)
C(b8)–C(b7)–C(a7)	106.75(12)	H(5b)–C(4′)–H(5C)	60(2)
C(b8)–C(b7)–H(b7)	126.6	C(3′)–C(4′)–H(4′a)	125.4
C(a7)–C(b7)–H(b7)	126.6	N(5′)–C(4′)–H(4′a)	125.4
C(b7)–C(b8)–C(a8)	107.23(13)	H(5b)–C(4′)–H(4′a)	66.3
C(b7)–C(b8)–H(b8)	126.4	H(5C)–C(4′)–H(4′a)	76.1
C(a8)–C(b8)–H(b8)	126.4	C(2′)–C(5′)–H(5′a)	109.5
C(a3)–C(m1)–C(a2)	123.09(13)	C(2′)–C(5′)–H(5′b)	109.5
C(a3)–C(m1)–C(11)	119.13(12)	H(5′a)–C(5′)–H(5′b)	109.5
C(a2)–C(m1)–C(11)	117.78(13)	C(2′)–C(5′)–H(5′C)	109.5
C(a4)–C(m2)–C(a5)	123.25(14)	H(5′a)–C(5′)–H(5′C)	109.5
C(a4)–C(m2)–C(21)	117.76(13)	H(5′b)–C(5′)–H(5′C)	109.5
C(a5)–C(m2)–C(21)	118.75(13)	N(6′)–C(6′)–H(6b)	120(4)
C(a7)–C(m3)–C(a6)	123.71(13)	N(6′)–C(6′)–H(6′a)	109.5
C(a7)–C(m3)–C(31)	119.28(12)	H(6b)–C(6′)–H(6′a)	115.5
C(a6)–C(m3)–C(31)	116.74(12)	N(6′)–C(6′)–H(6′b)	109.5
C(a8)–C(m4)–C(a1)	122.68(13)	H(6b)–C(6′)–H(6′b)	90.9
C(a8)–C(m4)–C(41)	118.24(12)	H(6′a)–C(6′)–H(6′b)	109.5
C(a1)–C(m4)–C(41)	119.03(13)	N(6′)–C(6′)–H(6′C)	109.5
C(12)–C(11)–C(16)	118.66(14)	H(6′a)–C(6′)–H(6′C)	109.5
C(12)–C(11)–C(m1)	118.44(13)	H(6′b)–C(6′)–H(6′C)	109.5
C(16)–C(11)–C(m1)	122.88(14)	C(56)–C(51)–C(55)	120.0
C(11)–C(12)–C(13)	121.24(15)	C(56)–C(51)–H(51a)	120.0
C(11)–C(12)–H(12)	119.4	C(55)–C(51)–H(51a)	120.0
C(13)–C(12)–H(12)	119.4	C(52)–C(56)–C(51)	120.0
C(14)–C(13)–C(12)	119.31(16)	C(52)–C(56)–H(56a)	120.0
C(14)–C(13)–H(13)	120.3	C(51)–C(56)–H(56a)	120.0
C(12)–C(13)–H(13)	120.3	C(56)–C(52)–C(54)	120.0

Table S5. Continued

angle	degree	angle	degree
C(13)–C(14)–C(15)	120.24(14)	C(56)–C(52)–H(52a)	120.0
C(13)–C(14)–H(14)	119.9	C(54)–C(52)–H(52a)	120.0
C(15)–C(14)–H(14)	119.9	C(53)–C(54)–C(52)	120.0
C(14)–C(15)–C(16)	120.19(14)	C(53)–C(54)–H(54a)	120.0
C(14)–C(15)–H(15)	119.9	C(52)–C(54)–H(54a)	120.0
C(16)–C(15)–H(15)	119.9	C(54)–C(53)–C(55)	120.0
C(11)–C(16)–C(15)	120.33(15)	C(54)–C(53)–H(53a)	120.0
C(11)–C(16)–H(16)	119.8	C(55)–C(53)–H(53a)	120.0
C(15)–C(16)–H(16)	119.8	C(53)–C(55)–C(51)	120.0
C(22)–C(21)–C(26)	118.16(15)	C(53)–C(55)–C(57)	117.6(5)
C(22)–C(21)–C(m2)	121.03(14)	C(51)–C(55)–C(57)	122.4(5)
C(26)–C(21)–C(m2)	120.79(15)	C(55)–C(57)–H(57a)	109.5
C(21)–C(22)–C(23)	121.19(17)	C(55)–C(57)–H(57b)	109.5
C(21)–C(22)–H(22)	119.4	H(57a)–C(57)–H(57b)	109.5
C(23)–C(22)–H(22)	119.4	C(55)–C(57)–H(57C)	109.5
C(24)–C(23)–C(22)	119.90(18)	H(57a)–C(57)–H(57C)	109.5
C(24)–C(23)–H(23)	120.0	H(57b)–C(57)–H(57C)	109.5
C(22)–C(23)–H(23)	120.0	C(60)–C(61)–C(62)	120.0
C(25)–C(24)–C(23)	119.64(17)	C(71)–C(70)–C(72)#2	105(2)
C(25)–C(24)–H(24)	120.2	C(71)–C(70)–C(76)	56.2(17)
C(23)–C(24)–H(24)	120.2	C(72)#2–C(70)–C(76)	161.3(15)
C(24)–C(25)–C(26)	120.68(18)	C(72)#2–C(70)–C(72)	77.2(11)
C(24)–C(25)–H(25)	119.7	C(76)–C(70)–C(72)	84.1(8)
C(26)–C(25)–H(25)	119.7	C(70)–C(71)–C(72)	139(2)
C(25)–C(26)–C(21)	120.42(18)	C(70)–C(71)–C(76)	101(2)
C(25)–C(26)–H(26)	119.8	C(72)–C(71)–C(76)	120.0
C(21)–C(26)–H(26)	119.8	C(70)–C(71)–C(72)#2	52.8(16)
C(36)–C(31)–C(32)	118.78(13)	C(72)–C(71)–C(72)#2	86.4(10)
C(36)–C(31)–C(m3)	120.58(13)	C(76)–C(71)–C(72)#2	153.4(11)
C(32)–C(31)–C(m3)	120.50(13)	C(73)–C(72)–C(71)	120.0
C(31)–C(32)–C(33)	120.68(15)	C(73)–C(72)–C(70)#2	124.5(10)
C(31)–C(32)–H(32)	119.7	C(71)–C(72)–C(70)#2	115.5(10)
C(33)–C(32)–H(32)	119.7	C(73)–C(72)–C(71)#2	146.2(8)
C(34)–C(33)–C(32)	119.83(15)	C(71)–C(72)–C(71)#2	93.6(8)

Table S5. Continued

angle	degree	angle	degree
C(34)–C(33)–H(33)	120.1	C(73)–C(72)–C(70)	132.7(7)
C(32)–C(33)–H(33)	120.1	C(70)#2–C(72)–C(70)	102.8(10)
C(33)–C(34)–C(35)	120.04(14)	C(71)#2–C(72)–C(70)	80.7(7)
C(33)–C(34)–H(34)	120.0	C(72)–C(73)–C(74)	120.0
C(35)–C(34)–H(34)	120.0	C(73)–C(74)–C(75)	120.0
C(34)–C(35)–C(36)	119.86(15)	C(76)–C(75)–C(74)	120.0
C(34)–C(35)–H(35)	120.1	C(75)–C(76)–C(71)	120.0
C(36)–C(35)–H(35)	120.1	C(75)–C(76)–C(70)	142.9(7)
C(31)–C(36)–C(35)	120.71(14)		
C(31)–C(36)–H(36)	119.6		

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

Table S6. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1,2-DiMeIm)]·C_7H_8[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0192(1)	0.0129(1)	0.0173(1)	−0.0010(1)	0.0049(1)	−0.0019(1)
N(1)	0.0177(5)	0.0174(5)	0.0199(5)	−0.0031(4)	0.0030(4)	−0.0020(4)
N(2)	0.0224(5)	0.0158(5)	0.0240(6)	−0.0028(4)	0.0093(5)	−0.0044(4)
N(3)	0.0236(6)	0.0151(5)	0.0230(6)	−0.0024(4)	0.0096(5)	−0.0041(4)
N(4)	0.0188(5)	0.0155(5)	0.0196(5)	−0.0017(4)	0.0037(4)	−0.0005(4)
C(A1)	0.0172(6)	0.0209(6)	0.0223(6)	−0.0038(5)	0.0053(5)	−0.0021(5)
C(A2)	0.0195(6)	0.0189(6)	0.0189(6)	−0.0033(5)	0.0025(5)	−0.0007(5)
C(A3)	0.0252(7)	0.0158(6)	0.0228(6)	−0.0028(5)	0.0073(5)	−0.0035(5)
C(A4)	0.0248(7)	0.0183(6)	0.0280(7)	−0.0047(5)	0.0098(6)	−0.0062(5)
C(A5)	0.0248(7)	0.0185(6)	0.0261(7)	−0.0016(5)	0.0121(6)	−0.0049(5)
C(A6)	0.0272(7)	0.0151(6)	0.0209(6)	−0.0007(5)	0.0097(5)	−0.0023(5)
C(A7)	0.0223(6)	0.0140(6)	0.0182(6)	−0.0010(5)	0.0023(5)	0.0000(5)
C(A8)	0.0183(6)	0.0159(6)	0.0235(6)	−0.0023(5)	0.0034(5)	−0.0009(5)
C(B1)	0.0209(6)	0.0269(7)	0.0263(7)	−0.0067(6)	0.0081(6)	−0.0044(5)
C(B2)	0.0220(6)	0.0258(7)	0.0244(7)	−0.0074(6)	0.0061(5)	−0.0019(5)
C(B3)	0.0301(7)	0.0174(6)	0.0325(8)	−0.0066(6)	0.0114(6)	−0.0070(6)
C(B4)	0.0286(7)	0.0205(7)	0.0369(8)	−0.0075(6)	0.0136(7)	−0.0091(6)
C(B5)	0.0266(7)	0.0219(7)	0.0291(7)	−0.0032(6)	0.0142(6)	−0.0041(6)
C(B6)	0.0290(7)	0.0199(7)	0.0241(7)	−0.0021(5)	0.0140(6)	−0.0030(5)
C(B7)	0.0239(7)	0.0173(6)	0.0233(6)	−0.0041(5)	0.0020(5)	−0.0017(5)
C(B8)	0.0204(6)	0.0180(6)	0.0282(7)	−0.0045(5)	0.0027(5)	−0.0021(5)
C(M1)	0.0232(6)	0.0157(6)	0.0201(6)	−0.0021(5)	0.0039(5)	−0.0011(5)
C(M2)	0.0240(7)	0.0203(7)	0.0276(7)	−0.0035(5)	0.0102(6)	−0.0065(5)
C(M3)	0.0265(7)	0.0142(6)	0.0189(6)	−0.0002(5)	0.0058(5)	−0.0002(5)
C(M4)	0.0181(6)	0.0190(6)	0.0250(7)	−0.0024(5)	0.0045(5)	−0.0026(5)
C(11)	0.0234(6)	0.0170(6)	0.0249(7)	−0.0039(5)	0.0083(5)	−0.0029(5)
C(12)	0.0293(8)	0.0238(7)	0.0287(7)	−0.0062(6)	0.0028(6)	0.0014(6)
C(13)	0.0283(7)	0.0248(7)	0.0360(8)	−0.0027(6)	0.0071(7)	0.0048(6)
C(14)	0.0271(7)	0.0201(7)	0.0361(8)	−0.0068(6)	0.0147(6)	−0.0015(6)
C(15)	0.0313(8)	0.0233(7)	0.0264(7)	−0.0076(6)	0.0091(6)	−0.0041(6)
C(16)	0.0281(7)	0.0199(7)	0.0248(7)	−0.0040(5)	0.0065(6)	−0.0025(5)
C(21)	0.0253(7)	0.0206(7)	0.0371(8)	−0.0067(6)	0.0143(6)	−0.0068(6)
C(22)	0.0275(7)	0.0225(7)	0.0395(9)	−0.0063(6)	0.0121(7)	−0.0026(6)
C(23)	0.0258(8)	0.0256(8)	0.0530(11)	−0.0101(7)	0.0097(7)	−0.0033(6)

Table S6. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.0280(8)	0.0329(9)	0.0685(14)	−0.0099(9)	0.0207(9)	−0.0101(7)
C(25)	0.0400(10)	0.0393(10)	0.0558(12)	−0.0037(9)	0.0276(9)	−0.0135(8)
C(26)	0.0358(9)	0.0351(9)	0.0389(9)	−0.0047(7)	0.0178(8)	−0.0133(7)
C(31)	0.0245(6)	0.0168(6)	0.0203(6)	−0.0026(5)	0.0071(5)	−0.0025(5)
C(32)	0.0367(8)	0.0215(7)	0.0227(7)	0.0024(5)	0.0087(6)	−0.0002(6)
C(33)	0.0397(9)	0.0322(8)	0.0201(7)	−0.0025(6)	0.0110(6)	−0.0061(7)
C(34)	0.0295(7)	0.0289(8)	0.0276(7)	−0.0116(6)	0.0122(6)	−0.0075(6)
C(35)	0.0298(7)	0.0197(7)	0.0304(8)	−0.0063(6)	0.0075(6)	0.0000(6)
C(36)	0.0305(7)	0.0186(6)	0.0209(6)	−0.0019(5)	0.0057(6)	−0.0015(5)
C(41)	0.0206(6)	0.0210(7)	0.0271(7)	−0.0060(5)	0.0071(5)	−0.0054(5)
C(42)	0.0280(8)	0.0238(7)	0.0404(9)	−0.0013(6)	0.0107(7)	−0.0036(6)
C(43)	0.0377(9)	0.0258(8)	0.0423(9)	−0.0020(7)	0.0154(8)	−0.0098(7)
C(44)	0.0325(8)	0.0366(9)	0.0358(9)	−0.0112(7)	0.0152(7)	−0.0163(7)
C(45)	0.0215(7)	0.0363(9)	0.0410(9)	−0.0082(7)	0.0109(7)	−0.0067(6)
C(46)	0.0216(7)	0.0270(8)	0.0360(8)	−0.0052(6)	0.0084(6)	−0.0037(6)
C(1)	0.0207(6)	0.0224(7)	0.0246(7)	−0.0002(5)	0.0081(5)	−0.0001(5)
N(5)	0.0233(12)	0.0183(10)	0.0221(10)	−0.0005(8)	0.0072(9)	0.0033(9)
C(2)	0.0258(12)	0.0224(11)	0.0205(10)	−0.0024(9)	0.0017(9)	0.0049(9)
N(6)	0.0376(17)	0.025(3)	0.022(2)	0.0098(19)	0.0026(15)	0.0080(14)
C(3)	0.0432(16)	0.0286(13)	0.0294(13)	0.0083(11)	0.0024(12)	−0.0064(12)
C(4)	0.0307(14)	0.0260(13)	0.0264(12)	0.0062(10)	0.0036(10)	−0.0090(11)
C(5)	0.0205(13)	0.0443(18)	0.0341(15)	0.0032(13)	0.0043(13)	0.0071(14)
C(6)	0.0450(15)	0.0401(16)	0.0447(15)	0.0172(12)	0.0003(14)	0.0108(13)
N(5')	0.0212(19)	0.0180(16)	0.0208(16)	0.0009(12)	0.0129(15)	0.0067(14)
C(2')	0.030(2)	0.0209(18)	0.0240(18)	0.0048(14)	0.0115(16)	0.0016(15)
N(6')	0.036(3)	0.030(5)	0.033(5)	0.005(4)	0.005(3)	−0.003(3)
C(3')	0.029(2)	0.038(2)	0.040(2)	0.0101(18)	0.0031(17)	0.0042(17)
C(4')	0.0143(18)	0.0243(19)	0.032(2)	0.0032(16)	0.0072(17)	0.0033(17)
C(5')	0.028(2)	0.037(3)	0.037(3)	0.016(2)	0.0094(19)	−0.0034(19)
C(6')	0.0450(15)	0.0401(16)	0.0447(15)	0.0172(12)	0.0003(14)	0.0108(13)
O(1)	0.0550(9)	0.0480(8)	0.0419(8)	0.0231(7)	0.0155(7)	0.0192(7)

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

Table S7. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1,2-DiMeIm)]·C_7H_8[a]

atom	x	y	z	U(eq)
H(B1	0.0494	0.1951	0.8062	0.029
H(B2	0.1314	0.2897	0.8411	0.029
H(B3	0.4796	0.3822	0.7833	0.031
H(B4	0.6330	0.3426	0.7303	0.033
H(B5	0.6870	0.1631	0.5177	0.030
H(B6	0.5616	0.0993	0.4170	0.028
H(B7	0.1667	0.0450	0.3997	0.026
H(B8	0.0519	0.0556	0.5156	0.027
H(12)	0.1647	0.3828	0.6916	0.033
H(13)	0.1208	0.4705	0.7480	0.036
H(14)	0.2082	0.5025	0.8955	0.032
H(15)	0.3365	0.4467	0.9866	0.026(5)
H(16)	0.3828	0.3599	0.9287	0.029
H(22)	0.7552	0.2515	0.7783	0.035
H(23)	0.9252	0.2818	0.7834	0.041
H(24)	0.9800	0.3037	0.6436	0.050
H(25)	0.8635	0.2976	0.5001	0.051
H(26)	0.6931	0.2687	0.4943	0.042
H(32)	0.3276	0.1179	0.2649	0.032
H(33)	0.3571	0.0571	0.1454	0.036
H(34)	0.4183	−0.0345	0.1827	0.033
H(35)	0.4383	−0.0676	0.3376	0.032
H(36)	0.4046	−0.0075	0.4562	0.028
H(42)	0.1145	0.0322	0.7333	0.036
H(43)	−0.0230	−0.0179	0.7751	0.041
H(44)	−0.1888	0.0217	0.7497	0.041
H(45)	−0.2176	0.1112	0.6814	0.039
H(46)	−0.0807	0.1625	0.6423	0.033
H(3A)	0.3487	0.3529	0.3926	0.041
H(4A)	0.4438	0.2851	0.5089	0.034
H(5A)	0.112(3)	0.2239(16)	0.553(3)	0.053
H(5B)	0.085(3)	0.2221(18)	0.439(3)	0.053
H(5C)	0.056(3)	0.2672(17)	0.477(3)	0.053
H(6A)	0.081(3)	0.3108(16)	0.307(3)	0.053

Table S7. Continued

atom	x	y	z	U(eq)
H(6B)	0.157(3)	0.3667(18)	0.323(3)	0.053
H(6C)	0.092(3)	0.3644(16)	0.387(3)	0.053
H(3'A)	0.0460	0.2895	0.4012	0.044
H(4'A)	0.1112	0.2181	0.5234	0.028
H(5'A)	0.4403	0.2770	0.4781	0.050
H(5'B)	0.4148	0.3358	0.5234	0.050
H(5'C)	0.3952	0.3288	0.4112	0.050
H(6'A)	0.2585	0.3583	0.3182	0.067
H(6'B)	0.2001	0.3952	0.3842	0.067
H(6'C)	0.1345	0.3580	0.3007	0.067
H(51A)	0.2692	0.1140	−0.0674	0.078
H(56A)	0.3997	0.0492	−0.0815	0.073
H(52A)	0.3803	−0.0465	−0.0472	0.070
H(54A)	0.2303	−0.0774	0.0014	0.115
H(53A)	0.0998	−0.0126	0.0155	0.107
H(57A)	0.0301	0.0750	0.0055	0.144
H(57B)	0.0602	0.1159	−0.0729	0.144
H(57C)	0.1131	0.1245	0.0358	0.144

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

Table S8. Complete Crystallographic Details for [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8

formula	$C_{56}H_{34}FeN_6O$
FW, amu	862.74
a, Å	13.1961(2)
b, Å	23.4514(3)
c, Å	14.2630(2)
β, deg	105.1980(10)
V, Å^3	4259.55(10)
space group	P2(1)/n
Z	4
D_c, g/cm^3	1.345
F(000)	1784
μ, mm^{-1}	0.404
crystal dimensions, mm	0.66 × 0.39 × 0.27
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.72–32.50
index range	$-19 \leq h \leq 19$
	$-35 \leq k \leq 35$
	$-21 \leq l \leq 21$
total data collected	66278
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.8987 and 0.7759
unique data	15413 (R_{int} = 0.037)
unique observed data [I > 2σ(I)]	12118
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	15413/0/623
goodness-of-fit (pased on F^2)	1.028
final R indices [I > 2σ(I)]	R_1 = 0.0446, wR_2 = 0.1139
final R indices (all data)	R_1 = 0.0618, wR_2 = 0.1252

Table S9. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8[a]

atom	x	y	z	U(eq)
Fe	0.34102(1)	0.20289(1)	0.60944(1)	0.0128(1)
N(1)	0.23397(8)	0.22432(5)	0.67805(8)	0.0148(2)
N(2)	0.42934(8)	0.26923(5)	0.66914(8)	0.0148(2)
N(3)	0.44757(8)	0.18138(5)	0.53965(8)	0.0149(2)
N(4)	0.24956(8)	0.13898(5)	0.54669(8)	0.0143(2)
C(a1)	0.15577(10)	0.18982(6)	0.69436(9)	0.0162(2)
C(a2)	0.23327(10)	0.27259(5)	0.73185(9)	0.0163(2)
C(a3)	0.39787(10)	0.31471(5)	0.71571(9)	0.0157(2)
C(a4)	0.52989(10)	0.28124(6)	0.66470(10)	0.0162(2)
C(a5)	0.54904(10)	0.20141(5)	0.55793(9)	0.0160(2)
C(a6)	0.44005(10)	0.13766(5)	0.47350(9)	0.0153(2)
C(a7)	0.26231(10)	0.10527(5)	0.47162(9)	0.0149(2)
C(a8)	0.16067(10)	0.11909(5)	0.56900(9)	0.0151(2)
C(b1)	0.10837(11)	0.21632(6)	0.76358(10)	0.0202(3)
C(b2)	0.15378(11)	0.26836(6)	0.78411(10)	0.0209(3)
C(b3)	0.48007(11)	0.35702(6)	0.73911(10)	0.0194(2)
C(b4)	0.56227(11)	0.33585(6)	0.70989(11)	0.0200(2)
C(b5)	0.60664(10)	0.16867(6)	0.50338(10)	0.0183(2)
C(b6)	0.53881(10)	0.13003(6)	0.44993(10)	0.0177(2)
C(b7)	0.17527(10)	0.06663(5)	0.44135(10)	0.0168(2)
C(b8)	0.11304(10)	0.07453(5)	0.50233(10)	0.0167(2)
C(m1)	0.30390(10)	0.31797(5)	0.74268(9)	0.0165(2)
C(m2)	0.58927(10)	0.24851(6)	0.61657(10)	0.0167(2)
C(m3)	0.35172(10)	0.10350(5)	0.43699(9)	0.0152(2)
C(m4)	0.11980(10)	0.13984(5)	0.64343(9)	0.0159(2)
C(11)	0.27646(10)	0.37121(6)	0.78822(10)	0.0182(2)
C(12)	0.33044(12)	0.38878(6)	0.88115(11)	0.0220(3)
C(13)	0.30108(13)	0.43846(6)	0.92042(11)	0.0246(3)
C(14)	0.21827(12)	0.47116(6)	0.86756(12)	0.0237(3)
C(15)	0.16292(12)	0.45362(7)	0.77580(13)	0.0285(3)
C(16)	0.19175(12)	0.40354(7)	0.73678(12)	0.0262(3)
C(21)	0.69883(11)	0.26714(6)	0.62212(11)	0.0194(2)
C(22)	0.72703(13)	0.28360(7)	0.53846(12)	0.0277(3)
C(23)	0.82934(14)	0.30074(8)	0.54352(15)	0.0349(4)

Table S9. Continued

atom	x	y	z	U(eq)
C(24)	0.90389(13)	0.30218(7)	0.63189(15)	0.0333(4)
C(25)	0.87666(12)	0.28640(7)	0.71556(13)	0.0285(3)
C(26)	0.77465(11)	0.26908(6)	0.71114(11)	0.0222(3)
C(31)	0.35959(10)	0.05824(5)	0.36510(9)	0.0159(2)
C(32)	0.39005(11)	0.00291(6)	0.39659(10)	0.0197(2)
C(33)	0.40615(12)	−0.03844(6)	0.33168(11)	0.0221(3)
C(34)	0.38933(12)	−0.02498(6)	0.23393(11)	0.0221(3)
C(35)	0.35577(13)	0.02932(6)	0.20120(11)	0.0241(3)
C(36)	0.34109(12)	0.07081(6)	0.26660(10)	0.0213(3)
C(41)	0.03196(10)	0.10846(6)	0.66815(10)	0.0175(2)
C(42)	−0.06763(11)	0.13295(6)	0.65320(11)	0.0209(3)
C(43)	−0.14658(11)	0.10449(7)	0.68266(11)	0.0244(3)
C(44)	−0.12665(12)	0.05170(7)	0.72802(11)	0.0260(3)
C(45)	−0.02861(13)	0.02699(7)	0.74152(12)	0.0263(3)
C(46)	0.05009(12)	0.05465(6)	0.71076(11)	0.0227(3)
C(1)	0.40501(10)	0.16115(6)	0.70817(10)	0.0180(2)
O(1)	0.45089(10)	0.13633(5)	0.77538(9)	0.0315(3)
C(2)	0.17470(11)	0.27010(6)	0.44663(10)	0.0211(3)
C(3)	0.27402(14)	0.33322(7)	0.39577(12)	0.0299(3)
C(4)	0.33531(12)	0.29777(6)	0.46188(11)	0.0241(3)
N(5)	0.27289(9)	0.25833(5)	0.49439(8)	0.0179(2)
C(5)	0.07710(12)	0.24058(7)	0.45239(12)	0.0284(3)
N(6)	0.17295(11)	0.31523(6)	0.38669(10)	0.0273(3)
C(51)	0.0559(3)	−0.02292(15)	0.9895(3)	0.0653(14)
C(52)	0.1385(3)	−0.03519(13)	0.9490(3)	0.0785(19)
C(53)	0.2019(3)	0.00854(19)	0.9308(3)	0.095(3)
C(55)	0.1826(3)	0.06455(16)	0.9531(3)	0.090(2)
C(54)	0.1001(4)	0.07682(13)	0.9935(3)	0.0736(16)
C(56)	0.0367(3)	0.03309(18)	1.0117(3)	0.0742(19)
C(57)	−0.0164(7)	−0.0688(3)	1.0046(5)	0.082(2)
C(61)	0.5277(3)	−0.0285(3)	1.0176(4)	0.085(3)
C(62)	0.5370(5)	0.0291(3)	0.9982(5)	0.134(7)
C(63)	0.4475(7)	0.06180(18)	0.9616(4)	0.129(5)
C(64)	0.3487(5)	0.0369(3)	0.9443(3)	0.153(6)

Table S9. Continued

atom	x	y	z	U(eq)
C(65)	0.3394(3)	−0.0207(3)	0.9637(3)	0.081(2)
C(66)	0.4289(4)	−0.05335(18)	1.0003(3)	0.079(2)
C(67)	0.2386(11)	−0.0437(7)	0.9490(8)	0.142(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 S10. Bond Lengths for [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8[a]

bond	length (Å)	bond	length (Å)
Fe–C(1)	1.7410(14)	C(31)–C(36)	1.3930(19)
Fe–N(1)	1.9825(11)	C(31)–C(32)	1.3974(19)
Fe–N(4)	1.9843(11)	C(32)–C(33)	1.3950(19)
Fe–N(3)	1.9891(11)	C(32)–H(32)	0.9500
Fe–N(2)	1.9959(11)	C(33)–C(34)	1.389(2)
Fe–N(5)	2.1018(12)	C(33)–H(33)	0.9500
N(1)–C(a2)	1.3689(16)	C(34)–C(35)	1.388(2)
N(1)–C(a1)	1.3782(17)	C(34)–H(34)	0.9500
N(2)–C(a4)	1.3740(17)	C(35)–C(36)	1.3960(19)
N(2)–C(a3)	1.3769(16)	C(35)–H(35)	0.9500
N(3)–C(a5)	1.3778(16)	C(36)–H(36)	0.9500
N(3)–C(a6)	1.3793(16)	C(41)–C(46)	1.394(2)
N(4)–C(a8)	1.3750(16)	C(41)–C(42)	1.398(2)
N(4)–C(a7)	1.3763(16)	C(42)–C(43)	1.392(2)
C(a1)–C(m4)	1.3950(18)	C(42)–H(42)	0.9500
C(a1)–C(b1)	1.4407(18)	C(43)–C(44)	1.390(2)
C(a2)–C(m1)	1.3962(18)	C(43)–H(43)	0.9500
C(a2)–C(b2)	1.4408(19)	C(44)–C(45)	1.384(2)
C(a3)–C(m1)	1.3934(18)	C(44)–H(44)	0.9500
C(a3)–C(b3)	1.4432(18)	C(45)–C(46)	1.390(2)
C(a4)–C(m2)	1.3987(19)	C(45)–H(45)	0.9500
C(a4)–C(b4)	1.4470(18)	C(46)–H(46)	0.9500
C(a5)–C(m2)	1.4031(18)	C(1)–O(1)	1.1488(17)
C(a5)–C(b5)	1.4430(18)	C(2)–N(5)	1.3252(18)
C(a6)–C(m3)	1.3976(18)	C(2)–N(6)	1.3569(19)
C(a6)–C(b6)	1.4398(18)	C(2)–C(5)	1.483(2)
C(a7)–C(m3)	1.3941(18)	C(3)–C(4)	1.354(2)
C(a7)–C(b7)	1.4375(17)	C(3)–N(6)	1.372(2)
C(a8)–C(m4)	1.3983(18)	C(3)–H(3)	0.9500
C(a8)–C(b8)	1.4413(17)	C(4)–N(5)	1.3962(19)
C(b1)–C(b2)	1.3573(19)	C(4)–H(4)	0.9500
C(b1)–H(b1)	0.9500	C(5)–H(5a)	0.9800
C(b2)–H(b2)	0.9500	C(5)–H(5b)	0.9800
C(b3)–C(b4)	1.354(2)	C(5)–H(5c)	0.9800

Table S10. Continued

bond	length (Å)	bond	length (Å)
C(b3)–H(b3)	0.9500	N(6)–H(6)	0.79(3)
C(b4)–H(b4)	0.9500	C(51)–C(56)#1)	1.242(8)
C(b5)–C(b6)	1.3587(19)	C(51)–C(52)	1.3900
C(b5)–H(b5)	0.9500	C(51)–C(56)	1.3900
C(b6)–H(b6)	0.9500	C(51)–C(57)	1.492(9)
C(b7)–C(b8)	1.3564(19)	C(52)–C(53)	1.3900
C(b7)–H(b7)	0.9500	C(53)–C(55)	1.3900
C(b8)–H(b8)	0.9500	C(55)–C(54)	1.3900
C(m1)–C(11)	1.4952(18)	C(54)–C(57)#1)	1.127(9)
C(m2)–C(21)	1.4924(18)	C(54)–C(56)	1.3900
C(m3)–C(31)	1.4981(17)	C(56)–C(57)#1)	0.892(7)
C(m4)–C(41)	1.4913(18)	C(56)–C(51)#1)	1.242(7)
C(11)–C(16)	1.390(2)	C(57)–C(56)#1)	0.892(8)
C(11)–C(12)	1.3924(19)	C(57)–C(54)#1)	1.127(11)
C(12)–C(13)	1.391(2)	C(61)–C(62)#2)	0.824(9)
C(12)–H(12)	0.9500	C(61)–C(63)#2)	0.869(12)
C(13)–C(14)	1.385(2)	C(61)–C(62)	1.3900
C(13)–H(13)	0.9500	C(61)–C(64)#2)	1.591(9)
C(14)–C(15)	1.384(2)	C(62)–C(66)#2)	0.722(7)
C(14)–H(14)	0.9500	C(62)–C(61)#2)	0.824(9)
C(15)–C(16)	1.395(2)	C(62)–C(63)	1.3900
C(15)–H(15)	0.9500	C(62)–C(65)#2)	1.591(14)
C(16)–H(16)	0.9500	C(62)–C(62)#2)	1.687(7)
C(21)–C(22)	1.394(2)	C(63)–C(61)#2)	0.869(11)
C(21)–C(26)	1.396(2)	C(63)–C(64)	1.3900
C(22)–C(23)	1.392(2)	C(63)–C(66)#2)	1.591(18)
C(22)–H(22)	0.9500	C(64)–C(65)	1.3900
C(23)–C(24)	1.381(3)	C(64)–C(61)#2)	1.591(10)
C(23)–H(23)	0.9500	C(65)–C(66)	1.3900
C(24)–C(25)	1.384(3)	C(65)–C(67)	1.400(14)
C(24)–H(24)	0.9500	C(65)–C(62)#2)	1.591(9)
C(25)–C(26)	1.392(2)	C(66)–C(62)#2)	0.722(7)
C(25)–H(25)	0.9500	C(66)–C(63)#2)	1.591(11)
C(26)–H(26)	0.9500		

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

Table S11. Bond Angles for [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8[a]

angle	degree	angle	degree
C(1)–Fe–N(1)	90.03(5)	C(33)–C(32)–C(31)	120.88(13)
C(1)–Fe–N(4)	92.80(5)	C(33)–C(32)–H(32)	119.6
N(1)–Fe–N(4)	89.22(4)	C(31)–C(32)–H(32)	119.6
C(1)–Fe–N(3)	90.32(5)	C(34)–C(33)–C(32)	119.73(13)
N(1)–Fe–N(3)	179.56(4)	C(34)–C(33)–H(33)	120.1
N(4)–Fe–N(3)	90.51(4)	C(32)–C(33)–H(33)	120.1
C(1)–Fe–N(2)	89.32(5)	C(35)–C(34)–C(33)	119.93(13)
N(1)–Fe–N(2)	90.21(4)	C(35)–C(34)–H(34)	120.0
N(4)–Fe–N(2)	177.81(5)	C(33)–C(34)–H(34)	120.0
N(3)–Fe–N(2)	90.05(4)	C(34)–C(35)–C(36)	120.17(13)
C(1)–Fe–N(5)	175.42(5)	C(34)–C(35)–H(35)	119.9
N(1)–Fe–N(5)	90.82(5)	C(36)–C(35)–H(35)	119.9
N(4)–Fe–N(5)	91.72(4)	C(31)–C(36)–C(35)	120.54(13)
N(3)–Fe–N(5)	88.85(5)	C(31)–C(36)–H(36)	119.7
N(2)–Fe–N(5)	86.18(4)	C(35)–C(36)–H(36)	119.7
C(a2)–N(1)–C(a1)	105.99(11)	C(46)–C(41)–C(42)	119.04(13)
C(a2)–N(1)–Fe	126.64(9)	C(46)–C(41)–C(m4)	119.64(12)
C(a1)–N(1)–Fe	126.61(9)	C(42)–C(41)–C(m4)	121.26(12)
C(a4)–N(2)–C(a3)	106.30(10)	C(43)–C(42)–C(41)	120.33(14)
C(a4)–N(2)–Fe	127.08(9)	C(43)–C(42)–H(42)	119.8
C(a3)–N(2)–Fe	126.40(9)	C(41)–C(42)–H(42)	119.8
C(a5)–N(3)–C(a6)	105.96(10)	C(44)–C(43)–C(42)	120.17(14)
C(a5)–N(3)–Fe	126.74(9)	C(44)–C(43)–H(43)	119.9
C(a6)–N(3)–Fe	126.68(9)	C(42)–C(43)–H(43)	119.9
C(a8)–N(4)–C(a7)	105.71(10)	C(45)–C(44)–C(43)	119.58(14)
C(a8)–N(4)–Fe	127.36(8)	C(45)–C(44)–H(44)	120.2
C(a7)–N(4)–Fe	126.93(9)	C(43)–C(44)–H(44)	120.2
N(1)–C(a1)–C(m4)	124.96(12)	C(44)–C(45)–C(46)	120.61(15)
N(1)–C(a1)–C(b1)	109.96(11)	C(44)–C(45)–H(45)	119.7
C(m4)–C(a1)–C(b1)	124.72(12)	C(46)–C(45)–H(45)	119.7
N(1)–C(a2)–C(m1)	126.15(12)	C(45)–C(46)–C(41)	120.22(14)
N(1)–C(a2)–C(b2)	110.23(11)	C(45)–C(46)–H(46)	119.9
C(m1)–C(a2)–C(b2)	123.41(12)	C(41)–C(46)–H(46)	119.9
N(2)–C(a3)–C(m1)	125.34(12)	O(1)–C(1)–Fe	175.96(13)

Table S11. Continued

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	109.91(11)	N(5)–C(2)–N(6)	109.83(13)
C(m1)–C(a3)–C(b3)	124.60(12)	N(5)–C(2)–C(5)	128.34(13)
N(2)–C(a4)–C(m2)	125.61(12)	N(6)–C(2)–C(5)	121.82(13)
N(2)–C(a4)–C(b4)	109.68(11)	C(4)–C(3)–N(6)	105.38(14)
C(m2)–C(a4)–C(b4)	124.49(12)	C(4)–C(3)–H(3)	127.3
N(3)–C(a5)–C(m2)	125.33(12)	N(6)–C(3)–H(3)	127.3
N(3)–C(a5)–C(b5)	109.86(11)	C(3)–C(4)–N(5)	109.95(14)
C(m2)–C(a5)–C(b5)	124.73(12)	C(3)–C(4)–H(4)	125.0
N(3)–C(a6)–C(m3)	125.76(12)	N(5)–C(4)–H(4)	125.0
N(3)–C(a6)–C(b6)	110.17(11)	C(2)–N(5)–C(4)	105.89(12)
C(m3)–C(a6)–C(b6)	124.01(12)	C(2)–N(5)–Fe	133.68(10)
N(4)–C(a7)–C(m3)	125.46(11)	C(4)–N(5)–Fe	120.02(9)
N(4)–C(a7)–C(b7)	110.17(11)	C(2)–C(5)–H(5a)	109.5
C(m3)–C(a7)–C(b7)	123.95(12)	C(2)–C(5)–H(5b)	109.5
N(4)–C(a8)–C(m4)	125.44(11)	H(5a)–C(5)–H(5b)	109.5
N(4)–C(a8)–C(b8)	110.14(11)	C(2)–C(5)–H(5c)	109.5
C(m4)–C(a8)–C(b8)	124.40(12)	H(5a)–C(5)–H(5c)	109.5
C(b2)–C(b1)–C(a1)	106.81(12)	H(5b)–C(5)–H(5c)	109.5
C(b2)–C(b1)–H(b1)	126.6	C(2)–N(6)–C(3)	108.95(13)
C(a1)–C(b1)–H(b1)	126.6	C(2)–N(6)–H(6)	121(2)
C(b1)–C(b2)–C(a2)	106.88(12)	C(3)–N(6)–H(6)	130(2)
C(b1)–C(b2)–H(b2)	126.6	C(56)#1–C(51)–C(52)	146.2(5)
C(a2)–C(b2)–H(b2)	126.6	C(56)#1–C(51)–C(56)	86.9(6)
C(b4)–C(b3)–C(a3)	106.91(12)	C(52)–C(51)–C(56)	120.0
C(b4)–C(b3)–H(b3)	126.5	C(52)–C(51)–C(57)	120.8(4)
C(a3)–C(b3)–H(b3)	126.5	C(56)–C(51)–C(57)	119.1(4)
C(b3)–C(b4)–C(a4)	107.15(12)	C(52)–C(51)–C(51)#1	154.5(3)
C(b3)–C(b4)–H(b4)	126.4	C(57)–C(51)–C(51)#1	80.4(4)
C(a4)–C(b4)–H(b4)	126.4	C(53)–C(52)–C(51)	120.0
C(b6)–C(b5)–C(a5)	107.14(12)	C(52)–C(53)–C(55)	120.0
C(b6)–C(b5)–H(b5)	126.4	C(54)–C(55)–C(53)	120.0
C(a5)–C(b5)–H(b5)	126.4	C(57)#1–C(54)–C(55)	148.7(4)
C(b5)–C(b6)–C(a6)	106.84(11)	C(55)–C(54)–C(56)	120.0
C(b5)–C(b6)–H(b6)	126.6	C(57)#1–C(56)–C(51)#1	87.1(7)

Table S11. Continued

angle	degree	angle	degree
C(a6)–C(b6)–H(b6)	126.6	C(57)#1–C(56)–C(54)	54.0(6)
C(b8)–C(b7)–C(a7)	106.95(11)	C(51)#1–C(56)–C(54)	141.1(5)
C(b8)–C(b7)–H(b7)	126.5	C(57)#1–C(56)–C(51)	152.7(5)
C(a7)–C(b7)–H(b7)	126.5	C(51)#1–C(56)–C(51)	93.1(5)
C(b7)–C(b8)–C(a8)	106.83(11)	C(54)–C(56)–C(51)	120.0
C(b7)–C(b8)–H(b8)	126.6	C(57)#1–C(56)–C(56)#1	130.3(7)
C(a8)–C(b8)–H(b8)	126.6	C(54)–C(56)–C(56)#1	156.3(3)
C(a3)–C(m1)–C(a2)	122.97(12)	C(56)#1–C(57)–C(54)#1	86.2(8)
C(a3)–C(m1)–C(11)	120.01(11)	C(56)#1–C(57)–C(51)	56.2(6)
C(a2)–C(m1)–C(11)	117.00(12)	C(54)#1–C(57)–C(51)	142.3(6)
C(a4)–C(m2)–C(a5)	123.46(12)	C(62)#2–C(61)–C(63)#2	110.3(11)
C(a4)–C(m2)–C(21)	118.22(12)	C(62)#2–C(61)–C(62)	95.9(6)
C(a5)–C(m2)–C(21)	118.16(12)	C(63)#2–C(61)–C(62)	153.7(9)
C(a7)–C(m3)–C(a6)	123.48(12)	C(63)#2–C(61)–C(66)	86.3(9)
C(a7)–C(m3)–C(31)	118.73(11)	C(62)–C(61)–C(66)	120.0
C(a6)–C(m3)–C(31)	117.40(11)	C(62)#2–C(61)–C(61)#2	63.8(6)
C(a1)–C(m4)–C(a8)	122.79(12)	C(63)#2–C(61)–C(61)#2	173.8(10)
C(a1)–C(m4)–C(41)	118.10(11)	C(66)–C(61)–C(61)#2	87.9(3)
C(a8)–C(m4)–C(41)	119.09(11)	C(62)#2–C(61)–C(64)#2	170.8(12)
C(16)–C(11)–C(12)	118.75(13)	C(63)#2–C(61)–C(64)#2	60.7(5)
C(16)–C(11)–C(m1)	118.62(12)	C(62)–C(61)–C(64)#2	93.0(8)
C(12)–C(11)–C(m1)	122.61(13)	C(66)–C(61)–C(64)#2	147.0(8)
C(13)–C(12)–C(11)	120.27(14)	C(61)#2–C(61)–C(64)#2	125.1(9)
C(13)–C(12)–H(12)	119.9	C(62)#2–C(61)–C(66)#2	106.7(10)
C(11)–C(12)–H(12)	119.9	C(63)#2–C(61)–C(66)#2	142.8(8)
C(14)–C(13)–C(12)	120.52(14)	C(66)–C(61)–C(66)#2	130.9(5)
C(14)–C(13)–H(13)	119.7	C(64)#2–C(61)–C(66)#2	82.1(4)
C(12)–C(13)–H(13)	119.7	C(66)#2–C(62)–C(61)#2	128(2)
C(15)–C(14)–C(13)	119.72(13)	C(66)#2–C(62)–C(61)	147.8(17)
C(15)–C(14)–H(14)	120.1	C(61)#2–C(62)–C(61)	84.1(7)
C(13)–C(14)–H(14)	120.1	C(66)#2–C(62)–C(63)	92.2(17)
C(14)–C(15)–C(16)	119.75(15)	C(61)–C(62)–C(63)	120.0
C(14)–C(15)–H(15)	120.1	C(66)#2–C(62)–C(65)#2	60.8(10)
C(16)–C(15)–H(15)	120.1	C(61)#2–C(62)–C(65)#2	170.9(14)

Table S11. Continued

angle	degree	angle	degree
C(11)–C(16)–C(15)	120.96(14)	C(61)–C(62)–C(65)#2	87.0(8)
C(11)–C(16)–H(16)	119.5	C(63)–C(62)–C(65)#2	153.0(8)
C(15)–C(16)–H(16)	119.5	C(66)#2–C(62)–C(62)#2	176.1(17)
C(22)–C(21)–C(26)	118.74(13)	C(63)–C(62)–C(62)#2	90.9(3)
C(22)–C(21)–C(m2)	120.52(13)	C(65)#2–C(62)–C(62)#2	116.0(9)
C(26)–C(21)–C(m2)	120.73(13)	C(61)#2–C(63)–C(64)	86.3(5)
C(23)–C(22)–C(21)	120.55(16)	C(64)–C(63)–C(62)	120.0
C(23)–C(22)–H(22)	119.7	C(61)#2–C(63)–C(66)#2	60.7(7)
C(21)–C(22)–H(22)	119.7	C(64)–C(63)–C(66)#2	147.0(5)
C(24)–C(23)–C(22)	120.22(17)	C(65)–C(64)–C(63)	120.0
C(24)–C(23)–H(23)	119.9	C(65)–C(64)–C(61)#2	87.0(3)
C(22)–C(23)–H(23)	119.9	C(64)–C(65)–C(66)	120.0
C(23)–C(24)–C(25)	119.77(15)	C(64)–C(65)–C(67)	118.4(8)
C(23)–C(24)–H(24)	120.1	C(66)–C(65)–C(67)	121.5(8)
C(25)–C(24)–H(24)	120.1	C(64)–C(65)–C(62)#2	93.0(3)
C(24)–C(25)–C(26)	120.38(16)	C(67)–C(65)–C(62)#2	148.4(9)
C(24)–C(25)–H(25)	119.8	C(62)#2–C(66)–C(65)	92.2(8)
C(26)–C(25)–H(25)	119.8	C(65)–C(66)–C(61)	120.0
C(25)–C(26)–C(21)	120.32(15)	C(62)#2–C(66)–C(63)#2	60.8(8)
C(25)–C(26)–H(26)	119.8	C(65)–C(66)–C(63)#2	153.0(5)
C(21)–C(26)–H(26)	119.8	C(65)–C(66)–C(61)#2	70.9(3)
C(36)–C(31)–C(32)	118.70(12)	C(63)#2–C(66)–C(61)#2	82.2(4)
C(36)–C(31)–C(m3)	121.01(12)		
C(32)–C(31)–C(m3)	120.24(12)		

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

Table S12. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe	0.0112(1)	0.0126(1)	0.0144(1)	−0.0022(1)	0.0028(1)	−0.0012(1)
N(1)	0.0135(5)	0.0143(4)	0.0167(5)	−0.0028(4)	0.0040(4)	−0.0026(4)
N(2)	0.0131(5)	0.0144(4)	0.0168(5)	−0.0023(4)	0.0037(4)	−0.0016(4)
N(3)	0.0128(4)	0.0148(4)	0.0170(5)	−0.0021(4)	0.0038(4)	−0.0015(4)
N(4)	0.0130(4)	0.0141(4)	0.0160(5)	−0.0025(3)	0.0041(4)	−0.0012(4)
C(a1)	0.0142(5)	0.0174(5)	0.0176(5)	−0.0038(4)	0.0053(4)	−0.0020(4)
C(a2)	0.0152(5)	0.0159(5)	0.0179(6)	−0.0048(4)	0.0047(4)	−0.0016(4)
C(a3)	0.0148(5)	0.0141(5)	0.0178(5)	−0.0028(4)	0.0035(4)	−0.0016(4)
C(a4)	0.0134(5)	0.0158(5)	0.0186(6)	−0.0013(4)	0.0030(4)	−0.0025(4)
C(a5)	0.0129(5)	0.0172(5)	0.0178(5)	−0.0007(4)	0.0042(4)	−0.0010(4)
C(a6)	0.0151(5)	0.0155(5)	0.0158(5)	−0.0016(4)	0.0049(4)	−0.0001(4)
C(a7)	0.0143(5)	0.0142(5)	0.0156(5)	−0.0022(4)	0.0027(4)	−0.0013(4)
C(a8)	0.0133(5)	0.0136(5)	0.0180(5)	−0.0020(4)	0.0035(4)	−0.0014(4)
C(b1)	0.0189(6)	0.0227(6)	0.0213(6)	−0.0072(5)	0.0096(5)	−0.0055(5)
C(b2)	0.0193(6)	0.0225(6)	0.0230(6)	−0.0094(5)	0.0095(5)	−0.0043(5)
C(b3)	0.0181(6)	0.0153(5)	0.0247(6)	−0.0042(5)	0.0052(5)	−0.0035(5)
C(b4)	0.0171(6)	0.0170(6)	0.0257(6)	−0.0039(5)	0.0052(5)	−0.0049(5)
C(b5)	0.0148(5)	0.0202(6)	0.0212(6)	−0.0015(5)	0.0067(5)	−0.0003(5)
C(b6)	0.0161(6)	0.0193(6)	0.0195(6)	−0.0020(4)	0.0080(5)	0.0001(5)
C(b7)	0.0165(6)	0.0148(5)	0.0183(6)	−0.0037(4)	0.0030(4)	−0.0021(4)
C(b8)	0.0150(5)	0.0141(5)	0.0206(6)	−0.0027(4)	0.0037(4)	−0.0022(4)
C(m1)	0.0155(5)	0.0152(5)	0.0181(5)	−0.0038(4)	0.0032(4)	−0.0013(4)
C(m2)	0.0127(5)	0.0174(5)	0.0197(6)	−0.0014(4)	0.0036(4)	−0.0024(4)
C(m3)	0.0155(5)	0.0138(5)	0.0164(5)	−0.0019(4)	0.0046(4)	−0.0002(4)
C(m4)	0.0137(5)	0.0156(5)	0.0186(6)	−0.0021(4)	0.0046(4)	−0.0027(4)
C(11)	0.0164(6)	0.0164(5)	0.0227(6)	−0.0050(5)	0.0067(5)	−0.0027(4)
C(12)	0.0254(7)	0.0175(6)	0.0222(6)	−0.0041(5)	0.0048(5)	−0.0010(5)
C(13)	0.0315(8)	0.0192(6)	0.0238(7)	−0.0063(5)	0.0085(6)	−0.0037(6)
C(14)	0.0244(7)	0.0167(6)	0.0341(8)	−0.0074(5)	0.0150(6)	−0.0030(5)
C(15)	0.0206(7)	0.0244(7)	0.0390(9)	−0.0070(6)	0.0051(6)	0.0043(6)
C(16)	0.0200(6)	0.0257(7)	0.0298(7)	−0.0098(6)	0.0011(6)	0.0017(5)
C(21)	0.0148(6)	0.0173(5)	0.0265(6)	−0.0041(5)	0.0063(5)	−0.0023(5)
C(22)	0.0220(7)	0.0325(8)	0.0302(8)	−0.0011(6)	0.0098(6)	−0.0064(6)
C(23)	0.0291(8)	0.0372(9)	0.0444(10)	−0.0013(7)	0.0205(8)	−0.0091(7)

Table S12. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.0184(7)	0.0299(8)	0.0540(11)	−0.0098(7)	0.0139(7)	−0.0077(6)
C(25)	0.0146(6)	0.0261(7)	0.0423(9)	−0.0120(6)	0.0033(6)	−0.0022(5)
C(26)	0.0157(6)	0.0213(6)	0.0284(7)	−0.0060(5)	0.0036(5)	−0.0012(5)
C(31)	0.0148(5)	0.0155(5)	0.0182(5)	−0.0036(4)	0.0057(4)	−0.0012(4)
C(32)	0.0221(6)	0.0179(6)	0.0192(6)	−0.0005(5)	0.0057(5)	0.0013(5)
C(33)	0.0237(7)	0.0171(6)	0.0263(7)	−0.0026(5)	0.0080(5)	0.0014(5)
C(34)	0.0241(7)	0.0206(6)	0.0244(6)	−0.0071(5)	0.0112(5)	−0.0018(5)
C(35)	0.0325(8)	0.0232(6)	0.0188(6)	−0.0033(5)	0.0107(6)	−0.0016(6)
C(36)	0.0270(7)	0.0178(6)	0.0201(6)	−0.0009(5)	0.0080(5)	0.0006(5)
C(41)	0.0175(6)	0.0174(5)	0.0190(6)	−0.0051(4)	0.0071(5)	−0.0044(5)
C(42)	0.0173(6)	0.0223(6)	0.0241(6)	−0.0038(5)	0.0072(5)	−0.0038(5)
C(43)	0.0178(6)	0.0291(7)	0.0285(7)	−0.0076(6)	0.0099(5)	−0.0059(5)
C(44)	0.0259(7)	0.0285(7)	0.0277(7)	−0.0091(6)	0.0142(6)	−0.0129(6)
C(45)	0.0315(8)	0.0209(6)	0.0291(7)	−0.0017(5)	0.0126(6)	−0.0079(6)
C(46)	0.0229(7)	0.0186(6)	0.0283(7)	−0.0019(5)	0.0097(6)	−0.0028(5)
C(1)	0.0156(5)	0.0175(6)	0.0209(6)	−0.0039(4)	0.0045(5)	−0.0009(4)
O(1)	0.0326(6)	0.0304(6)	0.0269(6)	0.0042(4)	−0.0004(5)	0.0066(5)
C(2)	0.0199(6)	0.0226(6)	0.0196(6)	0.0005(5)	0.0028(5)	0.0023(5)
C(3)	0.0312(8)	0.0288(7)	0.0279(7)	0.0084(6)	0.0045(6)	−0.0040(6)
C(4)	0.0235(7)	0.0249(7)	0.0229(6)	0.0034(5)	0.0043(5)	−0.0033(5)
N(5)	0.0174(5)	0.0182(5)	0.0171(5)	−0.0016(4)	0.0031(4)	−0.0001(4)
C(5)	0.0171(6)	0.0348(8)	0.0306(8)	0.0063(6)	0.0015(6)	−0.0003(6)
N(6)	0.0245(6)	0.0283(6)	0.0253(6)	0.0083(5)	0.0001(5)	0.0031(5)
C(51)	0.079(4)	0.077(4)	0.033(2)	0.001(2)	0.003(2)	0.015(3)
C(52)	0.096(5)	0.064(3)	0.059(3)	−0.008(3)	−0.007(3)	0.027(3)
C(53)	0.153(7)	0.057(3)	0.052(3)	−0.010(3)	−0.015(4)	0.016(4)
C(55)	0.116(6)	0.083(4)	0.049(3)	−0.014(3)	−0.016(3)	0.014(4)
C(54)	0.096(5)	0.071(4)	0.046(3)	−0.012(2)	0.006(3)	0.000(4)
C(56)	0.119(6)	0.058(3)	0.040(2)	0.002(2)	0.011(3)	0.023(4)
C(57)	0.117(6)	0.061(4)	0.059(3)	−0.013(3)	0.007(4)	0.012(4)
C(61)	0.108(7)	0.108(7)	0.051(4)	−0.010(4)	0.041(4)	−0.047(6)
C(62)	0.242(17)	0.115(8)	0.092(7)	−0.062(6)	0.127(10)	−0.120(11)
C(63)	0.271(16)	0.093(6)	0.058(4)	0.031(4)	0.105(8)	0.059(8)
C(64)	0.293(18)	0.134(9)	0.066(5)	−0.045(5)	0.106(8)	−0.114(11)

Table S12. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(65)	0.106(6)	0.107(6)	0.036(3)	−0.015(3)	0.029(3)	−0.005(5)
C(66)	0.095(5)	0.107(6)	0.042(3)	−0.031(4)	0.032(3)	−0.028(5)
C(67)	0.132(10)	0.216(15)	0.082(6)	−0.038(8)	0.037(6)	−0.014(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 S13. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(CO)(2-MeHIm)]·C_7H_8[a]

atom	x	y	z	U(eq)
H(b1	0.0555	0.2004	0.7898	0.024
H(b2	0.1365	0.2966	0.8251	0.025
H(b3	0.4771	0.3929	0.7692	0.023
H(b4	0.6287	0.3535	0.7176	0.024
H(b5	0.6785	0.1733	0.5046	0.022
H(b6	0.5537	0.1031	0.4055	0.021
H(b7	0.1636	0.0405	0.3887	0.020
H(b8	0.0501	0.0545	0.5013	0.020
H(12)	0.3875	0.3667	0.9179	0.026
H(13)	0.3381	0.4500	0.9840	0.030
H(14)	0.1996	0.5055	0.8942	0.028
H(15)	0.1055	0.4756	0.7395	0.034
H(16)	0.1529	0.3913	0.6741	0.031
H(22)	0.6760	0.2831	0.4775	0.033
H(23)	0.8479	0.3115	0.4860	0.042
H(24)	0.9736	0.3140	0.6352	0.040
H(25)	0.9279	0.2874	0.7764	0.034
H(26)	0.7565	0.2585	0.7690	0.027
H(32)	0.3999	−0.0067	0.4631	0.024
H(33)	0.4285	−0.0757	0.3542	0.027
H(34)	0.4008	−0.0529	0.1895	0.027
H(35)	0.3428	0.0383	0.1341	0.029
H(36)	0.3183	0.1079	0.2437	0.026
H(42)	−0.0815	0.1692	0.6228	0.025
H(43)	−0.2143	0.1212	0.6717	0.029
H(44)	−0.1800	0.0327	0.7496	0.031
H(45)	−0.0150	−0.0092	0.7721	0.032
H(46)	0.1165	0.0368	0.7188	0.027
H(3)	0.2963	0.3640	0.3627	0.036
H(4)	0.4098	0.2995	0.4830	0.029
H(5a)	0.0685	0.2442	0.5183	0.043
H(5b)	0.0816	0.2001	0.4366	0.043
H(5c)	0.0167	0.2579	0.4061	0.043
H(6)	0.120(2)	0.3254(12)	0.350(2)	0.060(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 S14. Complete Crystallographic Details for [Fe(TPP)(CO)(1,2-DiMeIm)]

formula	$C_{50}H_{36}FeN_6O$
FW, amu	792.70
a, Å	15.0577(8)
b, Å	18.8294(10)
c, Å	13.7197(7)
β, deg	102.8940(10)
V, Å^3	3791.8(3)
space group	C2/c
Z	4
D_c, g/cm^3	1.389
F(000)	1648
μ, mm^{-1}	0.447
crystal dimensions, mm	0.4 × 0.3 × 0.2
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.76–28.29
index range	$-19 \leq h \leq 20$
	$-25 \leq k \leq 25$
	$-18 \leq l \leq 18$
total data collected	20612
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	1.0000 and 0.8883
unique data	4695 (R_{int} = 0.0376)
unique observed data [I > 2σ(I)]	4169
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	4695/0/294
goodness-of-fit (pased on F^2)	1.052
final R indices [I > 2σ(I)]	R_1 = 0.0406, wR_2 = 0.1073
final R indices (all data)	R_1 = 0.0453, wR_2 = 0.1115

Table S15. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1,2-DiMeIm)][a]

atom	x	y	z	U(eq)
Fe	1.0000	0.87267(1)	0.2500	0.0182(1)
N(1)	0.86716(8)	0.87229(6)	0.18397(9)	0.0202(2)
N(2)	0.96876(9)	0.87341(6)	0.38463(9)	0.0208(2)
C(a4)	1.02836(10)	0.87507(7)	0.47692(11)	0.0215(3)
C(a3)	0.88284(10)	0.87072(8)	0.40451(11)	0.0224(3)
C(a2)	0.79480(10)	0.87565(8)	0.23045(11)	0.0221(3)
C(a1)	0.82929(10)	0.87760(7)	0.08311(11)	0.0218(3)
C(b4)	0.97883(11)	0.86997(8)	0.55564(12)	0.0255(3)
C(b3)	0.88937(11)	0.86733(8)	0.51096(12)	0.0265(3)
C(b2)	0.71033(10)	0.88365(9)	0.15694(12)	0.0267(3)
C(b1)	0.73164(10)	0.88467(9)	0.06629(12)	0.0260(3)
C(m1)	0.80068(10)	0.87300(8)	0.33349(12)	0.0229(3)
C(m2)	0.87682(10)	0.87740(7)	0.00633(11)	0.0215(3)
C(11)	0.71360(11)	0.87712(9)	0.36925(12)	0.0285(3)
C(12)	0.69517(12)	0.93678(11)	0.42203(13)	0.0368(4)
C(13)	0.61222(13)	0.94308(13)	0.45050(15)	0.0485(5)
C(14)	0.54796(12)	0.89050(16)	0.42686(14)	0.0548(6)
C(15)	0.56566(13)	0.83104(16)	0.37676(15)	0.0543(6)
C(16)	0.64882(12)	0.82376(12)	0.34781(14)	0.0407(4)
C(21)	0.82290(10)	0.87614(8)	−0.09959(11)	0.0221(3)
C(22)	0.82735(10)	0.93234(8)	−0.16480(11)	0.0255(3)
C(23)	0.77853(11)	0.92988(9)	−0.26388(12)	0.0295(3)
C(24)	0.72479(11)	0.87124(9)	−0.29894(12)	0.0296(3)
C(25)	0.71997(10)	0.81513(9)	−0.23451(12)	0.0285(3)
C(26)	0.76871(10)	0.81737(8)	−0.13583(11)	0.0259(3)
C(1)	1.0000	0.96634(11)	0.2500	0.0212(4)
O(1)	1.0000	1.02677(9)	0.2500	0.0314(4)
C(3)	0.9781(2)	0.65576(17)	0.1523(2)	0.0252(6)
C(4)	0.9760(2)	0.72646(18)	0.1407(3)	0.0239(6)
N(5)	0.9969(6)	0.76005(13)	0.2329(3)	0.0205(10)
C(2)	1.01118(19)	0.70785(16)	0.3001(3)	0.0206(5)
N(6)	1.0000	0.64359(10)	0.2500	0.0240(4)
C(5)	1.0368(2)	0.71493(18)	0.4095(3)	0.0264(7)
C(6)	1.0140(3)	0.57362(17)	0.2996(3)	0.0332(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 S16. Bond Lengths for [Fe(TPP)(CO)(1,2-DiMeIm)][a]

bond	length (Å)	bond	length (Å)
Fe–C(1)	1.764(2)	C(23)–H(23)	0.9500
Fe–N(1)	2.0032(12)	C(24)–C(25)	1.390(2)
Fe–N(1)#1)	2.0032(12)	C(24)–H(24)	0.9500
Fe–N(2)	2.0052(13)	C(25)–C(26)	1.389(2)
Fe–N(2)#1)	2.0052(13)	C(25)–H(25)	0.9500
Fe–N(5)#1)	2.133(2)	C(26)–H(26)	0.9500
Fe–N(5)	2.133(2)	C(1)–O(1)	1.138(3)
N(1)–C(a1)	1.3776(18)	C(3)–C(2)#1)	1.170(4)
N(1)–C(a2)	1.3812(18)	C(3)–N(6)	1.327(3)
N(2)–C(a4)	1.3793(19)	C(3)–C(4)	1.340(5)
N(2)–C(a3)	1.3815(19)	C(3)–C(5)#1)	1.388(5)
C(a4)–C(m2#1)	1.395(2)	C(3)–C(6)#1)	1.675(4)
C(a4)–C(b4)	1.446(2)	C(3)–H(2)	0.9246
C(a3)–C(m1)	1.394(2)	C(4)–C(5)#1)	0.707(4)
C(a3)–C(b3)	1.443(2)	C(4)–C(2)#1)	0.866(4)
C(a2)–C(m1)	1.398(2)	C(4)–N(5)	1.387(5)
C(a2)–C(b2)	1.444(2)	C(4)–N(5)#1)	1.805(6)
C(a1)–C(m2)	1.399(2)	C(4)–H(3)	1.0967
C(a1)–C(b1)	1.443(2)	N(5)–N(5)#1)	0.457(7)
C(b4)–C(b3)	1.351(2)	N(5)–C(2)#1)	1.078(4)
C(b4)–H(b4)	0.9500	N(5)–C(2)	1.331(4)
C(b3)–H(b3)	0.9500	N(5)–C(4)#1)	1.805(6)
C(b2)–C(b1)	1.352(2)	C(2)–C(4)#1)	0.866(4)
C(b2)–H(b2)	0.9500	C(2)–N(5)#1)	1.078(4)
C(b1)–H(b1)	0.9500	C(2)–C(3)#1)	1.170(4)
C(m1)–C(11)	1.501(2)	C(2)–C(2)#1)	1.339(7)
C(m2)–C(a4#1)	1.395(2)	C(2)–N(6)	1.383(4)
C(m2)–C(21)	1.498(2)	C(2)–C(5)	1.471(5)
C(11)–C(16)	1.385(3)	N(6)–C(3)#1)	1.327(3)
C(11)–C(12)	1.398(3)	N(6)–C(2)#1)	1.383(4)
C(12)–C(13)	1.394(2)	N(6)–C(6)#1)	1.476(3)
C(12)–H(12)	0.9500	N(6)–C(6)	1.476(3)
C(13)–C(14)	1.372(4)	C(5)–C(4)#1)	0.707(4)
C(13)–H(13)	0.9500	C(5)–C(3)#1)	1.388(5)

Table S16. Continued

bond	length (Å)	bond	length (Å)
C(14)–C(15)	1.371(4)	C(5)–H(4a)	0.8167
C(14)–H(14)	0.9500	C(5)–H(4b)	0.8807
C(15)–C(16)	1.402(3)	C(5)–H(4c)	0.9619
C(15)–H(15)	0.9500	C(6)–C(6)#1)	1.332(7)
C(16)–H(16)	0.9028	C(6)–C(3)#1)	1.675(4)
C(21)–C(22)	1.397(2)	C(6)–H(5a)	0.9472
C(21)–C(26)	1.399(2)	C(6)–H(5b)	0.8458
C(22)–C(23)	1.394(2)	C(6)–H(5c)	0.9181
C(22)–H(22)	0.9500		
C(23)–C(24)	1.390(2)		

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

Table S17. Bond Angles for [Fe(TPP)(CO)(1,2-DiMeIm)][a]

angle	degree	angle	degree
C(1)–Fe–N(1)	90.21(3)	C(2)#1–C(3)–C(6)#1	124.4(3)
C(1)–Fe–N(1)#1	90.21(3)	N(6)–C(3)–C(6)#1	57.51(17)
N(1)–Fe–N(1)#1	179.58(7)	C(4)–C(3)–C(6)#1	164.0(3)
C(1)–Fe–N(2)	89.60(3)	C(5)#1–C(3)–C(6)#1	165.8(3)
N(1)–Fe–N(2)	90.05(5)	C(2)#1–C(3)–H(2)	173.8
N(1)#1–Fe–N(2)	89.96(5)	N(6)–C(3)–H(2)	119.3
C(1)–Fe–N(2)#1	89.60(3)	C(4)–C(3)–H(2)	134.1
N(1)–Fe–N(2)#1	89.96(5)	C(5)#1–C(3)–H(2)	104.2
N(1)#1–Fe–N(2)#1	90.05(5)	C(6)#1–C(3)–H(2)	61.8
N(2)–Fe–N(2)#1	179.21(7)	C(5)#1–C(4)–C(2)#1	138.2(6)
C(1)–Fe–N(5)#1	173.85(9)	C(5)#1–C(4)–C(3)	78.7(5)
N(1)–Fe–N(5)#1	92.4(2)	C(2)#1–C(4)–C(3)	59.5(3)
N(1)#1–Fe–N(5)#1	87.2(2)	C(5)#1–C(4)–N(5)	170.6(5)
N(2)–Fe–N(5)#1	84.81(13)	C(2)#1–C(4)–N(5)	51.0(3)
N(2)#1–Fe–N(5)#1	95.98(13)	C(3)–C(4)–N(5)	110.5(3)
C(1)–Fe–N(5)	173.85(9)	C(5)#1–C(4)–N(5)#1	176.3(5)
N(1)–Fe–N(5)	87.2(2)	C(3)–C(4)–N(5)#1	103.9(3)
N(1)#1–Fe–N(5)	92.4(2)	C(5)#1–C(4)–H(3)	53.4
N(2)–Fe–N(5)	95.98(13)	C(2)#1–C(4)–H(3)	166.0
N(2)#1–Fe–N(5)	84.81(13)	C(3)–C(4)–H(3)	130.5
N(5)#1–Fe–N(5)	12.29(18)	N(5)–C(4)–H(3)	117.9
C(a1)–N(1)–C(a2)	105.55(12)	N(5)#1–C(4)–H(3)	124.6
C(a1)–N(1)–Fe	126.99(10)	N(5)#1–N(5)–C(2)#1	114.1(3)
C(a2)–N(1)–Fe	127.01(10)	N(5)#1–N(5)–C(2)	47.6(2)
C(a4)–N(2)–C(a3)	105.41(12)	C(2)#1–N(5)–C(2)	66.6(4)
C(a4)–N(2)–Fe	127.41(10)	N(5)#1–N(5)–C(4)	152.7(3)
C(a3)–N(2)–Fe	127.17(10)	C(2)–N(5)–C(4)	105.3(3)
N(2)–C(a4)–C(m2#1	125.74(14)	C(2)#1–N(5)–C(4)#1	93.7(3)
N(2)–C(a4)–C(b4)	110.23(13)	C(4)–N(5)–C(4)#1	132.3(3)
C(m2#1–C(a4)–C(b4)	123.94(14)	N(5)#1–N(5)–Fe	83.85(9)
N(2)–C(a3)–C(m1)	125.80(14)	C(2)#1–N(5)–Fe	161.9(3)
N(2)–C(a3)–C(b3)	110.25(13)	C(2)–N(5)–Fe	131.4(3)
C(m1)–C(a3)–C(b3)	123.93(14)	C(4)–N(5)–Fe	123.3(2)
N(1)–C(a2)–C(m1)	125.95(14)	C(4)#1–N(5)–Fe	104.38(19)

Table S17. Continued

angle	degree	angle	degree
N(1)–C(a2)–C(b2)	110.18(13)	C(4)#1–C(2)–N(5)#1	90.3(4)
C(m1)–C(a2)–C(b2)	123.86(14)	C(4)#1–C(2)–C(3)#1	80.8(3)
N(1)–C(a1)–C(m2)	126.11(14)	N(5)#1–C(2)–C(3)#1	171.2(4)
N(1)–C(a1)–C(b1)	110.25(13)	C(4)#1–C(2)–N(5)	108.5(4)
C(m2)–C(a1)–C(b1)	123.64(14)	C(3)#1–C(2)–N(5)	170.6(4)
C(b3)–C(b4)–C(a4)	106.96(13)	C(4)#1–C(2)–C(2)#1	156.1(3)
C(b3)–C(b4)–H(b4)	126.5	N(5)#1–C(2)–C(2)#1	65.8(2)
C(a4)–C(b4)–H(b4)	126.5	C(3)#1–C(2)–C(2)#1	123.0(2)
C(b4)–C(b3)–C(a3)	107.07(13)	N(5)–C(2)–C(2)#1	47.6(2)
C(b4)–C(b3)–H(b3)	126.5	C(4)#1–C(2)–N(6)	142.8(4)
C(a3)–C(b3)–H(b3)	126.5	N(5)#1–C(2)–N(6)	126.8(3)
C(b1)–C(b2)–C(a2)	106.92(13)	C(3)#1–C(2)–N(6)	62.0(2)
C(b1)–C(b2)–H(b2)	126.5	N(5)–C(2)–N(6)	108.6(3)
C(a2)–C(b2)–H(b2)	126.5	C(2)#1–C(2)–N(6)	61.04(14)
C(b2)–C(b1)–C(a1)	107.10(13)	N(5)#1–C(2)–C(5)	109.0(3)
C(b2)–C(b1)–H(b1)	126.4	C(3)#1–C(2)–C(5)	62.2(3)
C(a1)–C(b1)–H(b1)	126.4	N(5)–C(2)–C(5)	127.2(3)
C(a3)–C(m1)–C(a2)	123.64(14)	C(2)#1–C(2)–C(5)	174.75(18)
C(a3)–C(m1)–C(11)	118.48(14)	N(6)–C(2)–C(5)	124.2(3)
C(a2)–C(m1)–C(11)	117.78(13)	C(3)–N(6)–C(3)#1	160.1(3)
C(a4#1–C(m2)–C(a1)	123.54(14)	C(3)–N(6)–C(2)	109.0(2)
C(a4#1–C(m2)–C(21)	118.19(13)	C(3)#1–N(6)–C(2)	51.08(19)
C(a1)–C(m2)–C(21)	118.20(13)	C(3)–N(6)–C(2)#1	51.09(19)
C(16)–C(11)–C(12)	118.77(16)	C(3)#1–N(6)–C(2)#1	109.0(2)
C(16)–C(11)–C(m1)	121.21(15)	C(2)–N(6)–C(2)#1	57.9(3)
C(12)–C(11)–C(m1)	119.98(15)	C(3)–N(6)–C(6)#1	73.19(19)
C(13)–C(12)–C(11)	120.49(19)	C(3)#1–N(6)–C(6)#1	126.7(2)
C(13)–C(12)–H(12)	119.8	C(2)–N(6)–C(6)#1	177.20(19)
C(11)–C(12)–H(12)	119.8	C(2)#1–N(6)–C(6)#1	124.25(19)
C(14)–C(13)–C(12)	120.1(2)	C(3)–N(6)–C(6)	126.7(2)
C(14)–C(13)–H(13)	120.0	C(3)#1–N(6)–C(6)	73.19(19)
C(12)–C(13)–H(13)	120.0	C(2)–N(6)–C(6)	124.25(19)
C(15)–C(14)–C(13)	120.15(17)	C(2)#1–N(6)–C(6)	177.2(2)
C(15)–C(14)–H(14)	119.9	C(6)#1–N(6)–C(6)	53.6(3)

Table S17. Continued

angle	degree	angle	degree
C(13)–C(14)–H(14)	119.9	C(4)#1–C(5)–C(3)#1	71.3(4)
C(14)–C(15)–C(16)	120.5(2)	C(3)#1–C(5)–C(2)	48.2(2)
C(14)–C(15)–H(15)	119.7	C(4)#1–C(5)–H(4a)	98.0
C(16)–C(15)–H(15)	119.7	C(3)#1–C(5)–H(4a)	127.4
C(11)–C(16)–C(15)	120.0(2)	C(2)–C(5)–H(4a)	112.2
C(11)–C(16)–H(16)	124.4	C(4)#1–C(5)–H(4b)	89.2
C(15)–C(16)–H(16)	115.6	C(3)#1–C(5)–H(4b)	138.0
C(22)–C(21)–C(26)	118.63(14)	C(2)–C(5)–H(4b)	106.5
C(22)–C(21)–C(m2)	121.07(13)	H(4a)–C(5)–H(4b)	91.1
C(26)–C(21)–C(m2)	120.28(13)	C(4)#1–C(5)–H(4c)	131.4
C(23)–C(22)–C(21)	120.60(15)	C(3)#1–C(5)–H(4c)	60.8
C(23)–C(22)–H(22)	119.7	C(2)–C(5)–H(4c)	108.4
C(21)–C(22)–H(22)	119.7	H(4a)–C(5)–H(4c)	116.5
C(24)–C(23)–C(22)	120.22(15)	H(4b)–C(5)–H(4c)	121.1
C(24)–C(23)–H(23)	119.9	C(6)#1–C(6)–N(6)	63.18(14)
C(22)–C(23)–H(23)	119.9	C(6)#1–C(6)–C(3)#1	112.39(15)
C(25)–C(24)–C(23)	119.52(14)	N(6)–C(6)–C(3)#1	49.31(14)
C(25)–C(24)–H(24)	120.2	C(6)#1–C(6)–H(5a)	45.3
C(23)–C(24)–H(24)	120.2	N(6)–C(6)–H(5a)	108.5
C(26)–C(25)–C(24)	120.38(15)	C(3)#1–C(6)–H(5a)	157.5
C(26)–C(25)–H(25)	119.8	C(6)#1–C(6)–H(5b)	130.6
C(24)–C(25)–H(25)	119.8	N(6)–C(6)–H(5b)	112.0
C(25)–C(26)–C(21)	120.65(14)	C(3)#1–C(6)–H(5b)	78.3
C(25)–C(26)–H(26)	119.7	H(5a)–C(6)–H(5b)	113.2
C(21)–C(26)–H(26)	119.7	C(6)#1–C(6)–H(5c)	117.5
O(1)–C(1)–Fe	180.000(1)	N(6)–C(6)–H(5c)	115.7
C(2)#1–C(3)–N(6)	66.9(2)	C(3)#1–C(6)–H(5c)	95.8
N(6)–C(3)–C(4)	106.6(3)	H(5a)–C(6)–H(5c)	98.4
C(2)#1–C(3)–C(5)#1	69.6(3)	H(5b)–C(6)–H(5c)	108.5
N(6)–C(3)–C(5)#1	136.5(3)		

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

Table S18. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1,2-DiMeIm)][a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe	0.0135(2)	0.0228(2)	0.0189(2)	0.000	0.0046(1)	0.000
N(1)	0.0154(5)	0.0258(6)	0.0201(6)	0.0007(4)	0.0052(4)	−0.0004(4)
N(2)	0.0162(5)	0.0264(6)	0.0202(6)	0.0016(4)	0.0047(4)	0.0007(4)
C(a4)	0.0199(7)	0.0250(7)	0.0205(7)	−0.0004(5)	0.0065(5)	0.0005(5)
C(a3)	0.0186(7)	0.0286(7)	0.0212(7)	0.0019(5)	0.0070(5)	0.0007(5)
C(a2)	0.0155(6)	0.0280(7)	0.0232(7)	0.0012(5)	0.0054(5)	0.0000(5)
C(a1)	0.0169(7)	0.0264(7)	0.0219(7)	0.0023(5)	0.0036(5)	−0.0007(5)
C(b4)	0.0207(7)	0.0360(8)	0.0211(7)	0.0006(6)	0.0073(5)	0.0003(6)
C(b3)	0.0199(7)	0.0390(9)	0.0222(7)	0.0019(6)	0.0081(6)	0.0008(6)
C(b2)	0.0152(6)	0.0399(8)	0.0252(7)	0.0035(6)	0.0049(5)	0.0014(6)
C(b1)	0.0165(7)	0.0375(8)	0.0233(7)	0.0034(6)	0.0033(5)	0.0010(6)
C(m1)	0.0163(7)	0.0298(7)	0.0241(7)	0.0016(5)	0.0075(5)	0.0002(5)
C(m2)	0.0192(7)	0.0248(7)	0.0204(7)	0.0023(5)	0.0044(5)	−0.0010(5)
C(11)	0.0162(7)	0.0493(10)	0.0207(7)	0.0049(6)	0.0056(5)	0.0021(6)
C(12)	0.0279(8)	0.0535(11)	0.0316(8)	0.0034(8)	0.0125(7)	0.0094(7)
C(13)	0.0319(10)	0.0840(16)	0.0333(9)	0.0068(10)	0.0149(8)	0.0205(10)
C(14)	0.0184(8)	0.124(2)	0.0237(8)	0.0081(11)	0.0087(6)	0.0097(10)
C(15)	0.0244(9)	0.107(2)	0.0326(10)	0.0012(11)	0.0080(7)	−0.0195(10)
C(16)	0.0260(8)	0.0657(13)	0.0318(9)	−0.0015(8)	0.0096(7)	−0.0106(8)
C(21)	0.0164(6)	0.0303(7)	0.0201(7)	0.0020(5)	0.0052(5)	0.0011(5)
C(22)	0.0214(7)	0.0304(7)	0.0253(7)	0.0031(6)	0.0062(5)	−0.0014(6)
C(23)	0.0266(8)	0.0377(8)	0.0245(7)	0.0083(6)	0.0065(6)	0.0015(6)
C(24)	0.0224(7)	0.0458(10)	0.0197(7)	0.0004(6)	0.0029(6)	0.0006(6)
C(25)	0.0216(7)	0.0374(8)	0.0262(7)	−0.0043(6)	0.0047(6)	−0.0052(6)
C(26)	0.0225(7)	0.0303(8)	0.0252(7)	0.0020(6)	0.0062(5)	−0.0018(6)
C(1)	0.0168(9)	0.0290(10)	0.0193(9)	0.000	0.0070(7)	0.000
O(1)	0.0349(9)	0.0270(8)	0.0363(9)	0.000	0.0164(7)	0.000
C(3)	0.0274(15)	0.0287(15)	0.0183(12)	−0.0039(11)	0.0023(11)	−0.0015(12)
C(4)	0.0237(15)	0.0336(17)	0.0128(18)	−0.0001(16)	0.0010(13)	−0.0003(12)
N(5)	0.0166(14)	0.0271(10)	0.018(3)	0.0008(10)	0.004(3)	0.0016(12)
C(2)	0.0163(13)	0.0274(16)	0.0183(16)	−0.0008(13)	0.0040(10)	0.0001(10)
N(6)	0.0233(9)	0.0241(8)	0.0240(9)	0.000	0.0038(7)	0.000
C(5)	0.0309(17)	0.0287(17)	0.0189(18)	−0.0021(14)	0.0041(14)	0.0032(12)
C(6)	0.045(2)	0.0253(15)	0.0291(17)	0.0012(12)	0.0076(14)	0.0029(13)

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

Table S19. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for [Fe(TPP)(CO)(1,2-DiMeIm)][a]

atom	x	y	z	U(eq)
H(b4	1.0044	0.8687	0.6255	0.031
H(b3	0.8401	0.8639	0.5435	0.032
H(b2	0.6511	0.8875	0.1698	0.032
H(b1	0.6901	0.8892	0.0034	0.031
H(12)	0.7395	0.9733	0.4386	0.044
H(13)	0.6002	0.9838	0.4863	0.058
H(14)	0.4911	0.8953	0.4453	0.066
H(15)	0.5212	0.7945	0.3615	0.065
H(16)	0.6546	0.7842	0.3126	0.049
H(22)	0.8640	0.9726	−0.1414	0.031
H(23)	0.7820	0.9684	−0.3076	0.035
H(24)	0.6916	0.8695	−0.3665	0.036
H(25)	0.6831	0.7750	−0.2581	0.034
H(26)	0.7652	0.7786	−0.0925	0.031
H(2)	0.9689	0.6177	0.1086	0.030
H(3)	0.9733	0.7590	0.0738	0.029
H(4a)	0.9990	0.7373	0.4314	0.032
H(4b)	1.0756	0.7506	0.4224	0.032
H(4c)	1.0525	0.6687	0.4379	0.032
H(5a)	1.0000	0.5379	0.2500	0.040
H(5b)	0.9843	0.5695	0.3449	0.040
H(5c)	1.0736	0.5613	0.3260	0.040

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

Table S20. Complete Crystallographic Details for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6

formula	$C_{55}H_{40}FeN_6O$
FW, amu	856.78
a, Å	9.6313(19)
b, Å	13.189(3)
c, Å	17.622(4)
α, deg	75.25(3)
β, deg	88.95(3)
γ, deg	81.52(3)
V, Å^3	2140.6(7)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.329
F(000)	892
μ, mm^{-1}	0.402
crystal dimensions, mm	0.29 × 0.26 × 0.10
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.61–33.84
index range	$-14 \leq h \leq 14$
	$-20 \leq k \leq 20$
	$-27 \leq l \leq 27$
total data collected	45838
absorption correction	Semi-empirical fromequiv
relative transmission coefficients (I)	0.9610 and 0.8924
unique data	15633 (R_{int} = 0.035)
unique observed data [I > 2σ(I)]	11562
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	12321/0/600
goodness-of-fit (pased on F^2)	1.024
final R indices [I > 2σ(I)]	R_1 = 0.0459, wR_2 = 0.1155
final R indices (all data)	R_1 = 0.0615, wR_2 = 0.1259

Table S21. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6[a]

atom	x	y	z	U(eq)
Fe	0.25690(2)	0.15564(2)	0.21231(1)	0.0149(1)
N(1)	0.26909(13)	0.15431(10)	0.09911(7)	0.0165(2)
N(2)	0.26855(13)	0.31192(10)	0.18337(7)	0.0159(2)
N(3)	0.25526(13)	0.15608(10)	0.32583(7)	0.0164(2)
N(4)	0.24186(13)	0.00042(10)	0.24047(7)	0.0169(2)
C(a1)	0.26521(15)	0.06914(12)	0.06747(9)	0.0172(3)
C(a2)	0.27501(15)	0.24008(12)	0.03601(9)	0.0168(3)
C(a3)	0.26269(15)	0.37776(12)	0.10883(9)	0.0169(3)
C(a4)	0.26171(16)	0.37784(12)	0.23323(9)	0.0172(3)
C(a5)	0.26727(16)	0.23976(12)	0.35742(9)	0.0172(3)
C(a6)	0.25622(16)	0.06901(12)	0.38840(9)	0.0174(3)
C(a7)	0.22679(16)	−0.06236(12)	0.31460(9)	0.0186(3)
C(a8)	0.23072(16)	−0.06268(12)	0.19005(9)	0.0181(3)
C(b1)	0.27476(16)	0.10180(13)	−0.01677(9)	0.0192(3)
C(b2)	0.27991(16)	0.20715(12)	−0.03638(9)	0.0186(3)
C(b3)	0.24941(17)	0.48734(12)	0.11182(9)	0.0199(3)
C(b4)	0.24870(17)	0.48753(12)	0.18873(9)	0.0201(3)
C(b5)	0.28253(17)	0.20323(13)	0.44178(9)	0.0206(3)
C(b6)	0.27521(17)	0.09774(13)	0.46094(9)	0.0206(3)
C(b7)	0.20465(18)	−0.16734(13)	0.31067(10)	0.0226(3)
C(b8)	0.20707(18)	−0.16745(13)	0.23374(9)	0.0223(3)
C(m1)	0.26864(15)	0.34533(12)	0.03918(9)	0.0169(3)
C(m2)	0.26643(16)	0.34532(12)	0.31515(9)	0.0174(3)
C(m3)	0.23792(16)	−0.03247(12)	0.38438(9)	0.0179(3)
C(m4)	0.24475(15)	−0.03279(12)	0.10893(9)	0.0173(3)
C(11)	0.26356(16)	0.42873(12)	−0.03692(9)	0.0177(3)
C(12)	0.13571(17)	0.46896(13)	−0.07710(10)	0.0225(3)
C(13)	0.12882(19)	0.54849(13)	−0.14685(10)	0.0247(3)
C(14)	0.24942(19)	0.58862(13)	−0.17670(9)	0.0238(3)
C(15)	0.37692(18)	0.54803(14)	−0.13786(10)	0.0252(3)
C(16)	0.38409(17)	0.46811(13)	−0.06837(9)	0.0229(3)
C(21)	0.27535(17)	0.42647(12)	0.36005(9)	0.0201(3)
C(22)	0.1736(2)	0.44509(15)	0.41427(11)	0.0301(4)
C(23)	0.1877(2)	0.51594(17)	0.45922(12)	0.0390(5)

Table S21. Continued

atom	x	y	z	U(eq)
C(24)	0.3026(3)	0.56884(15)	0.45060(11)	0.0373(5)
C(25)	0.4029(2)	0.55243(14)	0.39616(11)	0.0324(4)
C(26)	0.38943(19)	0.48185(13)	0.35086(10)	0.0241(3)
C(31)	0.22982(17)	−0.11471(12)	0.45999(9)	0.0186(3)
C(32)	0.10087(19)	−0.13506(15)	0.49228(11)	0.0293(4)
C(33)	0.0947(2)	−0.21262(17)	0.56218(11)	0.0352(4)
C(34)	0.2167(2)	−0.27040(14)	0.59980(10)	0.0312(4)
C(35)	0.3450(2)	−0.24936(14)	0.56851(10)	0.0279(4)
C(36)	0.35198(18)	−0.17177(13)	0.49908(10)	0.0235(3)
C(41)	0.23239(16)	−0.11153(12)	0.06200(9)	0.0178(3)
C(42)	0.10274(17)	−0.13955(13)	0.04978(10)	0.0224(3)
C(43)	0.09072(18)	−0.20855(14)	0.00304(10)	0.0246(3)
C(44)	0.20793(18)	−0.25054(12)	−0.03207(9)	0.0219(3)
C(45)	0.33773(18)	−0.22388(13)	−0.02008(10)	0.0239(3)
C(46)	0.34990(17)	−0.15484(13)	0.02694(10)	0.0229(3)
C(1)	0.07229(17)	0.18184(12)	0.20742(9)	0.0189(3)
O(1)	−0.04732(13)	0.19476(10)	0.20664(8)	0.0311(3)
C(2)	0.55898(16)	0.05827(13)	0.18906(9)	0.0204(3)
C(3)	0.68819(18)	0.10020(15)	0.27313(10)	0.0270(4)
C(4)	0.55306(18)	0.14518(16)	0.27709(11)	0.0291(4)
C(5)	0.81569(17)	−0.01431(14)	0.19099(10)	0.0257(3)
N(5)	0.47112(13)	0.11882(10)	0.22381(7)	0.0177(2)
N(6)	0.69125(14)	0.04510(11)	0.21667(8)	0.0196(3)
C(51)	0.8338(5)	0.6519(4)	0.3012(3)	0.0479(11)
C(52)	0.8306(6)	0.7246(5)	0.3511(3)	0.0559(12)
C(53)	0.7121(5)	0.7983(3)	0.3512(2)	0.0362(9)
C(54)	0.5969(4)	0.8021(3)	0.3030(2)	0.0329(9)
C(55)	0.6014(5)	0.7339(4)	0.2557(2)	0.0358(9)
C(56)	0.7149(5)	0.6590(3)	0.2555(2)	0.0340(9)
C(61)	0.5937(9)	0.7744(8)	0.2890(6)	0.062(2)
C(62)	0.6636(8)	0.8067(5)	0.3391(4)	0.0367(14)
C(63)	0.8033(7)	0.7656(6)	0.3580(3)	0.0385(14)
C(64)	0.8705(7)	0.6844(5)	0.3244(4)	0.0440(15)
C(65)	0.7852(9)	0.6521(5)	0.2717(5)	0.0497(16)

Table S21. Continued

atom	x	y	z	U(eq)
C(66)	0.6524(11)	0.6987(8)	0.2567(5)	0.065(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 S22. Bond Lengths for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6[a]

bond	length (Å)	bond	length (Å)
Fe–C(1)	1.7600(17)	C(24)–H(24)	0.9500
Fe–N(1)	2.0005(13)	C(25)–C(26)	1.392(2)
Fe–N(3)	2.0016(13)	C(25)–H(25)	0.9500
Fe–N(4)	2.0064(14)	C(26)–H(26)	0.9500
Fe–N(2)	2.0129(14)	C(31)–C(36)	1.389(2)
Fe–N(5)	2.0503(14)	C(31)–C(32)	1.390(2)
N(1)–C(a2)	1.377(2)	C(32)–C(33)	1.393(2)
N(1)–C(a1)	1.3807(19)	C(32)–H(32)	0.9500
N(2)–C(a3)	1.3747(19)	C(33)–C(34)	1.382(3)
N(2)–C(a4)	1.3792(19)	C(33)–H(33)	0.9500
N(3)–C(a6)	1.3737(19)	C(34)–C(35)	1.381(3)
N(3)–C(a5)	1.3763(19)	C(34)–H(34)	0.9500
N(4)–C(a7)	1.375(2)	C(35)–C(36)	1.389(2)
N(4)–C(a8)	1.3783(19)	C(35)–H(35)	0.9500
C(a1)–C(m4)	1.397(2)	C(36)–H(36)	0.9500
C(a1)–C(b1)	1.442(2)	C(41)–C(42)	1.389(2)
C(a2)–C(m1)	1.396(2)	C(41)–C(46)	1.397(2)
C(a2)–C(b2)	1.446(2)	C(42)–C(43)	1.392(2)
C(a3)–C(m1)	1.396(2)	C(42)–H(42)	0.9500
C(a3)–C(b3)	1.446(2)	C(43)–C(44)	1.389(2)
C(a4)–C(m2)	1.397(2)	C(43)–H(43)	0.9500
C(a4)–C(b4)	1.448(2)	C(44)–C(45)	1.381(2)
C(a5)–C(m2)	1.401(2)	C(44)–H(44)	0.9500
C(a5)–C(b5)	1.444(2)	C(45)–C(46)	1.396(2)
C(a6)–C(m3)	1.395(2)	C(45)–H(45)	0.9500
C(a6)–C(b6)	1.445(2)	C(46)–H(46)	0.9500
C(a7)–C(m3)	1.394(2)	C(1)–O(1)	1.139(2)
C(a7)–C(b7)	1.451(2)	C(2)–N(5)	1.327(2)
C(a8)–C(m4)	1.393(2)	C(2)–N(6)	1.343(2)
C(a8)–C(b8)	1.449(2)	C(2)–H(2)	0.9500
C(b1)–C(b2)	1.352(2)	C(3)–C(4)	1.357(2)
C(b1)–H(b1)	0.9500	C(3)–N(6)	1.371(2)
C(b2)–H(b2)	0.9500	C(3)–H(3)	0.9500
C(b3)–C(b4)	1.356(2)	C(4)–N(5)	1.378(2)

Table S22. Continued

bond	length (Å)	bond	length (Å)
C(b3)–H(b3)	0.9500	C(4)–H(4)	0.9500
C(b4)–H(b4)	0.9500	C(5)–N(6)	1.462(2)
C(b5)–C(b6)	1.358(2)	C(5)–H(5a)	0.9800
C(b5)–H(b5)	0.9500	C(5)–H(5b)	0.9800
C(b6)–H(b6)	0.9500	C(5)–H(5c)	0.9800
C(b7)–C(b8)	1.356(2)	C(51)–C(52)	1.454(7)
C(b7)–H(b7)	0.9500	C(51)–C(56)	1.390(6)
C(b8)–H(b8)	0.9500	C(51)–H(51)	0.9500
C(m1)–C(11)	1.499(2)	C(52)–C(53)	1.385(7)
C(m2)–C(21)	1.496(2)	C(52)–H(52)	0.9500
C(m3)–C(31)	1.498(2)	C(53)–C(54)	1.397(6)
C(m4)–C(41)	1.501(2)	C(53)–H(53)	0.9500
C(11)–C(16)	1.390(2)	C(54)–C(55)	1.369(6)
C(11)–C(12)	1.395(2)	C(54)–H(54)	0.9500
C(12)–C(13)	1.393(2)	C(55)–C(56)	1.362(5)
C(12)–H(12)	0.9500	C(55)–H(55)	0.9500
C(13)–C(14)	1.387(3)	C(56)–H(56)	0.9500
C(13)–H(13)	0.9500	C(61)–C(62)	1.309(11)
C(14)–C(15)	1.383(2)	C(61)–C(66)	1.324(13)
C(14)–H(14)	0.9500	C(61)–H(61)	0.9500
C(15)–C(16)	1.393(2)	C(62)–C(63)	1.387(9)
C(15)–H(15)	0.9500	C(62)–H(62)	0.9500
C(16)–H(16)	0.9500	C(63)–C(64)	1.422(9)
C(21)–C(26)	1.392(2)	C(63)–H(63)	0.9500
C(21)–C(22)	1.395(2)	C(64)–C(65)	1.433(10)
C(22)–C(23)	1.392(3)	C(64)–H(64)	0.9500
C(22)–H(22)	0.9500	C(65)–C(66)	1.335(12)
C(23)–C(24)	1.379(3)	C(65)–H(65)	0.9500
C(23)–H(23)	0.9500	C(66)–H(66)	0.9500
C(24)–C(25)	1.382(3)		

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

Table S23. Bond Angles for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6[a]

angle	degree	angle	degree
C(1)–Fe–N(1)	92.33(7)	C(23)–C(22)–H(22)	119.7
C(1)–Fe–N(3)	90.55(7)	C(21)–C(22)–H(22)	119.7
N(1)–Fe–N(3)	177.12(5)	C(24)–C(23)–C(22)	120.30(19)
C(1)–Fe–N(4)	88.23(7)	C(24)–C(23)–H(23)	119.8
N(1)–Fe–N(4)	89.46(6)	C(22)–C(23)–H(23)	119.8
N(3)–Fe–N(4)	90.85(6)	C(23)–C(24)–C(25)	119.67(17)
C(1)–Fe–N(2)	90.84(7)	C(23)–C(24)–H(24)	120.2
N(1)–Fe–N(2)	90.28(6)	C(25)–C(24)–H(24)	120.2
N(3)–Fe–N(2)	89.45(6)	C(24)–C(25)–C(26)	120.38(18)
N(4)–Fe–N(2)	179.02(5)	C(24)–C(25)–H(25)	119.8
C(1)–Fe–N(5)	176.78(6)	C(26)–C(25)–H(25)	119.8
N(1)–Fe–N(5)	89.95(6)	C(21)–C(26)–C(25)	120.50(17)
N(3)–Fe–N(5)	87.19(6)	C(21)–C(26)–H(26)	119.8
N(4)–Fe–N(5)	89.51(6)	C(25)–C(26)–H(26)	119.8
N(2)–Fe–N(5)	91.43(6)	C(36)–C(31)–C(32)	118.97(15)
C(a2)–N(1)–C(a1)	105.58(12)	C(36)–C(31)–C(m3)	120.15(15)
C(a2)–N(1)–Fe	126.82(10)	C(32)–C(31)–C(m3)	120.88(14)
C(a1)–N(1)–Fe	127.50(10)	C(31)–C(32)–C(33)	120.35(17)
C(a3)–N(2)–C(a4)	105.51(12)	C(31)–C(32)–H(32)	119.8
C(a3)–N(2)–Fe	126.51(10)	C(33)–C(32)–H(32)	119.8
C(a4)–N(2)–Fe	127.28(10)	C(34)–C(33)–C(32)	120.23(18)
C(a6)–N(3)–C(a5)	106.00(12)	C(34)–C(33)–H(33)	119.9
C(a6)–N(3)–Fe	126.05(10)	C(32)–C(33)–H(33)	119.9
C(a5)–N(3)–Fe	127.65(10)	C(35)–C(34)–C(33)	119.58(16)
C(a7)–N(4)–C(a8)	105.76(12)	C(35)–C(34)–H(34)	120.2
C(a7)–N(4)–Fe	126.35(11)	C(33)–C(34)–H(34)	120.2
C(a8)–N(4)–Fe	127.61(10)	C(34)–C(35)–C(36)	120.46(17)
N(1)–C(a1)–C(m4)	125.98(14)	C(34)–C(35)–H(35)	119.8
N(1)–C(a1)–C(b1)	110.17(13)	C(36)–C(35)–H(35)	119.8
C(m4)–C(a1)–C(b1)	123.69(14)	C(35)–C(36)–C(31)	120.38(17)
N(1)–C(a2)–C(m1)	126.03(14)	C(35)–C(36)–H(36)	119.8
N(1)–C(a2)–C(b2)	110.20(13)	C(31)–C(36)–H(36)	119.8
C(m1)–C(a2)–C(b2)	123.66(14)	C(42)–C(41)–C(46)	118.53(14)
N(2)–C(a3)–C(m1)	125.69(14)	C(42)–C(41)–C(m4)	120.63(14)

Table S23. Continued

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	110.49(13)	C(46)–C(41)–C(m4)	120.80(14)
C(m1)–C(a3)–C(b3)	123.82(14)	C(41)–C(42)–C(43)	120.42(15)
N(2)–C(a4)–C(m2)	125.73(14)	C(41)–C(42)–H(42)	119.8
N(2)–C(a4)–C(b4)	110.40(13)	C(43)–C(42)–H(42)	119.8
C(m2)–C(a4)–C(b4)	123.88(14)	C(44)–C(43)–C(42)	120.64(15)
N(3)–C(a5)–C(m2)	125.87(14)	C(44)–C(43)–H(43)	119.7
N(3)–C(a5)–C(b5)	110.09(13)	C(42)–C(43)–H(43)	119.7
C(m2)–C(a5)–C(b5)	124.04(14)	C(45)–C(44)–C(43)	119.59(15)
N(3)–C(a6)–C(m3)	126.02(14)	C(45)–C(44)–H(44)	120.2
N(3)–C(a6)–C(b6)	110.10(13)	C(43)–C(44)–H(44)	120.2
C(m3)–C(a6)–C(b6)	123.85(14)	C(44)–C(45)–C(46)	119.80(15)
N(4)–C(a7)–C(m3)	125.54(14)	C(44)–C(45)–H(45)	120.1
N(4)–C(a7)–C(b7)	110.29(14)	C(46)–C(45)–H(45)	120.1
C(m3)–C(a7)–C(b7)	124.09(14)	C(45)–C(46)–C(41)	121.02(15)
N(4)–C(a8)–C(m4)	125.66(14)	C(45)–C(46)–H(46)	119.5
N(4)–C(a8)–C(b8)	110.28(13)	C(41)–C(46)–H(46)	119.5
C(m4)–C(a8)–C(b8)	124.02(14)	O(1)–C(1)–Fe	177.03(15)
C(b2)–C(b1)–C(a1)	107.09(14)	N(5)–C(2)–N(6)	112.04(14)
C(b2)–C(b1)–H(b1)	126.5	N(5)–C(2)–H(2)	124.0
C(a1)–C(b1)–H(b1)	126.5	N(6)–C(2)–H(2)	124.0
C(b1)–C(b2)–C(a2)	106.90(14)	C(4)–C(3)–N(6)	106.77(15)
C(b1)–C(b2)–H(b2)	126.6	C(4)–C(3)–H(3)	126.6
C(a2)–C(b2)–H(b2)	126.6	N(6)–C(3)–H(3)	126.6
C(b4)–C(b3)–C(a3)	106.89(14)	C(3)–C(4)–N(5)	109.57(15)
C(b4)–C(b3)–H(b3)	126.6	C(3)–C(4)–H(4)	125.2
C(a3)–C(b3)–H(b3)	126.6	N(5)–C(4)–H(4)	125.2
C(b3)–C(b4)–C(a4)	106.70(14)	N(6)–C(5)–H(5a)	109.5
C(b3)–C(b4)–H(b4)	126.6	N(6)–C(5)–H(5b)	109.5
C(a4)–C(b4)–H(b4)	126.6	H(5a)–C(5)–H(5b)	109.5
C(b6)–C(b5)–C(a5)	106.83(14)	N(6)–C(5)–H(5c)	109.5
C(b6)–C(b5)–H(b5)	126.6	H(5a)–C(5)–H(5c)	109.5
C(a5)–C(b5)–H(b5)	126.6	H(5b)–C(5)–H(5c)	109.5
C(b5)–C(b6)–C(a6)	106.92(14)	C(2)–N(5)–C(4)	105.02(13)
C(b5)–C(b6)–H(b6)	126.5	C(2)–N(5)–Fe	129.25(11)

Table S23. Continued

angle	degree	angle	degree
C(a6)–C(b6)–H(b6)	126.5	C(4)–N(5)–Fe	125.46(11)
C(b8)–C(b7)–C(a7)	106.83(14)	C(2)–N(6)–C(3)	106.61(13)
C(b8)–C(b7)–H(b7)	126.6	C(2)–N(6)–C(5)	127.22(14)
C(a7)–C(b7)–H(b7)	126.6	C(3)–N(6)–C(5)	126.17(14)
C(b7)–C(b8)–C(a8)	106.84(14)	C(52)–C(51)–C(56)	117.6(4)
C(b7)–C(b8)–H(b8)	126.6	C(52)–C(51)–H(51)	121.2
C(a8)–C(b8)–H(b8)	126.6	C(56)–C(51)–H(51)	121.2
C(a2)–C(m1)–C(a3)	123.95(14)	C(53)–C(52)–C(51)	119.9(5)
C(a2)–C(m1)–C(11)	117.87(13)	C(53)–C(52)–H(52)	120.1
C(a3)–C(m1)–C(11)	118.15(13)	C(51)–C(52)–H(52)	120.1
C(a4)–C(m2)–C(a5)	123.18(14)	C(52)–C(53)–C(54)	119.5(4)
C(a4)–C(m2)–C(21)	118.54(14)	C(52)–C(53)–H(53)	120.2
C(a5)–C(m2)–C(21)	118.26(13)	C(54)–C(53)–H(53)	120.2
C(a7)–C(m3)–C(a6)	124.27(14)	C(53)–C(54)–C(55)	120.2(4)
C(a7)–C(m3)–C(31)	117.87(14)	C(53)–C(54)–H(54)	119.9
C(a6)–C(m3)–C(31)	117.86(14)	C(55)–C(54)–H(54)	119.9
C(a8)–C(m4)–C(a1)	123.35(14)	C(54)–C(55)–C(56)	121.7(4)
C(a8)–C(m4)–C(41)	119.37(14)	C(54)–C(55)–H(55)	119.1
C(a1)–C(m4)–C(41)	117.24(13)	C(56)–C(55)–H(55)	119.1
C(16)–C(11)–C(12)	118.86(14)	C(55)–C(56)–C(51)	121.0(4)
C(16)–C(11)–C(m1)	121.28(14)	C(55)–C(56)–H(56)	119.5
C(12)–C(11)–C(m1)	119.86(14)	C(51)–C(56)–H(56)	119.5
C(13)–C(12)–C(11)	120.48(16)	C(62)–C(61)–C(66)	121.1(9)
C(13)–C(12)–H(12)	119.8	C(62)–C(61)–H(61)	119.5
C(11)–C(12)–H(12)	119.8	C(66)–C(61)–H(61)	119.5
C(14)–C(13)–C(12)	120.05(16)	C(61)–C(62)–C(63)	121.2(7)
C(14)–C(13)–H(13)	120.0	C(61)–C(62)–H(62)	119.4
C(12)–C(13)–H(13)	120.0	C(63)–C(62)–H(62)	119.4
C(15)–C(14)–C(13)	119.81(15)	C(62)–C(63)–C(64)	119.5(6)
C(15)–C(14)–H(14)	120.1	C(62)–C(63)–H(63)	120.2
C(13)–C(14)–H(14)	120.1	C(64)–C(63)–H(63)	120.3
C(14)–C(15)–C(16)	120.19(16)	C(65)–C(64)–C(63)	115.6(6)
C(14)–C(15)–H(15)	119.9	C(65)–C(64)–H(64)	122.2
C(16)–C(15)–H(15)	119.9	C(63)–C(64)–H(64)	122.2

Table S23. Continued

angle	degree	angle	degree
C(11)–C(16)–C(15)	120.59(15)	C(64)–C(65)–C(66)	119.8(7)
C(11)–C(16)–H(16)	119.7	C(64)–C(65)–H(65)	120.1
C(15)–C(16)–H(16)	119.7	C(66)–C(65)–H(65)	120.1
C(26)–C(21)–C(22)	118.54(15)	C(65)–C(66)–C(61)	122.9(9)
C(26)–C(21)–C(m2)	120.25(14)	C(65)–C(66)–H(66)	118.6
C(22)–C(21)–C(m2)	121.15(15)	C(61)–C(66)–H(66)	118.6
C(23)–C(22)–C(21)	120.58(18)		

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

Table S24. Anisotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
FeH(3a)	0.0166(1)	0.0139(1)	0.0146(1)	−0.0032(1)	0.0003(1)	−0.0045(1)
N(1)	0.0174(6)	0.0164(6)	0.0165(6)	−0.0040(5)	−0.0006(4)	−0.0047(5)
N(2)	0.0168(6)	0.0162(6)	0.0149(6)	−0.0033(4)	0.0000(4)	−0.0040(5)
N(3)	0.0181(6)	0.0151(6)	0.0164(6)	−0.0036(5)	0.0007(4)	−0.0045(5)
N(4)	0.0193(6)	0.0160(6)	0.0163(6)	−0.0042(5)	0.0001(4)	−0.0050(5)
C(a1)	0.0164(6)	0.0184(7)	0.0177(7)	−0.0056(5)	0.0001(5)	−0.0039(5)
C(a2)	0.0163(6)	0.0188(7)	0.0156(6)	−0.0035(5)	−0.0005(5)	−0.0049(5)
C(a3)	0.0164(6)	0.0152(7)	0.0189(7)	−0.0032(5)	−0.0009(5)	−0.0039(5)
C(a4)	0.0183(7)	0.0148(7)	0.0188(7)	−0.0040(5)	−0.0003(5)	−0.0039(5)
C(a5)	0.0185(7)	0.0185(7)	0.0156(6)	−0.0055(5)	0.0017(5)	−0.0039(5)
C(a6)	0.0184(7)	0.0186(7)	0.0152(6)	−0.0031(5)	0.0011(5)	−0.0049(5)
C(a7)	0.0215(7)	0.0148(7)	0.0190(7)	−0.0025(5)	0.0006(5)	−0.0046(5)
C(a8)	0.0203(7)	0.0154(7)	0.0195(7)	−0.0047(5)	−0.0008(5)	−0.0052(5)
C(b1)	0.0203(7)	0.0214(7)	0.0174(7)	−0.0065(6)	0.0014(5)	−0.0053(6)
C(b2)	0.0200(7)	0.0208(7)	0.0161(7)	−0.0053(5)	0.0011(5)	−0.0049(6)
C(b3)	0.0237(7)	0.0154(7)	0.0204(7)	−0.0034(5)	−0.0023(6)	−0.0038(6)
C(b4)	0.0240(7)	0.0147(7)	0.0215(7)	−0.0046(6)	−0.0019(6)	−0.0028(6)
C(b5)	0.0263(8)	0.0204(7)	0.0168(7)	−0.0059(6)	0.0010(6)	−0.0066(6)
C(b6)	0.0265(8)	0.0211(7)	0.0148(7)	−0.0037(6)	0.0008(6)	−0.0072(6)
C(b7)	0.0307(8)	0.0156(7)	0.0222(7)	−0.0035(6)	0.0002(6)	−0.0078(6)
C(b8)	0.0300(8)	0.0157(7)	0.0225(8)	−0.0049(6)	−0.0009(6)	−0.0076(6)
C(m1)	0.0160(6)	0.0178(7)	0.0159(6)	−0.0013(5)	−0.0019(5)	−0.0040(5)
C(m2)	0.0182(7)	0.0173(7)	0.0181(7)	−0.0063(5)	0.0014(5)	−0.0043(5)
C(m3)	0.0191(7)	0.0166(7)	0.0173(7)	−0.0020(5)	0.0008(5)	−0.0043(5)
C(m4)	0.0165(6)	0.0173(7)	0.0192(7)	−0.0060(5)	0.0000(5)	−0.0038(5)
C(11)	0.0221(7)	0.0155(7)	0.0152(6)	−0.0028(5)	−0.0005(5)	−0.0039(5)
C(12)	0.0231(7)	0.0207(8)	0.0228(8)	−0.0028(6)	−0.0024(6)	−0.0046(6)
C(13)	0.0290(8)	0.0212(8)	0.0219(8)	−0.0029(6)	−0.0072(6)	−0.0006(6)
C(14)	0.0342(9)	0.0195(7)	0.0156(7)	−0.0023(6)	0.0002(6)	−0.0013(6)
C(15)	0.0273(8)	0.0241(8)	0.0214(8)	−0.0005(6)	0.0052(6)	−0.0052(6)
C(16)	0.0222(7)	0.0231(8)	0.0208(7)	−0.0006(6)	−0.0002(6)	−0.0041(6)
C(21)	0.0263(8)	0.0165(7)	0.0182(7)	−0.0053(5)	−0.0014(6)	−0.0036(6)
C(22)	0.0351(9)	0.0280(9)	0.0320(9)	−0.0158(7)	0.0084(7)	−0.0069(7)
C(23)	0.0564(13)	0.0330(10)	0.0332(10)	−0.0198(8)	0.0111(9)	−0.0056(9)

Table S24. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.0659(14)	0.0233(9)	0.0267(9)	−0.0120(7)	−0.0043(9)	−0.0091(9)
C(25)	0.0491(11)	0.0221(8)	0.0286(9)	−0.0053(7)	−0.0077(8)	−0.0148(8)
C(26)	0.0313(8)	0.0190(7)	0.0225(8)	−0.0038(6)	−0.0017(6)	−0.0073(6)
C(31)	0.0250(7)	0.0154(7)	0.0159(7)	−0.0040(5)	−0.0006(5)	−0.0051(6)
C(32)	0.0250(8)	0.0322(9)	0.0253(8)	0.0029(7)	0.0021(6)	−0.0052(7)
C(33)	0.0375(10)	0.0383(11)	0.0257(9)	0.0028(8)	0.0082(7)	−0.0130(8)
C(34)	0.0530(12)	0.0241(8)	0.0163(7)	−0.0014(6)	−0.0015(7)	−0.0109(8)
C(35)	0.0398(10)	0.0205(8)	0.0219(8)	−0.0035(6)	−0.0107(7)	−0.0013(7)
C(36)	0.0268(8)	0.0203(8)	0.0229(8)	−0.0039(6)	−0.0026(6)	−0.0043(6)
C(41)	0.0206(7)	0.0164(7)	0.0169(7)	−0.0041(5)	−0.0003(5)	−0.0042(5)
C(42)	0.0195(7)	0.0242(8)	0.0274(8)	−0.0120(6)	0.0038(6)	−0.0059(6)
C(43)	0.0215(7)	0.0262(8)	0.0308(9)	−0.0135(7)	−0.0008(6)	−0.0074(6)
C(44)	0.0297(8)	0.0164(7)	0.0204(7)	−0.0062(6)	−0.0012(6)	−0.0029(6)
C(45)	0.0247(8)	0.0195(8)	0.0277(8)	−0.0083(6)	0.0035(6)	−0.0007(6)
C(46)	0.0185(7)	0.0216(8)	0.0307(8)	−0.0098(6)	0.0017(6)	−0.0041(6)
C(1)	0.0251(8)	0.0140(7)	0.0179(7)	−0.0032(5)	0.0007(5)	−0.0056(6)
O(1)	0.0199(6)	0.0301(7)	0.0407(7)	−0.0043(6)	0.0008(5)	−0.0041(5)
C(2)	0.0211(7)	0.0229(8)	0.0189(7)	−0.0076(6)	−0.0004(5)	−0.0045(6)
C(3)	0.0215(8)	0.0382(10)	0.0278(8)	−0.0182(7)	0.0008(6)	−0.0075(7)
C(4)	0.0213(8)	0.0395(10)	0.0355(9)	−0.0246(8)	0.0016(7)	−0.0069(7)
C(5)	0.0221(8)	0.0284(9)	0.0283(8)	−0.0121(7)	0.0016(6)	−0.0009(6)
N(5)	0.0198(6)	0.0173(6)	0.0174(6)	−0.0051(5)	0.0017(5)	−0.0062(5)
N(6)	0.0193(6)	0.0201(6)	0.0205(6)	−0.0066(5)	0.0009(5)	−0.0032(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 S25. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6[a]

atom	x	y	z	U(eq)
H(b1	0.2770	0.0576	−0.0519	0.023
H(b2	0.2857	0.2512	−0.0879	0.022
H(b3	0.2425	0.5477	0.0682	0.024
H(b4	0.2411	0.5479	0.2094	0.024
H(b5	0.2953	0.2450	0.4771	0.025
H(b6	0.2814	0.0516	0.5123	0.025
H(b7	0.1911	−0.2250	0.3537	0.027
H(b8	0.1955	−0.2252	0.2125	0.027
H(12)	0.0528	0.4419	−0.0567	0.027
H(13)	0.0414	0.5752	−0.1740	0.030
H(14)	0.2445	0.6438	−0.2237	0.029
H(15)	0.4598	0.5748	−0.1586	0.030
H(16)	0.4721	0.4403	−0.0422	0.027
H(22)	0.0940	0.4091	0.4206	0.036
H(23)	0.1179	0.5279	0.4960	0.047
H(24)	0.3128	0.6163	0.4819	0.045
H(25)	0.4815	0.5895	0.3896	0.039
H(26)	0.4587	0.4714	0.3134	0.029
H(32)	0.0166	−0.0959	0.4665	0.035
H(33)	0.0062	−0.2258	0.5840	0.042
H(34)	0.2124	−0.3243	0.6469	0.037
H(35)	0.4291	−0.2882	0.5947	0.033
H(36)	0.4408	−0.1576	0.4782	0.028
H(42)	0.0217	−0.1114	0.0735	0.027
H(43)	0.0015	−0.2271	−0.0049	0.030
H(44)	0.1989	−0.2973	−0.0641	0.026
H(45)	0.4185	−0.2524	−0.0438	0.029
H(46)	0.4395	−0.1370	0.0352	0.027
H(2)	0.5316	0.0278	0.1493	0.024
H(3)	0.7657	0.1058	0.3036	0.032
H(4)	0.5200	0.1882	0.3113	0.035
H(5a)	0.7938	−0.0827	0.1862	0.039
H(5b)	0.8922	−0.0263	0.2296	0.039
H(5c)	0.8445	0.0263	0.1400	0.039

Table S25. Continued

atom	x	y	z	U(eq)
H(51)	0.9143	0.6012	0.2999	0.057
H(52)	0.9095	0.7216	0.3836	0.067
H(53)	0.7093	0.8459	0.3838	0.043
H(54)	0.5152	0.8522	0.3030	0.040
H(55)	0.5232	0.7389	0.2222	0.043
H(56)	0.7128	0.6110	0.2236	0.041
H(61)	0.4992	0.8059	0.2755	0.075
H(62)	0.6179	0.8591	0.3631	0.044
H(63)	0.8537	0.7916	0.3930	0.046
H(64)	0.9657	0.6536	0.3361	0.053
H(65)	0.8230	0.5977	0.2475	0.060
H(66)	0.5976	0.6765	0.2214	0.078

[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 S26. Orthogonal Coordinates (Å) of the Rigid Group Imidazole Ring used in the Refinement of [Fe(TPP)(CO)(1,2-DiMeIm)]·C_7H_8.

atom	x	y	z
N5	0.00000	0.00000	0.00000
C1	0.43751	0.62032	1.08059
N6	−0.38643	0.42602	2.12490
C2	−1.42304	−0.37659	1.68181
C3	−1.17985	−0.62875	0.37657
C4	1.66759	1.44674	1.16572
C5	−0.21245	0.88816	3.49236

Supporting Information

Table S19. Hydrogen Coordinates and Isotropic Displacement Parameters for [Fe(TPP)(CO)(1,2-DiMeIm)].

Table S20. Complete Crystallographic Details for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6.

Table S21. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6.

Table S22. Bond Lengths for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6.

Table S23. Bond Angles for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6.

Table S24. Anisotropic Isotropic Displacement Parameters for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6.

Table S25. Hydrogen Coordinates and Isotropic Displacement Parameters for [Fe(TPP)(CO)(1-MeIm)]·C_6H_6.

Table S26. Orthogonal Coordinates of the Rigid Group Imidazole Ring used in the Refinement of [Fe(TPP)(CO)(1,2-DiMeIm)].

References and Notes

(1) A linear correlation coefficient, Pearson's R, was used to judge the fit to the data.

$$R = \sum_i (x_i - \bar{x})(y_i - \bar{y}) / \sqrt{\sum_i (x_i - \bar{x})^2} \sqrt{\sum_i (y_i - \bar{y})^2}$$