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Table S17. Bond lengths [A] and angles [deg] for Os(OEP)(CO)(1-MeIM).

Os(1)-C(41)	1.817(13)
Os(1)-N(3)	2.057(8)
Os(1)-N(2)	2.058(8)
Os(1)-N(4)	2.061(8)
Os(1)-N(1)	2.063(8)
Os(1)-N(5)	2.177(9)
O(1)-C(41)	1.171(13)
N(1)-C(4)	1.379(12)
N(1)-C(1)	1.389(12)
N(2)-C(9)	1.370(13)
N(2)-C(6)	1.383(13)
N(3)-C(14)	1.362(12)
N(3)-C(11)	1.383(12)
N(4)-C(16)	1.359(12)
N(4)-C(19)	1.382(12)
N(5)-C(37)	1.308(13)
N(5)-C(39)	1.378(13)
N(6)-C(37)	1.343(14)
N(6)-C(38)	1.365(14)
N(6)-C(40)	1.461(14)
C(1)-C(20)	1.392(14)
C(1)-C(2)	1.450(13)
C(2)-C(3)	1.366(14)
C(2)-C(21)	1.502(14)
C(3)-C(4)	1.440(14)
C(3)-C(23)	1.503(13)
C(4)-C(5)	1.405(14)
C(5)-C(6)	1.41(2)
C(6)-C(7)	1.45(2)
C(7)-C(8)	1.35(2)
C(7)-C(25)	1.52(2)
C(8)-C(9)	1.46(2)
C(8)-C(27)	1.56(2)
C(9)-C(10)	1.405(14)
C(10)-C(11)	1.371(14)
C(11)-C(12)	1.461(14)
C(12)-C(13)	1.354(14)
C(12)-C(29)	1.494(14)
C(13)-C(14)	1.462(13)
C(13)-C(31)	1.513(14)
C(14)-C(15)	1.402(14)
C(15)-C(16)	1.408(14)
C(16)-C(17)	1.450(14)
C(17)-C(18)	1.356(14)
C(17)-C(33)	1.524(14)
C(18)-C(19)	1.450(14)
C(18)-C(35A)	1.53(3)
C(18)-C(35B)	1.58(3)
C(19)-C(20)	1.397(14)
C(21)-C(22)	1.51(2)
C(23)-C(24)	1.50(2)
C(25)-C(26)	1.48(2)
C(27)-C(28)	1.46(2)

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C(29)-C(30)	1.51(2)
C(31)-C(32)	1.50(2)
C(33)-C(34)	1.52(2)
C(35A)-C(36A)	1.54(5)
C(35B)-C(36B)	1.52(4)
C(38)-C(39)	1.35(2)
C(42)-Cl(2)	1.69(2)
C(42)-Cl(1)	1.80(2)

C(41)-Os(1)-N(3)	91.7(4)
C(41)-Os(1)-N(2)	94.2(4)
N(3)-Os(1)-N(2)	89.4(3)
C(41)-Os(1)-N(4)	91.9(4)
N(3)-Os(1)-N(4)	89.9(3)
N(2)-Os(1)-N(4)	173.9(4)
C(41)-Os(1)-N(1)	94.2(4)
N(3)-Os(1)-N(1)	174.1(4)
N(2)-Os(1)-N(1)	89.9(3)
N(4)-Os(1)-N(1)	90.2(3)
C(41)-Os(1)-N(5)	177.9(4)
N(3)-Os(1)-N(5)	86.2(3)
N(2)-Os(1)-N(5)	86.1(3)
N(4)-Os(1)-N(5)	87.8(3)
N(1)-Os(1)-N(5)	87.9(3)
C(4)-N(1)-C(1)	106.7(8)
C(4)-N(1)-Os(1)	127.3(7)
C(1)-N(1)-Os(1)	126.0(6)
C(9)-N(2)-C(6)	106.2(8)
C(9)-N(2)-Os(1)	126.9(7)
C(6)-N(2)-Os(1)	126.8(7)
C(14)-N(3)-C(11)	106.9(8)
C(14)-N(3)-Os(1)	126.4(7)
C(11)-N(3)-Os(1)	126.6(6)
C(16)-N(4)-C(19)	106.5(8)
C(16)-N(4)-Os(1)	127.2(7)
C(19)-N(4)-Os(1)	126.1(6)
C(37)-N(5)-C(39)	104.1(9)
C(37)-N(5)-Os(1)	127.9(8)
C(39)-N(5)-Os(1)	128.0(7)
C(37)-N(6)-C(38)	105.7(10)
C(37)-N(6)-C(40)	127.4(10)
C(38)-N(6)-C(40)	126.9(11)
N(1)-C(1)-C(20)	124.9(9)
N(1)-C(1)-C(2)	108.9(8)
C(20)-C(1)-C(2)	126.0(9)
C(3)-C(2)-C(1)	107.4(9)
C(3)-C(2)-C(21)	127.1(9)
C(1)-C(2)-C(21)	125.5(9)
C(2)-C(3)-C(4)	107.0(9)
C(2)-C(3)-C(23)	127.5(10)
C(4)-C(3)-C(23)	125.5(10)
N(1)-C(4)-C(5)	123.4(9)
N(1)-C(4)-C(3)	109.9(9)
C(5)-C(4)-C(3)	126.6(9)
C(6)-C(5)-C(4)	128.4(10)
N(2)-C(6)-C(5)	124.0(10)
N(2)-C(6)-C(7)	110.0(9)

C(5)-C(6)-C(7)	126.0(10)
C(8)-C(7)-C(6)	106.8(10)
C(8)-C(7)-C(25)	129.0(11)
C(6)-C(7)-C(25)	124.1(11)
C(7)-C(8)-C(9)	107.4(10)
C(7)-C(8)-C(27)	127.6(10)
C(9)-C(8)-C(27)	124.9(10)
N(2)-C(9)-C(10)	124.2(9)
N(2)-C(9)-C(8)	109.6(9)
C(10)-C(9)-C(8)	126.1(10)
C(11)-C(10)-C(9)	127.8(9)
C(10)-C(11)-N(3)	124.8(9)
C(10)-C(11)-C(12)	125.9(9)
N(3)-C(11)-C(12)	109.3(8)
C(13)-C(12)-C(11)	106.9(9)
C(13)-C(12)-C(29)	128.2(9)
C(11)-C(12)-C(29)	124.8(9)
C(12)-C(13)-C(14)	106.9(9)
C(12)-C(13)-C(31)	128.2(9)
C(14)-C(13)-C(31)	124.9(9)
N(3)-C(14)-C(15)	124.8(9)
N(3)-C(14)-C(13)	109.9(9)
C(15)-C(14)-C(13)	125.2(9)
C(14)-C(15)-C(16)	127.7(9)
N(4)-C(16)-C(15)	123.8(9)
N(4)-C(16)-C(17)	110.7(9)
C(15)-C(16)-C(17)	125.5(9)
C(18)-C(17)-C(16)	106.1(9)
C(18)-C(17)-C(33)	128.2(10)
C(16)-C(17)-C(33)	125.6(9)
C(17)-C(18)-C(19)	107.5(9)
C(17)-C(18)-C(35A)	125.1(14)
C(19)-C(18)-C(35A)	123.5(14)
C(17)-C(18)-C(35B)	126.8(13)
C(19)-C(18)-C(35B)	123.1(13)
N(4)-C(19)-C(20)	124.9(9)
N(4)-C(19)-C(18)	109.1(9)
C(20)-C(19)-C(18)	126.0(9)
C(1)-C(20)-C(19)	127.5(10)
C(2)-C(21)-C(22)	113.5(10)
C(3)-C(23)-C(24)	112.6(10)
C(26)-C(25)-C(7)	113.2(13)
C(28)-C(27)-C(8)	108(2)
C(12)-C(29)-C(30)	113.0(9)
C(32)-C(31)-C(13)	113.7(9)
C(34)-C(33)-C(17)	113.3(10)
C(36A)-C(35A)-C(18)	106(3)
C(36B)-C(35B)-C(18)	106(2)
N(5)-C(37)-N(6)	113.5(11)
C(39)-C(38)-N(6)	106.8(11)
C(38)-C(39)-N(5)	110.0(10)
O(1)-C(41)-Os(1)	177.0(9)
Cl(2)-C(42)-Cl(1)	111.3(9)

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Table S18. Torsion angles [deg] for Os(OEP)(CO)(1-MeIM).

C(41)-Os(1)-N(1)-C(4)	91.4(9)
N(3)-Os(1)-N(1)-C(4)	-86(3)
N(2)-Os(1)-N(1)-C(4)	-2.8(9)
N(4)-Os(1)-N(1)-C(4)	-176.7(9)
N(5)-Os(1)-N(1)-C(4)	-88.9(9)
C(41)-Os(1)-N(1)-C(1)	-86.3(9)
N(3)-Os(1)-N(1)-C(1)	96(3)
N(2)-Os(1)-N(1)-C(1)	179.5(9)
N(4)-Os(1)-N(1)-C(1)	5.6(9)
N(5)-Os(1)-N(1)-C(1)	93.4(9)
C(41)-Os(1)-N(2)-C(9)	85.2(9)
N(3)-Os(1)-N(2)-C(9)	-6.5(9)
N(4)-Os(1)-N(2)-C(9)	-90(3)
N(1)-Os(1)-N(2)-C(9)	179.4(9)
N(5)-Os(1)-N(2)-C(9)	-92.7(9)
C(41)-Os(1)-N(2)-C(6)	-92.3(10)
N(3)-Os(1)-N(2)-C(6)	176.0(10)
N(4)-Os(1)-N(2)-C(6)	93(3)
N(1)-Os(1)-N(2)-C(6)	1.9(10)
N(5)-Os(1)-N(2)-C(6)	89.8(10)
C(41)-Os(1)-N(3)-C(14)	87.5(9)
N(2)-Os(1)-N(3)-C(14)	-178.3(9)
N(4)-Os(1)-N(3)-C(14)	-4.4(9)
N(1)-Os(1)-N(3)-C(14)	-95(3)
N(5)-Os(1)-N(3)-C(14)	-92.2(8)
C(41)-Os(1)-N(3)-C(11)	-88.9(9)
N(2)-Os(1)-N(3)-C(11)	5.3(8)
N(4)-Os(1)-N(3)-C(11)	179.2(8)
N(1)-Os(1)-N(3)-C(11)	89(3)
N(5)-Os(1)-N(3)-C(11)	91.4(8)
C(41)-Os(1)-N(4)-C(16)	-87.4(9)
N(3)-Os(1)-N(4)-C(16)	4.3(9)
N(2)-Os(1)-N(4)-C(16)	88(3)
N(1)-Os(1)-N(4)-C(16)	178.4(9)
N(5)-Os(1)-N(4)-C(16)	90.5(9)
C(41)-Os(1)-N(4)-C(19)	87.6(9)
N(3)-Os(1)-N(4)-C(19)	179.4(9)
N(2)-Os(1)-N(4)-C(19)	-97(3)
N(1)-Os(1)-N(4)-C(19)	-6.6(9)
N(5)-Os(1)-N(4)-C(19)	-94.5(9)
C(41)-Os(1)-N(5)-C(37)	-5(11)
N(3)-Os(1)-N(5)-C(37)	3.5(9)
N(2)-Os(1)-N(5)-C(37)	93.2(9)
N(4)-Os(1)-N(5)-C(37)	-86.5(9)
N(1)-Os(1)-N(5)-C(37)	-176.7(9)
C(41)-Os(1)-N(5)-C(39)	177(10)
N(3)-Os(1)-N(5)-C(39)	-174.4(8)
N(2)-Os(1)-N(5)-C(39)	-84.7(8)
N(4)-Os(1)-N(5)-C(39)	95.6(8)
N(1)-Os(1)-N(5)-C(39)	5.3(8)
C(4)-N(1)-C(1)-C(20)	177.7(11)
Os(1)-N(1)-C(1)-C(20)	-4(2)
C(4)-N(1)-C(1)-C(2)	1.5(12)

Os(1)-N(1)-C(1)-C(2)	179.6(7)
N(1)-C(1)-C(2)-C(3)	-1.4(13)
C(20)-C(1)-C(2)-C(3)	-177.6(11)
N(1)-C(1)-C(2)-C(21)	179.7(10)
C(20)-C(1)-C(2)-C(21)	4(2)
C(1)-C(2)-C(3)-C(4)	.7(13)
C(21)-C(2)-C(3)-C(4)	179.6(11)
C(1)-C(2)-C(3)-C(23)	-179.7(11)
C(21)-C(2)-C(3)-C(23)	-1(2)
C(1)-N(1)-C(4)-C(5)	-177.8(10)
Os(1)-N(1)-C(4)-C(5)	4(2)
C(1)-N(1)-C(4)-C(3)	-1.0(12)
Os(1)-N(1)-C(4)-C(3)	-179.1(7)
C(2)-C(3)-C(4)-N(1)	.2(13)
C(23)-C(3)-C(4)-N(1)	-179.4(10)
C(2)-C(3)-C(4)-C(5)	176.8(11)
C(23)-C(3)-C(4)-C(5)	-3(2)
N(1)-C(4)-C(5)-C(6)	-4(2)
C(3)-C(4)-C(5)-C(6)	179.8(12)
C(9)-N(2)-C(6)-C(5)	179.7(11)
Os(1)-N(2)-C(6)-C(5)	-2(2)
C(9)-N(2)-C(6)-C(7)	1.4(14)
Os(1)-N(2)-C(6)-C(7)	179.3(8)
C(4)-C(5)-C(6)-N(2)	3(2)
C(4)-C(5)-C(6)-C(7)	-178.8(12)
N(2)-C(6)-C(7)-C(8)	-2(2)
C(5)-C(6)-C(7)-C(8)	179.4(13)
N(2)-C(6)-C(7)-C(25)	175.6(13)
C(5)-C(6)-C(7)-C(25)	-3(2)
C(6)-C(7)-C(8)-C(9)	2(2)
C(25)-C(7)-C(8)-C(9)	-175.6(14)
C(6)-C(7)-C(8)-C(27)	-173.2(14)
C(25)-C(7)-C(8)-C(27)	9(3)
C(6)-N(2)-C(9)-C(10)	-176.2(12)
Os(1)-N(2)-C(9)-C(10)	6(2)
C(6)-N(2)-C(9)-C(8)	.0(13)
Os(1)-N(2)-C(9)-C(8)	-177.9(8)
C(7)-C(8)-C(9)-N(2)	-2(2)
C(27)-C(8)-C(9)-N(2)	174.1(13)
C(7)-C(8)-C(9)-C(10)	174.6(13)
C(27)-C(8)-C(9)-C(10)	-10(2)
N(2)-C(9)-C(10)-C(11)	-2(2)
C(8)-C(9)-C(10)-C(11)	-177.3(12)
C(9)-C(10)-C(11)-N(3)	1(2)
C(9)-C(10)-C(11)-C(12)	178.7(12)
C(14)-N(3)-C(11)-C(10)	179.6(11)
Os(1)-N(3)-C(11)-C(10)	-4(2)
C(14)-N(3)-C(11)-C(12)	1.0(11)
Os(1)-N(3)-C(11)-C(12)	178.0(7)
C(10)-C(11)-C(12)-C(13)	-179.2(11)
N(3)-C(11)-C(12)-C(13)	-.7(12)
C(10)-C(11)-C(12)-C(29)	-2(2)
N(3)-C(11)-C(12)-C(29)	176.6(9)
C(11)-C(12)-C(13)-C(14)	.1(12)
C(29)-C(12)-C(13)-C(14)	-177.1(10)
C(11)-C(12)-C(13)-C(31)	-179.8(10)
C(29)-C(12)-C(13)-C(31)	3(2)

C(11)-N(3)-C(14)-C(15)	-178.7(10)
Os(1)-N(3)-C(14)-C(15)	4(2)
C(11)-N(3)-C(14)-C(13)	-1.0(11)
Os(1)-N(3)-C(14)-C(13)	-177.9(6)
C(12)-C(13)-C(14)-N(3)	.5(12)
C(31)-C(13)-C(14)-N(3)	-179.5(9)
C(12)-C(13)-C(14)-C(15)	178.3(10)
C(31)-C(13)-C(14)-C(15)	-2(2)
N(3)-C(14)-C(15)-C(16)	-3(2)
C(13)-C(14)-C(15)-C(16)	-179.9(10)
C(19)-N(4)-C(16)-C(15)	-179.9(10)
Os(1)-N(4)-C(16)-C(15)	-4(2)
C(19)-N(4)-C(16)-C(17)	-.5(12)
Os(1)-N(4)-C(16)-C(17)	175.4(7)
C(14)-C(15)-C(16)-N(4)	2(2)
C(14)-C(15)-C(16)-C(17)	-177.0(11)
N(4)-C(16)-C(17)-C(18)	-.1(14)
C(15)-C(16)-C(17)-C(18)	179.3(12)
N(4)-C(16)-C(17)-C(33)	177.5(11)
C(15)-C(16)-C(17)-C(33)	-3(2)
C(16)-C(17)-C(18)-C(19)	1(2)
C(33)-C(17)-C(18)-C(19)	-176.9(12)
C(16)-C(17)-C(18)-C(35A)	159(2)
C(33)-C(17)-C(18)-C(35A)	-19(3)
C(16)-C(17)-C(18)-C(35B)	-162(2)
C(33)-C(17)-C(18)-C(35B)	21(3)
C(16)-N(4)-C(19)-C(20)	-177.8(11)
Os(1)-N(4)-C(19)-C(20)	6(2)
C(16)-N(4)-C(19)-C(18)	.8(13)
Os(1)-N(4)-C(19)-C(18)	-175.1(8)
C(17)-C(18)-C(19)-N(4)	-1(2)
C(35A)-C(18)-C(19)-N(4)	-160(2)
C(35B)-C(18)-C(19)-N(4)	162(2)
C(17)-C(18)-C(19)-C(20)	177.8(12)
C(35A)-C(18)-C(19)-C(20)	19(3)
C(35B)-C(18)-C(19)-C(20)	-19(2)
N(1)-C(1)-C(20)-C(19)	1(2)
C(2)-C(1)-C(20)-C(19)	177.0(12)
N(4)-C(19)-C(20)-C(1)	-3(2)
C(18)-C(19)-C(20)-C(1)	179.1(12)
C(3)-C(2)-C(21)-C(22)	-92(2)
C(1)-C(2)-C(21)-C(22)	86(2)
C(2)-C(3)-C(23)-C(24)	95(2)
C(4)-C(3)-C(23)-C(24)	-86.0(14)
C(8)-C(7)-C(25)-C(26)	-95(2)
C(6)-C(7)-C(25)-C(26)	88(2)
C(7)-C(8)-C(27)-C(28)	-98(2)
C(9)-C(8)-C(27)-C(28)	87(2)
C(13)-C(12)-C(29)-C(30)	90.1(14)
C(11)-C(12)-C(29)-C(30)	-86.6(13)
C(12)-C(13)-C(31)-C(32)	-95.8(14)
C(14)-C(13)-C(31)-C(32)	84.3(13)
C(18)-C(17)-C(33)-C(34)	97(2)
C(16)-C(17)-C(33)-C(34)	-80(2)
C(17)-C(18)-C(35A)-C(36A)	107(2)
C(19)-C(18)-C(35A)-C(36A)	-98(2)
C(35B)-C(18)-C(35A)-C(36A)	2(2)

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C(17)-C(18)-C(35B)-C(36B)	-94(2)
C(19)-C(18)-C(35B)-C(36B)	106(2)
C(35A)-C(18)-C(35B)-C(36B)	5(2)
C(39)-N(5)-C(37)-N(6)	-1.0(13)
Os(1)-N(5)-C(37)-N(6)	-179.3(7)
C(38)-N(6)-C(37)-N(5)	.3(14)
C(40)-N(6)-C(37)-N(5)	178.3(11)
C(37)-N(6)-C(38)-C(39)	.6(13)
C(40)-N(6)-C(38)-C(39)	-177.5(12)
N(6)-C(38)-C(39)-N(5)	-1.2(13)
C(37)-N(5)-C(39)-C(38)	1.3(12)
Os(1)-N(5)-C(39)-C(38)	179.6(8)
N(3)-Os(1)-C(41)-O(1)	-45(17)
N(2)-Os(1)-C(41)-O(1)	-135(17)
N(4)-Os(1)-C(41)-O(1)	45(17)
N(1)-Os(1)-C(41)-O(1)	135(17)
N(5)-Os(1)-C(41)-O(1)	-37(25)

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Table S19. Crystal data and structure refinement for Fe(TPP)(iPrNC)(1-MeIm).

Empirical formula	C54.50 H47 Fe N7	
Formula weight	855.84	
Temperature	198(2) K	
Wavelength	.71073 A	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.9981(7) A	alpha = 73.86 deg
	b = 13.2076(8) A	beta = 78.0500(10) deg
from 3532 reflns with 4<=theta<=28	c = 17.1650(11) A	gamma = 79.5640(10) deg
	V = 2322.9(3) A^3	Z = 2
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	0.369 mm^-1	
Crystal size	0.26 x 0.17 x 0.08 mm	
Crystal color	Black	
Theta range for data collection	1.78 to 24.00 deg	
Index ranges	-12<=h<=13, -12<=k<=16, -20<=l<=21	
Collection method	\w scans	
Reflections collected	11374 [R(int) = 0.0425]	
Independent reflections	7145 [4735 obs, I >2sigma(I)]	
Absorption correction	Semi-empirical from psi-scans	
Max. and min. transmission	1.00 and 0.8261	
Refinement (shift/err=0.066)	Full-matrix least-squares on F^2	
Data / restraints / parameters	7012 / 38 / 589	
Goodness-of-fit on F^2	1.075	
Final R indices (obs data)	R1 = 0.0659, wR2 = 0.1592	
R indices (all data)	R1 = 0.1132, wR2 = 0.1958	
calc w=1/[\s^2^(Fo^2^)+(0.0724P)^2^+3.9678P] where P=(Fo^2^+2Fc^2^)/3		
Largest diff. peak and hole	0.729 and -0.348 e.A^-3	

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Crystal preparation and structure refinement summary for Fe(TPP)(iPrNC)(1-MeIm).

Crystals were grown from dichloromethane-pentane.
The data crystal was mounted using oil (Paratone-N, Exxon) to a thin glass fiber with the (0 0 -1) scattering planes roughly normal to the spindle axis.

Systematic conditions suggested the ambiguous space group. The structure was solved by direct methods (Sheldrick, 1990). There is a solvent molecule (pentane) disorder which has been idealized. All the positions of the H-atoms have been calculated isotropically. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2^ (Sheldrick, 1993). The highest peaks in the difference Fourier map were in the vicinity of the disordered pentane molecule; the final map showed no other significant features. A final analysis of variance between observed an structure factors showed no dependence on amplitude or resolution.

Methyl H atom positions, R-CH~3~, were optimized by rotation about R-C bonds with idealized C-H, R--H and H--H distances. Remaining H atoms were included as fixed idealized contributors. H atom U's were assigned as 1.2 times Ueq of adjacent non-H atoms.

Sheldrick, G.M. (1990). SHELXS-86. Acta Cryst. A46, 467-473.

Sheldrick, G.M. (1993). SHELXL-93. Program for crystal structure refinement. Institute fur anorg chemie, G\"ottingen, Germany.

Siemens Industrial Automation, Incorporated. (1994). SAINT V4; SHELXTL V5; SMART V4. Madison, Wisconsin, USA.

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Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Fe(TPP)(iPrNC)(1-MeIm). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	8594(1)	8587(1)	7688(1)	23(1)
N(1)	7130(3)	9374(3)	7147(2)	23(1)
N(2)	8932(3)	9942(3)	7849(2)	23(1)
N(3)	10080(3)	7814(3)	8203(2)	25(1)
N(4)	8278(4)	7238(3)	7497(2)	28(1)
N(5)	6861(4)	7849(3)	9259(3)	34(1)
N(6)	9768(4)	8846(3)	6584(2)	27(1)
N(7)	11341(4)	9380(3)	5604(2)	37(1)
C(1)	6684(4)	10444(4)	7031(3)	28(1)
C(2)	5570(4)	10686(4)	6658(3)	29(1)
C(3)	5337(4)	9770(4)	6555(3)	27(1)
C(4)	6303(4)	8949(4)	6866(3)	24(1)
C(5)	6375(4)	7882(4)	6867(3)	28(1)
C(6)	7317(4)	7080(4)	7166(3)	30(1)
C(7)	7387(5)	5983(4)	7181(3)	41(1)
C(8)	8379(5)	5463(4)	7529(3)	41(1)
C(9)	8942(5)	6237(4)	7735(3)	31(1)
C(10)	9976(4)	5998(4)	8133(3)	28(1)
C(11)	10493(4)	6737(4)	8345(3)	26(1)
C(12)	11593(5)	6495(4)	8738(3)	33(1)
C(13)	11835(4)	7413(4)	8830(3)	32(1)
C(14)	10894(4)	8231(4)	8502(3)	26(1)
C(15)	10826(4)	9299(4)	8499(3)	26(1)
C(16)	9904(4)	10092(3)	8188(3)	25(1)
C(17)	9825(5)	11192(4)	8181(3)	32(1)
C(18)	8827(5)	11708(4)	7844(3)	33(1)
C(19)	8266(4)	10936(4)	7635(3)	28(1)
C(20)	7198(4)	11182(4)	7262(3)	28(1)
C(21)	5386(4)	7569(3)	6524(3)	26(1)
C(22)	5663(5)	7326(4)	5767(3)	37(1)
C(23)	4763(5)	7034(4)	5443(3)	43(1)
C(24)	3558(5)	6995(4)	5882(4)	43(1)
C(25)	3266(5)	7241(4)	6635(4)	42(1)
C(26)	4172(5)	7523(4)	6957(3)	37(1)
C(27)	10533(4)	4856(4)	8384(3)	31(1)
C(28)	10088(6)	4211(4)	9140(4)	48(2)
C(29)	10615(6)	3164(5)	9386(4)	57(2)
C(30)	11585(6)	2745(4)	8882(4)	50(2)
C(31)	12045(6)	3369(5)	8131(4)	57(2)
C(32)	11515(5)	4419(4)	7883(4)	53(2)
C(33)	11810(4)	9609(4)	8846(3)	27(1)
C(34)	11660(5)	9531(4)	9689(3)	36(1)
C(35)	12532(5)	9863(4)	10011(3)	39(1)
C(36)	13573(5)	10250(4)	9496(3)	37(1)
C(37)	13769(5)	10296(4)	8673(3)	42(1)
C(38)	12884(5)	9981(4)	8346(3)	39(1)
C(39)	6546(5)	12295(4)	7128(3)	32(1)

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C(40)	5876(5)	12667(4)	7796(4)	49(2)
C(41)	5238(6)	13693(5)	7689(5)	63(2)
C(42)	5265(6)	14356(5)	6905(5)	54(2)
C(43)	5943(7)	14011(5)	6248(4)	60(2)
C(44)	6584(6)	12974(4)	6357(3)	47(2)
C(46)	6086(5)	7129(4)	9872(3)	38(1)
C(45)	7528(4)	8215(4)	8674(3)	25(1)
C(47)	6719(6)	6006(5)	9935(5)	68(2)
C(48)	4795(6)	7295(5)	9648(5)	76(2)
C(49)	9831(5)	8389(4)	5937(3)	39(1)
C(50)	10798(5)	8727(4)	5333(3)	44(1)
C(51)	10696(5)	9428(4)	6353(3)	33(1)
C(52)	12452(5)	9894(5)	5183(4)	56(2)
C(71)	7987(14)	7617(12)	3688(10)	158(7)
C(72)	9051(15)	7179(10)	4198(10)	153(7)
C(73)	9089(16)	5966(10)	4528(14)	182(8)
C(74)	10107(26)	5536(15)	5077(14)	201(8)
C(75)	10121(29)	4327(15)	5426(16)	215(9)

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Table S21. Anisotropic displacement parameters (A^2 x 10^3) for Fe(TPP)(iPrNC)(1-MeIm). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	21(1)	24(1)	24(1)	-4(1)	-5(1)	-4(1)
N(1)	25(2)	24(2)	22(2)	-6(2)	-2(2)	-8(2)
N(2)	19(2)	27(2)	24(2)	-7(2)	-5(2)	-2(2)
N(3)	23(2)	27(2)	24(2)	-4(2)	-3(2)	-5(2)
N(4)	27(2)	26(2)	31(2)	-7(2)	-8(2)	-2(2)
N(5)	31(3)	37(3)	33(3)	-6(2)	-4(2)	-8(2)
N(6)	24(2)	28(2)	28(2)	-4(2)	-8(2)	2(2)
N(7)	30(3)	45(3)	29(2)	-3(2)	2(2)	-4(2)
C(1)	23(3)	29(3)	28(3)	-6(2)	0(2)	-2(2)
C(2)	26(3)	27(3)	33(3)	-4(2)	-9(2)	3(2)
C(3)	20(3)	32(3)	28(3)	-7(2)	-5(2)	-1(2)
C(4)	22(3)	29(3)	21(2)	-4(2)	-1(2)	-5(2)
C(5)	29(3)	31(3)	27(3)	-5(2)	-9(2)	-8(2)
C(6)	28(3)	34(3)	33(3)	-9(2)	-10(2)	-8(2)
C(7)	47(4)	26(3)	59(4)	-11(3)	-24(3)	-8(2)
C(8)	45(4)	21(3)	62(4)	-12(3)	-22(3)	-1(2)
C(9)	31(3)	26(3)	36(3)	-6(2)	-10(2)	-4(2)
C(10)	25(3)	27(3)	28(3)	-4(2)	-2(2)	-2(2)
C(11)	24(3)	26(3)	25(3)	-5(2)	-2(2)	-2(2)
C(12)	28(3)	30(3)	39(3)	-5(2)	-10(2)	0(2)
C(13)	23(3)	36(3)	39(3)	-9(2)	-11(2)	-1(2)
C(14)	22(3)	29(3)	28(3)	-8(2)	-8(2)	-4(2)
C(15)	24(3)	27(3)	24(3)	-4(2)	-2(2)	-3(2)
C(16)	27(3)	25(3)	26(3)	-8(2)	-4(2)	-4(2)
C(17)	28(3)	34(3)	37(3)	-10(2)	-9(2)	-8(2)
C(18)	32(3)	29(3)	38(3)	-8(2)	-8(2)	-4(2)
C(19)	28(3)	26(3)	31(3)	-9(2)	-7(2)	-5(2)
C(20)	27(3)	25(3)	30(3)	-7(2)	-4(2)	-3(2)
C(21)	27(3)	23(3)	31(3)	-3(2)	-11(2)	-6(2)
C(22)	34(3)	45(3)	32(3)	-8(2)	-8(2)	-7(2)
C(23)	51(4)	47(3)	37(3)	-10(3)	-22(3)	-8(3)
C(24)	45(4)	37(3)	54(4)	-4(3)	-31(3)	-10(3)
C(25)	28(3)	45(3)	54(4)	-12(3)	-10(3)	-9(2)
C(26)	34(3)	42(3)	39(3)	-12(3)	-7(3)	-12(2)
C(27)	25(3)	27(3)	46(3)	-12(2)	-11(2)	-2(2)
C(28)	50(4)	35(3)	49(4)	0(3)	-10(3)	3(3)
C(29)	65(5)	36(4)	60(4)	3(3)	-18(4)	0(3)
C(30)	45(4)	30(3)	82(5)	-13(3)	-30(4)	1(3)
C(31)	35(4)	42(4)	94(5)	-30(4)	-3(4)	8(3)
C(32)	46(4)	39(4)	67(4)	-15(3)	1(3)	1(3)
C(33)	22(3)	28(3)	30(3)	-6(2)	-9(2)	1(2)
C(34)	27(3)	47(3)	34(3)	-11(2)	-2(2)	-7(2)
C(35)	44(4)	44(3)	36(3)	-16(3)	-15(3)	-1(3)
C(36)	28(3)	34(3)	53(4)	-13(3)	-17(3)	2(2)
C(37)	25(3)	51(4)	50(4)	-11(3)	-1(3)	-11(2)
C(38)	34(3)	46(3)	40(3)	-14(3)	-9(3)	-6(2)
C(39)	27(3)	31(3)	41(3)	-8(2)	-12(2)	-6(2)

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C(40)	52(4)	29(3)	55(4)	-6(3)	2(3)	1(3)
C(41)	52(4)	46(4)	84(5)	-21(4)	5(4)	1(3)
C(42)	40(4)	36(4)	92(5)	-18(4)	-26(4)	2(3)
C(43)	91(5)	36(4)	62(4)	-2(3)	-50(4)	-3(3)
C(44)	70(4)	31(3)	44(3)	-11(3)	-25(3)	4(3)
C(46)	34(3)	43(3)	32(3)	-3(2)	5(2)	-14(2)
C(45)	25(3)	26(3)	26(3)	-5(2)	-8(2)	-4(2)
C(47)	51(4)	41(4)	96(5)	7(4)	-14(4)	-2(3)
C(48)	35(4)	55(4)	124(7)	7(4)	-17(4)	-9(3)
C(49)	44(4)	45(3)	32(3)	-14(3)	-6(3)	-9(3)
C(50)	41(4)	59(4)	29(3)	-17(3)	-3(3)	5(3)
C(51)	33(3)	31(3)	32(3)	-7(2)	0(2)	-4(2)
C(52)	41(4)	68(4)	49(4)	-2(3)	5(3)	-12(3)
C(71)	154(16)	236(14)	117(13)	-118(12)	85(10)	-116(14)
C(72)	153(15)	224(13)	119(12)	-127(12)	86(10)	-113(13)
C(73)	195(16)	223(12)	150(13)	-135(12)	96(11)	-88(14)
C(74)	220(16)	230(13)	167(15)	-126(14)	86(13)	-82(14)
C(75)	238(18)	233(14)	181(17)	-124(15)	93(15)	-81(15)

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Table S22. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Fe(TPP)(iPrNC)(1-MeIm). Treatment of hydrogen atoms not specifically described in the refinement summary was "noref."

	x	y	z	U(eq)
H(2)	5090(4)	11364(4)	6513(3)	35
H(3)	4665(4)	9680(4)	6321(3)	32
H(7)	6833(5)	5681(4)	6981(3)	50
H(8)	8659(5)	4722(4)	7623(3)	49
H(12)	12058(5)	5814(4)	8901(3)	40
H(13)	12502(4)	7502(4)	9068(3)	39
H(17)	10381(5)	11495(4)	8380(3)	38
H(18)	8539(5)	12447(4)	7758(3)	39
H(22)	6487(5)	7361(4)	5463(3)	44
H(23)	4972(5)	6863(4)	4925(3)	51
H(24)	2932(5)	6799(4)	5665(4)	51
H(25)	2438(5)	7216(4)	6935(4)	50
H(26)	3962(5)	7685(4)	7478(3)	44
H(28)	9410(6)	4493(4)	9495(4)	57
H(29)	10301(6)	2735(5)	9907(4)	68
H(30)	11940(6)	2024(4)	9050(4)	60
H(31)	12727(6)	3081(5)	7782(4)	69
H(32)	11833(5)	4843(4)	7361(4)	63
H(34)	10952(5)	9247(4)	10046(3)	43
H(35)	12411(5)	9824(4)	10583(3)	47
H(36)	14164(5)	10489(4)	9715(3)	44
H(37)	14505(5)	10541(4)	8327(3)	51
H(38)	13015(5)	10021(4)	7774(3)	47
H(40)	5854(5)	12213(4)	8334(4)	59
H(41)	4785(6)	13937(5)	8151(5)	76
H(42)	4812(6)	15051(5)	6827(5)	65
H(43)	5982(7)	14474(5)	5712(4)	72
H(44)	7050(6)	12739(4)	5894(3)	57
H(46)	6007(5)	7295(4)	10416(3)	45
H(47A)	6213(20)	5516(5)	10360(17)	82
H(47B)	7551(16)	5938(9)	10081(24)	82
H(47C)	6806(33)	5833(11)	9405(8)	82
H(48A)	4261(12)	6829(25)	10074(13)	92
H(48B)	4857(7)	7126(32)	9119(13)	92
H(48C)	4428(17)	8038(10)	9605(26)	92
H(49)	9287(5)	7916(4)	5918(3)	47
H(50)	11043(5)	8540(4)	4821(3)	53
H(51)	10888(5)	9835(4)	6679(3)	40
H(52A)	12379(15)	10212(23)	4603(6)	68
H(52B)	13201(6)	9365(7)	5220(18)	68
H(52C)	12519(18)	10450(18)	5443(13)	68
H(71A)	7963(14)	8389(12)	3478(10)	190
H(71B)	7184(14)	7455(12)	4035(10)	190
H(71C)	8135(14)	7287(12)	3226(10)	190

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H(72A)	8909(15)	7516(10)	4664(10)	184
H(72B)	9863(15)	7349(10)	3851(10)	184
H(73A)	9276(16)	5626(10)	4063(14)	219
H(73B)	8263(16)	5795(10)	4850(14)	219
H(74A)	10937(26)	5690(15)	4751(14)	241
H(74B)	9932(26)	5891(15)	5534(14)	241
H(75A)	10768(29)	4054(15)	5775(16)	258
H(75B)	10302(29)	3979(15)	4972(16)	258
H(75C)	9300(29)	4179(15)	5753(16)	258

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Table S23. Bond lengths [A] and angles [deg] for Fe(TPP)(iPrNC)(1-MeIm).

Fe(1)-C(45)	1.846(5)
Fe(1)-N(2)	1.994(4)
Fe(1)-N(3)	1.996(4)
Fe(1)-N(4)	2.000(4)
Fe(1)-N(1)	2.004(4)
Fe(1)-N(6)	2.041(4)
N(1)-C(4)	1.375(6)
N(1)-C(1)	1.383(6)
N(2)-C(19)	1.376(5)
N(2)-C(16)	1.384(6)
N(3)-C(14)	1.376(6)
N(3)-C(11)	1.382(6)
N(4)-C(6)	1.370(6)
N(4)-C(9)	1.386(6)
N(5)-C(45)	1.155(6)
N(5)-C(46)	1.450(6)
N(6)-C(51)	1.318(6)
N(6)-C(49)	1.388(6)
N(7)-C(51)	1.347(6)
N(7)-C(50)	1.357(7)
N(7)-C(52)	1.462(7)
C(1)-C(20)	1.390(6)
C(1)-C(2)	1.444(6)
C(2)-C(3)	1.345(6)
C(3)-C(4)	1.444(6)
C(4)-C(5)	1.396(6)
C(5)-C(6)	1.407(6)
C(5)-C(21)	1.504(6)
C(6)-C(7)	1.430(7)
C(7)-C(8)	1.338(7)
C(8)-C(9)	1.439(7)
C(9)-C(10)	1.390(6)
C(10)-C(11)	1.376(6)
C(10)-C(27)	1.500(6)
C(11)-C(12)	1.449(6)
C(12)-C(13)	1.343(7)
C(13)-C(14)	1.433(6)
C(14)-C(15)	1.398(6)
C(15)-C(16)	1.394(6)
C(15)-C(33)	1.502(6)
C(16)-C(17)	1.436(6)
C(17)-C(18)	1.333(6)
C(18)-C(19)	1.440(6)
C(19)-C(20)	1.397(6)
C(20)-C(39)	1.492(6)
C(21)-C(22)	1.384(7)
C(21)-C(26)	1.391(7)
C(22)-C(23)	1.387(7)
C(23)-C(24)	1.385(8)
C(24)-C(25)	1.380(8)
C(25)-C(26)	1.382(7)
C(27)-C(32)	1.380(7)
C(27)-C(28)	1.387(7)

C(28)-C(29)	1.383(7)
C(29)-C(30)	1.365(8)
C(30)-C(31)	1.373(9)
C(31)-C(32)	1.388(8)
C(33)-C(38)	1.388(7)
C(33)-C(34)	1.399(7)
C(34)-C(35)	1.387(7)
C(35)-C(36)	1.377(7)
C(36)-C(37)	1.371(7)
C(37)-C(38)	1.392(7)
C(39)-C(44)	1.374(7)
C(39)-C(40)	1.389(7)
C(40)-C(41)	1.390(8)
C(41)-C(42)	1.384(9)
C(42)-C(43)	1.361(9)
C(43)-C(44)	1.403(7)
C(46)-C(47)	1.504(7)
C(46)-C(48)	1.510(8)
C(49)-C(50)	1.365(7)
C(71)-C(72)	1.5395(11)
C(72)-C(73)	1.5400(11)
C(73)-C(74)	1.5402(11)
C(74)-C(75)	1.5402(11)

C(45)-Fe(1)-N(2)	96.1(2)
C(45)-Fe(1)-N(3)	91.4(2)
N(2)-Fe(1)-N(3)	89.9(2)
C(45)-Fe(1)-N(4)	85.3(2)
N(2)-Fe(1)-N(4)	178.5(2)
N(3)-Fe(1)-N(4)	90.3(2)
C(45)-Fe(1)-N(1)	89.9(2)
N(2)-Fe(1)-N(1)	89.92(14)
N(3)-Fe(1)-N(1)	178.7(2)
N(4)-Fe(1)-N(1)	89.9(2)
C(45)-Fe(1)-N(6)	174.1(2)
N(2)-Fe(1)-N(6)	89.7(2)
N(3)-Fe(1)-N(6)	87.7(2)
N(4)-Fe(1)-N(6)	88.9(2)
N(1)-Fe(1)-N(6)	90.96(14)
C(4)-N(1)-C(1)	105.5(4)
C(4)-N(1)-Fe(1)	127.2(3)
C(1)-N(1)-Fe(1)	127.2(3)
C(19)-N(2)-C(16)	104.8(4)
C(19)-N(2)-Fe(1)	127.6(3)
C(16)-N(2)-Fe(1)	127.6(3)
C(14)-N(3)-C(11)	105.5(4)
C(14)-N(3)-Fe(1)	127.7(3)
C(11)-N(3)-Fe(1)	126.8(3)
C(6)-N(4)-C(9)	105.0(4)
C(6)-N(4)-Fe(1)	128.1(3)
C(9)-N(4)-Fe(1)	126.7(3)
C(45)-N(5)-C(46)	162.6(5)
C(51)-N(6)-C(49)	104.8(4)
C(51)-N(6)-Fe(1)	127.1(3)
C(49)-N(6)-Fe(1)	127.9(3)
C(51)-N(7)-C(50)	106.9(4)
C(51)-N(7)-C(52)	126.3(5)

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C(50)-N(7)-C(52)	126.7(5)
N(1)-C(1)-C(20)	125.6(4)
N(1)-C(1)-C(2)	110.0(4)
C(20)-C(1)-C(2)	124.4(4)
C(3)-C(2)-C(1)	107.2(4)
C(2)-C(3)-C(4)	107.0(4)
N(1)-C(4)-C(5)	125.8(4)
N(1)-C(4)-C(3)	110.3(4)
C(5)-C(4)-C(3)	123.9(4)
C(4)-C(5)-C(6)	124.1(4)
C(4)-C(5)-C(21)	118.0(4)
C(6)-C(5)-C(21)	117.8(4)
N(4)-C(6)-C(5)	124.8(4)
N(4)-C(6)-C(7)	110.7(4)
C(5)-C(6)-C(7)	124.5(4)
C(8)-C(7)-C(6)	107.3(4)
C(7)-C(8)-C(9)	107.1(4)
N(4)-C(9)-C(10)	125.7(4)
N(4)-C(9)-C(8)	109.8(4)
C(10)-C(9)-C(8)	124.4(4)
C(11)-C(10)-C(9)	124.2(4)
C(11)-C(10)-C(27)	117.5(4)
C(9)-C(10)-C(27)	118.2(4)
C(10)-C(11)-N(3)	126.2(4)
C(10)-C(11)-C(12)	124.3(4)
N(3)-C(11)-C(12)	109.4(4)
C(13)-C(12)-C(11)	107.4(4)
C(12)-C(13)-C(14)	107.0(4)
N(3)-C(14)-C(15)	125.6(4)
N(3)-C(14)-C(13)	110.7(4)
C(15)-C(14)-C(13)	123.7(4)
C(16)-C(15)-C(14)	123.7(4)
C(16)-C(15)-C(33)	118.2(4)
C(14)-C(15)-C(33)	118.1(4)
N(2)-C(16)-C(15)	125.5(4)
N(2)-C(16)-C(17)	110.2(4)
C(15)-C(16)-C(17)	124.3(4)
C(18)-C(17)-C(16)	107.3(4)
C(17)-C(18)-C(19)	107.2(4)
N(2)-C(19)-C(20)	125.7(4)
N(2)-C(19)-C(18)	110.4(4)
C(20)-C(19)-C(18)	123.9(4)
C(1)-C(20)-C(19)	123.9(4)
C(1)-C(20)-C(39)	118.0(4)
C(19)-C(20)-C(39)	118.1(4)
C(22)-C(21)-C(26)	118.4(4)
C(22)-C(21)-C(5)	120.7(5)
C(26)-C(21)-C(5)	120.9(4)
C(21)-C(22)-C(23)	121.5(5)
C(24)-C(23)-C(22)	119.3(5)
C(25)-C(24)-C(23)	119.9(5)
C(24)-C(25)-C(26)	120.4(5)
C(25)-C(26)-C(21)	120.5(5)
C(32)-C(27)-C(28)	117.9(5)
C(32)-C(27)-C(10)	121.5(5)
C(28)-C(27)-C(10)	120.6(5)

C(29)-C(28)-C(27)	121.0(6)
C(30)-C(29)-C(28)	120.2(6)
C(29)-C(30)-C(31)	119.8(5)
C(30)-C(31)-C(32)	120.0(6)
C(27)-C(32)-C(31)	121.0(6)
C(38)-C(33)-C(34)	118.2(5)
C(38)-C(33)-C(15)	121.5(4)
C(34)-C(33)-C(15)	120.3(4)
C(35)-C(34)-C(33)	120.9(5)
C(36)-C(35)-C(34)	119.5(5)
C(37)-C(36)-C(35)	120.9(5)
C(36)-C(37)-C(38)	119.7(5)
C(33)-C(38)-C(37)	120.9(5)
C(44)-C(39)-C(40)	118.4(5)
C(44)-C(39)-C(20)	121.9(5)
C(40)-C(39)-C(20)	119.7(4)
C(39)-C(40)-C(41)	121.1(6)
C(42)-C(41)-C(40)	119.7(6)
C(43)-C(42)-C(41)	119.8(6)
C(42)-C(43)-C(44)	120.3(6)
C(39)-C(44)-C(43)	120.7(6)
N(5)-C(46)-C(47)	109.0(5)
N(5)-C(46)-C(48)	109.5(4)
C(47)-C(46)-C(48)	112.5(5)
N(5)-C(45)-Fe(1)	170.1(4)
C(50)-C(49)-N(6)	109.2(5)
N(7)-C(50)-C(49)	106.8(5)
N(6)-C(51)-N(7)	112.3(5)
C(71)-C(72)-C(73)	109.51(10)
C(72)-C(73)-C(74)	109.48(10)
C(75)-C(74)-C(73)	109.50(10)

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Table S24. Torsion angles [deg] for Fe(TPP)(iPrNC)(1-MeIm).

C(45)-Fe(1)-N(1)-C(4)	-80.8(4)
N(2)-Fe(1)-N(1)-C(4)	-176.9(4)
N(3)-Fe(1)-N(1)-C(4)	103(7)
N(4)-Fe(1)-N(1)-C(4)	4.6(4)
N(6)-Fe(1)-N(1)-C(4)	93.4(4)
C(45)-Fe(1)-N(1)-C(1)	94.0(4)
N(2)-Fe(1)-N(1)-C(1)	-2.1(4)
N(3)-Fe(1)-N(1)-C(1)	-83(7)
N(4)-Fe(1)-N(1)-C(1)	179.4(4)
N(6)-Fe(1)-N(1)-C(1)	-91.8(4)
C(45)-Fe(1)-N(2)-C(19)	-88.7(4)
N(3)-Fe(1)-N(2)-C(19)	179.8(4)
N(4)-Fe(1)-N(2)-C(19)	83(6)
N(1)-Fe(1)-N(2)-C(19)	1.2(4)
N(6)-Fe(1)-N(2)-C(19)	92.1(4)
C(45)-Fe(1)-N(2)-C(16)	92.6(4)
N(3)-Fe(1)-N(2)-C(16)	1.2(4)
N(4)-Fe(1)-N(2)-C(16)	-96(6)
N(1)-Fe(1)-N(2)-C(16)	-177.5(4)
N(6)-Fe(1)-N(2)-C(16)	-86.5(4)
C(45)-Fe(1)-N(3)-C(14)	-96.7(4)
N(2)-Fe(1)-N(3)-C(14)	-.6(4)
N(4)-Fe(1)-N(3)-C(14)	178.0(4)
N(1)-Fe(1)-N(3)-C(14)	80(7)
N(6)-Fe(1)-N(3)-C(14)	89.2(4)
C(45)-Fe(1)-N(3)-C(11)	82.3(4)
N(2)-Fe(1)-N(3)-C(11)	178.4(4)
N(4)-Fe(1)-N(3)-C(11)	-3.1(4)
N(1)-Fe(1)-N(3)-C(11)	-101(7)
N(6)-Fe(1)-N(3)-C(11)	-91.9(4)
C(45)-Fe(1)-N(4)-C(6)	86.0(4)
N(2)-Fe(1)-N(4)-C(6)	-85(6)
N(3)-Fe(1)-N(4)-C(6)	177.4(4)
N(1)-Fe(1)-N(4)-C(6)	-3.9(4)
N(6)-Fe(1)-N(4)-C(6)	-94.9(4)
C(45)-Fe(1)-N(4)-C(9)	-88.5(4)
N(2)-Fe(1)-N(4)-C(9)	100(6)
N(3)-Fe(1)-N(4)-C(9)	2.9(4)
N(1)-Fe(1)-N(4)-C(9)	-178.4(4)
N(6)-Fe(1)-N(4)-C(9)	90.6(4)
C(45)-Fe(1)-N(6)-C(51)	-147(2)
N(2)-Fe(1)-N(6)-C(51)	24.2(4)
N(3)-Fe(1)-N(6)-C(51)	-65.7(4)
N(4)-Fe(1)-N(6)-C(51)	-156.0(4)
N(1)-Fe(1)-N(6)-C(51)	114.1(4)
C(45)-Fe(1)-N(6)-C(49)	27(2)
N(2)-Fe(1)-N(6)-C(49)	-161.2(4)
N(3)-Fe(1)-N(6)-C(49)	108.9(4)
N(4)-Fe(1)-N(6)-C(49)	18.5(4)
N(1)-Fe(1)-N(6)-C(49)	-71.3(4)
C(4)-N(1)-C(1)-C(20)	177.0(5)
Fe(1)-N(1)-C(1)-C(20)	1.3(7)
C(4)-N(1)-C(1)-C(2)	-1.0(5)

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Fe(1)-N(1)-C(1)-C(2)	-176.7(3)
N(1)-C(1)-C(2)-C(3)	.5(5)
C(20)-C(1)-C(2)-C(3)	-177.6(5)
C(1)-C(2)-C(3)-C(4)	.2(5)
C(1)-N(1)-C(4)-C(5)	-179.5(4)
Fe(1)-N(1)-C(4)-C(5)	-3.8(7)
C(1)-N(1)-C(4)-C(3)	1.2(5)
Fe(1)-N(1)-C(4)-C(3)	176.9(3)
C(2)-C(3)-C(4)-N(1)	-.9(5)
C(2)-C(3)-C(4)-C(5)	179.8(5)
N(1)-C(4)-C(5)-C(6)	.5(8)
C(3)-C(4)-C(5)-C(6)	179.7(4)
N(1)-C(4)-C(5)-C(21)	-179.4(4)
C(3)-C(4)-C(5)-C(21)	-.1(7)
C(9)-N(4)-C(6)-C(5)	177.8(5)
Fe(1)-N(4)-C(6)-C(5)	2.3(7)
C(9)-N(4)-C(6)-C(7)	-1.0(5)
Fe(1)-N(4)-C(6)-C(7)	-176.5(3)
C(4)-C(5)-C(6)-N(4)	.3(8)
C(21)-C(5)-C(6)-N(4)	-179.9(4)
C(4)-C(5)-C(6)-C(7)	179.0(5)
C(21)-C(5)-C(6)-C(7)	-1.2(7)
N(4)-C(6)-C(7)-C(8)	.7(6)
C(5)-C(6)-C(7)-C(8)	-178.1(5)
C(6)-C(7)-C(8)-C(9)	-.1(6)
C(6)-N(4)-C(9)-C(10)	-177.4(5)
Fe(1)-N(4)-C(9)-C(10)	-1.8(7)
C(6)-N(4)-C(9)-C(8)	1.0(5)
Fe(1)-N(4)-C(9)-C(8)	176.5(3)
C(7)-C(8)-C(9)-N(4)	-.5(6)
C(7)-C(8)-C(9)-C(10)	177.8(5)
N(4)-C(9)-C(10)-C(11)	-.4(8)
C(8)-C(9)-C(10)-C(11)	-178.5(5)
N(4)-C(9)-C(10)-C(27)	176.8(4)
C(8)-C(9)-C(10)-C(27)	-1.3(8)
C(9)-C(10)-C(11)-N(3)	.2(8)
C(27)-C(10)-C(11)-N(3)	-177.0(4)
C(9)-C(10)-C(11)-C(12)	-178.1(5)
C(27)-C(10)-C(11)-C(12)	4.8(7)
C(14)-N(3)-C(11)-C(10)	-178.7(5)
Fe(1)-N(3)-C(11)-C(10)	2.2(7)
C(14)-N(3)-C(11)-C(12)	-.2(5)
Fe(1)-N(3)-C(11)-C(12)	-179.4(3)
C(10)-C(11)-C(12)-C(13)	178.5(5)
N(3)-C(11)-C(12)-C(13)	.0(6)
C(11)-C(12)-C(13)-C(14)	.2(6)
C(11)-N(3)-C(14)-C(15)	-179.0(4)
Fe(1)-N(3)-C(14)-C(15)	.1(7)
C(11)-N(3)-C(14)-C(13)	.4(5)
Fe(1)-N(3)-C(14)-C(13)	179.5(3)
C(12)-C(13)-C(14)-N(3)	-.4(6)
C(12)-C(13)-C(14)-C(15)	179.0(5)
N(3)-C(14)-C(15)-C(16)	.0(8)
C(13)-C(14)-C(15)-C(16)	-179.3(5)
N(3)-C(14)-C(15)-C(33)	-179.4(4)
C(13)-C(14)-C(15)-C(33)	1.3(7)
C(19)-N(2)-C(16)-C(15)	179.7(4)

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Fe(1)-N(2)-C(16)-C(15)	-1.4(7)
C(19)-N(2)-C(16)-C(17)	.1(5)
Fe(1)-N(2)-C(16)-C(17)	179.1(3)
C(14)-C(15)-C(16)-N(2)	.6(7)
C(33)-C(15)-C(16)-N(2)	-179.9(4)
C(14)-C(15)-C(16)-C(17)	-179.9(5)
C(33)-C(15)-C(16)-C(17)	-.4(7)
N(2)-C(16)-C(17)-C(18)	-.1(6)
C(15)-C(16)-C(17)-C(18)	-179.6(5)
C(16)-C(17)-C(18)-C(19)	.0(6)
C(16)-N(2)-C(19)-C(20)	179.5(5)
Fe(1)-N(2)-C(19)-C(20)	.6(7)
C(16)-N(2)-C(19)-C(18)	-.2(5)
Fe(1)-N(2)-C(19)-C(18)	-179.1(3)
C(17)-C(18)-C(19)-N(2)	.1(6)
C(17)-C(18)-C(19)-C(20)	-179.6(5)
N(1)-C(1)-C(20)-C(19)	1.2(8)
C(2)-C(1)-C(20)-C(19)	178.9(5)
N(1)-C(1)-C(20)-C(39)	-176.8(4)
C(2)-C(1)-C(20)-C(39)	1.0(7)
N(2)-C(19)-C(20)-C(1)	-2.2(8)
C(18)-C(19)-C(20)-C(1)	177.4(5)
N(2)-C(19)-C(20)-C(39)	175.8(4)
C(18)-C(19)-C(20)-C(39)	-4.6(7)
C(4)-C(5)-C(21)-C(22)	106.4(5)
C(6)-C(5)-C(21)-C(22)	-73.4(6)
C(4)-C(5)-C(21)-C(26)	-73.2(6)
C(6)-C(5)-C(21)-C(26)	107.0(5)
C(26)-C(21)-C(22)-C(23)	-.5(7)
C(5)-C(21)-C(22)-C(23)	179.9(4)
C(21)-C(22)-C(23)-C(24)	.7(8)
C(22)-C(23)-C(24)-C(25)	-.3(8)
C(23)-C(24)-C(25)-C(26)	-.2(8)
C(24)-C(25)-C(26)-C(21)	.4(8)
C(22)-C(21)-C(26)-C(25)	-.1(7)
C(5)-C(21)-C(26)-C(25)	179.6(4)
C(11)-C(10)-C(27)-C(32)	-89.3(6)
C(9)-C(10)-C(27)-C(32)	93.3(6)
C(11)-C(10)-C(27)-C(28)	89.3(6)
C(9)-C(10)-C(27)-C(28)	-88.0(6)
C(32)-C(27)-C(28)-C(29)	.3(8)
C(10)-C(27)-C(28)-C(29)	-178.4(5)
C(27)-C(28)-C(29)-C(30)	-.4(9)
C(28)-C(29)-C(30)-C(31)	.6(9)
C(29)-C(30)-C(31)-C(32)	-.7(9)
C(28)-C(27)-C(32)-C(31)	-.4(8)
C(10)-C(27)-C(32)-C(31)	178.3(5)
C(30)-C(31)-C(32)-C(27)	.6(9)
C(16)-C(15)-C(33)-C(38)	-85.5(6)
C(14)-C(15)-C(33)-C(38)	94.0(6)
C(16)-C(15)-C(33)-C(34)	94.3(5)
C(14)-C(15)-C(33)-C(34)	-86.3(6)
C(38)-C(33)-C(34)-C(35)	2.9(7)
C(15)-C(33)-C(34)-C(35)	-176.9(4)
C(33)-C(34)-C(35)-C(36)	-1.6(7)
C(34)-C(35)-C(36)-C(37)	-1.0(8)
C(35)-C(36)-C(37)-C(38)	2.2(8)

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C(34)-C(33)-C(38)-C(37)	-1.7(7)
C(15)-C(33)-C(38)-C(37)	178.0(4)
C(36)-C(37)-C(38)-C(33)	-.8(8)
C(1)-C(20)-C(39)-C(44)	-73.3(6)
C(19)-C(20)-C(39)-C(44)	108.6(6)
C(1)-C(20)-C(39)-C(40)	106.7(6)
C(19)-C(20)-C(39)-C(40)	-71.4(6)
C(44)-C(39)-C(40)-C(41)	1.3(9)
C(20)-C(39)-C(40)-C(41)	-178.7(5)
C(39)-C(40)-C(41)-C(42)	.1(10)
C(40)-C(41)-C(42)-C(43)	-1.7(10)
C(41)-C(42)-C(43)-C(44)	1.9(9)
C(40)-C(39)-C(44)-C(43)	-1.1(8)
C(20)-C(39)-C(44)-C(43)	178.8(5)
C(42)-C(43)-C(44)-C(39)	-.4(9)
C(45)-N(5)-C(46)-C(47)	38(2)
C(45)-N(5)-C(46)-C(48)	-86(2)
C(46)-N(5)-C(45)-Fe(1)	0(4)
N(2)-Fe(1)-C(45)-N(5)	-175(2)
N(3)-Fe(1)-C(45)-N(5)	-85(2)
N(4)-Fe(1)-C(45)-N(5)	5(2)
N(1)-Fe(1)-C(45)-N(5)	95(2)
N(6)-Fe(1)-C(45)-N(5)	-4(4)
C(51)-N(6)-C(49)-C(50)	-.6(5)
Fe(1)-N(6)-C(49)-C(50)	-176.1(3)
C(51)-N(7)-C(50)-C(49)	-.3(6)
C(52)-N(7)-C(50)-C(49)	176.9(5)
N(6)-C(49)-C(50)-N(7)	.6(6)
C(49)-N(6)-C(51)-N(7)	.4(5)
Fe(1)-N(6)-C(51)-N(7)	176.0(3)
C(50)-N(7)-C(51)-N(6)	-.1(6)
C(52)-N(7)-C(51)-N(6)	-177.3(5)
C(71)-C(72)-C(73)-C(74)	-177(2)
C(72)-C(73)-C(74)-C(75)	179(2)