Supplementary material

Table S1. Complete Crystallographic Details for [Fe(TEtP)(Cl)].

formula	$C_{28}H_{28}ClFeN_4$
FW, amu	511.84
a, Å	10.1710(5)
b, Å	11.309(3)
c, Å	12.170(3)
α, deg	91.774(9)
β, deg	113.170(14)
γ, deg	112.149(9)
V, Å^3	1165.2(4)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.459
F(000)	534
μ, mm^{-1}	0.787
power and current settings	50kV, 40mA
detector distance, mm	40
detector tilt angle, deg	−25
image time, sec	30
increment, deg	0.4
crystal dimensions, mm	0.43 × 0.30 × 0.03
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	130(2)
diffractometer	Enraf Nonius FAST
θ range for collected data, deg	2.31–29.75
index range	$-12 \leq h \leq 14$
	$-15 \leq k \leq 15$
	$-16 \leq l \leq 10$
total data collected	10744
absorption correction	DIFABS
relative transmission coefficients (I)	1.000 and 0.684
unique data	5831 (R_{int} = 0.0983)
unique observed data [I > 2σ(I)]	4545
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	5831/0/311
goodness-of-fit (based on F^2)	1.055
max($\Delta\rho$), e/Å^3	2.156
min($\Delta\rho$), e/Å^3	−1.094
final R indices [I > 2σ(I)]	R_1 = 0.0844, wR_2 = 0.2073
final R indices (all data)	R_1 = 0.1060, wR_2 = 0.2254

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

atom	x	y	z	U(eq)
Fe(1)	0.40905(7)	0.28864(5)	0.32123(5)	0.0274(2)
Cl	0.51041(14)	0.19808(11)	0.22573(10)	0.0394(3)
N(1)	0.2017(4)	0.1327(3)	0.2915(3)	0.0267(7)
N(2)	0.2728(4)	0.3526(3)	0.1851(3)	0.0285(7)
N(3)	0.5733(4)	0.4789(3)	0.3883(3)	0.0277(7)
N(4)	0.5040(4)	0.2575(3)	0.4946(3)	0.0268(7)
C(a1)	0.1885(5)	0.0335(4)	0.3565(4)	0.0282(8)
C(a2)	0.0591(5)	0.0884(4)	0.1876(4)	0.0320(9)
C(a3)	0.1206(6)	0.2782(5)	0.0958(4)	0.0362(10)
C(a4)	0.3275(6)	0.4693(5)	0.1485(4)	0.0387(10)
C(a5)	0.5870(5)	0.5778(4)	0.3236(4)	0.0320(9)
C(a6)	0.7118(5)	0.5265(4)	0.4952(4)	0.0305(8)
C(a7)	0.6523(5)	0.3342(4)	0.5864(4)	0.0314(8)
C(a8)	0.4491(5)	0.1415(4)	0.5316(4)	0.0294(8)
C(b1)	0.0353(5)	−0.0727(5)	0.2910(5)	0.0389(10)
C(b2)	−0.0425(5)	−0.0390(5)	0.1892(5)	0.0394(10)
C(b3)	0.0800(7)	0.3512(6)	0.0042(5)	0.0522(14)
C(b4)	0.2045(8)	0.4669(6)	0.0359(5)	0.0546(15)
C(b5)	0.7355(6)	0.6882(4)	0.3922(5)	0.0386(10)
C(b6)	0.8105(5)	0.6570(4)	0.4968(5)	0.0375(10)
C(b7)	0.6891(6)	0.2639(5)	0.6813(4)	0.0421(11)
C(b8)	0.5670(6)	0.1463(5)	0.6481(4)	0.0388(10)
C(m1)	0.3026(5)	0.0356(4)	0.4680(4)	0.0293(8)
C(m2)	0.0194(5)	0.1543(5)	0.0954(4)	0.0353(9)
C(m3)	0.4736(6)	0.5744(4)	0.2109(4)	0.0383(10)
C(m4)	0.7511(5)	0.4599(4)	0.5891(4)	0.0323(9)
C(11)	0.2642(6)	−0.0806(4)	0.5279(4)	0.0371(10)
C(21)	−0.1465(6)	0.0917(6)	−0.0078(5)	0.0493(13)
C(31)	0.5093(9)	0.6915(5)	0.1510(5)	0.0617(17)
C(41)	0.9127(5)	0.5273(5)	0.6983(4)	0.0437(11)
C(12)	0.1997(6)	−0.0638(5)	0.6170(5)	0.0408(10)
C(22)	−0.2637(7)	0.1220(7)	0.0263(6)	0.0598(16)
C(32)	0.5679(11)	0.6774(6)	0.0592(6)	0.085(3)
C(42)	1.0404(6)	0.5008(8)	0.6804(5)	0.0624(17)

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

Table S3. Bond Lengths for [Fe(TEtP)(Cl)][a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(3)	2.048(3)	C(a5)–C(m3)	1.390(6)
Fe(1)–N(4)	2.051(3)	C(a5)–C(b5)	1.435(6)
Fe(1)–N(2)	2.052(3)	C(a6)–C(m4)	1.398(6)
Fe(1)–N(1)	2.060(3)	C(a6)–C(b6)	1.433(6)
Fe(1)–Cl	2.2644(13)	C(a7)–C(m4)	1.388(6)
N(1)–C(a2)	1.386(5)	C(a7)–C(b7)	1.431(6)
N(1)–C(a1)	1.389(5)	C(a8)–C(m1)	1.394(6)
N(2)–C(a3)	1.387(6)	C(a8)–C(b8)	1.435(6)
N(2)–C(a4)	1.389(5)	C(b1)–C(b2)	1.338(7)
N(3)–C(a6)	1.382(5)	C(b3)–C(b4)	1.341(9)
N(3)–C(a5)	1.383(5)	C(b5)–C(b6)	1.339(7)
N(4)–C(a7)	1.379(5)	C(b7)–C(b8)	1.342(7)
N(4)–C(a8)	1.385(5)	C(m1)–C(11)	1.519(6)
C(a1)–C(m1)	1.388(6)	C(m2)–C(21)	1.518(6)
C(a1)–C(b1)	1.434(6)	C(m3)–C(31)	1.524(6)
C(a2)–C(m2)	1.379(6)	C(m4)–C(41)	1.523(6)
C(a2)–C(b2)	1.428(6)	C(11)–C(12)	1.512(7)
C(a3)–C(m2)	1.390(7)	C(21)–C(22)	1.548(8)
C(a3)–C(b3)	1.431(6)	C(31)–C(32)	1.488(10)
C(a4)–C(m3)	1.386(7)	C(41)–C(42)	1.529(8)
C(a4)–C(b4)	1.438(7)		

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

Table S4. Bond Angles for [Fe(TEtP)(Cl)][a]

angle	degree	angle	degree
N(3)–Fe(1)–N(4)	87.45(14)	N(3)–C(a5)–C(b5)	109.8(4)
N(3)–Fe(1)–N(2)	87.49(14)	C(m3)–C(a5)–C(b5)	124.2(4)
N(4)–Fe(1)–N(2)	155.21(14)	N(3)–C(a6)–C(m4)	126.1(4)
N(3)–Fe(1)–N(1)	154.47(14)	N(3)–C(a6)–C(b6)	109.5(4)
N(4)–Fe(1)–N(1)	87.54(14)	C(m4)–C(a6)–C(b6)	124.4(4)
N(2)–Fe(1)–N(1)	86.66(14)	N(4)–C(a7)–C(m4)	126.4(4)
N(3)–Fe(1)–Cl	103.55(11)	N(4)–C(a7)–C(b7)	109.0(4)
N(4)–Fe(1)–Cl	101.75(10)	C(m4)–C(a7)–C(b7)	124.6(4)
N(2)–Fe(1)–Cl	103.03(11)	N(4)–C(a8)–C(m1)	126.4(4)
N(1)–Fe(1)–Cl	101.98(10)	N(4)–C(a8)–C(b8)	109.3(4)
C(a2)–N(1)–C(a1)	105.9(3)	C(m1)–C(a8)–C(b8)	124.3(4)
C(a2)–N(1)–Fe(1)	126.7(3)	C(b2)–C(b1)–C(a1)	107.7(4)
C(a1)–N(1)–Fe(1)	125.5(3)	C(b1)–C(b2)–C(a2)	108.0(4)
C(a3)–N(2)–C(a4)	106.3(3)	C(b4)–C(b3)–C(a3)	107.9(4)
C(a3)–N(2)–Fe(1)	126.7(3)	C(b3)–C(b4)–C(a4)	107.9(5)
C(a4)–N(2)–Fe(1)	125.5(3)	C(b6)–C(b5)–C(a5)	107.2(4)
C(a6)–N(3)–C(a5)	105.6(3)	C(b5)–C(b6)–C(a6)	107.8(4)
C(a6)–N(3)–Fe(1)	126.5(3)	C(b8)–C(b7)–C(a7)	108.3(4)
C(a5)–N(3)–Fe(1)	126.3(3)	C(b7)–C(b8)–C(a8)	107.1(4)
C(a7)–N(4)–C(a8)	106.3(3)	C(a1)–C(m1)–C(a8)	123.6(4)
C(a7)–N(4)–Fe(1)	126.2(3)	C(a1)–C(m1)–C(11)	118.7(4)
C(a8)–N(4)–Fe(1)	125.7(3)	C(a8)–C(m1)–C(11)	117.6(4)
C(m1)–C(a1)–N(1)	126.3(4)	C(a2)–C(m2)–C(a3)	123.3(4)
C(m1)–C(a1)–C(b1)	124.7(4)	C(a2)–C(m2)–C(21)	118.2(5)
N(1)–C(a1)–C(b1)	109.1(4)	C(a3)–C(m2)–C(21)	118.4(4)
C(m2)–C(a2)–N(1)	126.3(4)	C(a4)–C(m3)–C(a5)	123.6(4)
C(m2)–C(a2)–C(b2)	124.4(4)	C(a4)–C(m3)–C(31)	117.3(5)
N(1)–C(a2)–C(b2)	109.3(4)	C(a5)–C(m3)–C(31)	119.1(5)
N(2)–C(a3)–C(m2)	126.3(4)	C(a7)–C(m4)–C(a6)	123.3(4)
N(2)–C(a3)–C(b3)	109.2(4)	C(a7)–C(m4)–C(41)	118.4(4)
C(m2)–C(a3)–C(b3)	124.5(4)	C(a6)–C(m4)–C(41)	118.3(4)
C(m3)–C(a4)–N(2)	126.6(4)	C(12)–C(11)–C(m1)	112.9(4)
C(m3)–C(a4)–C(b4)	124.6(4)	C(m2)–C(21)–C(22)	111.4(4)
N(2)–C(a4)–C(b4)	108.8(4)	C(32)–C(31)–C(m3)	113.9(6)
N(3)–C(a5)–C(m3)	125.9(4)	C(m4)–C(41)–C(42)	112.9(4)

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

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

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0276(3)	0.0270(3)	0.0222(3)	0.0061(2)	0.0061(2)	0.0111(2)
Cl	0.0448(6)	0.0414(6)	0.0361(6)	0.0071(4)	0.0176(5)	0.0224(5)
N(1)	0.0225(15)	0.0298(16)	0.0267(16)	0.0024(13)	0.0090(13)	0.0121(13)
N(2)	0.0365(18)	0.0305(16)	0.0187(14)	0.0071(12)	0.0090(13)	0.0175(14)
N(3)	0.0312(17)	0.0240(15)	0.0246(15)	0.0035(12)	0.0098(13)	0.0112(13)
N(4)	0.0275(16)	0.0295(16)	0.0240(15)	0.0063(12)	0.0103(13)	0.0138(13)
C(a1)	0.0290(19)	0.0300(18)	0.032(2)	0.0066(15)	0.0186(16)	0.0137(15)
C(a2)	0.0268(19)	0.034(2)	0.032(2)	−0.0020(16)	0.0103(16)	0.0130(16)
C(a3)	0.042(2)	0.044(2)	0.0225(19)	0.0056(17)	0.0055(17)	0.026(2)
C(a4)	0.056(3)	0.037(2)	0.025(2)	0.0122(17)	0.0149(19)	0.024(2)
C(a5)	0.045(2)	0.0250(18)	0.033(2)	0.0063(15)	0.0241(19)	0.0150(17)
C(a6)	0.0297(19)	0.0304(19)	0.031(2)	0.0015(15)	0.0137(16)	0.0120(16)
C(a7)	0.030(2)	0.041(2)	0.0221(18)	0.0049(16)	0.0078(15)	0.0174(17)
C(a8)	0.034(2)	0.035(2)	0.0277(19)	0.0130(16)	0.0154(16)	0.0207(17)
C(b1)	0.034(2)	0.033(2)	0.049(3)	0.0035(19)	0.024(2)	0.0081(18)
C(b2)	0.026(2)	0.039(2)	0.042(3)	−0.0016(19)	0.0102(18)	0.0086(17)
C(b3)	0.060(3)	0.054(3)	0.029(2)	0.012(2)	0.001(2)	0.029(3)
C(b4)	0.074(4)	0.053(3)	0.034(3)	0.021(2)	0.012(3)	0.035(3)
C(b5)	0.042(2)	0.0260(19)	0.052(3)	0.0041(18)	0.029(2)	0.0099(18)
C(b6)	0.026(2)	0.033(2)	0.049(3)	0.0002(18)	0.0188(19)	0.0069(16)
C(b7)	0.039(2)	0.054(3)	0.026(2)	0.0099(19)	0.0052(18)	0.022(2)
C(b8)	0.044(2)	0.051(3)	0.028(2)	0.0178(19)	0.0135(19)	0.028(2)
C(m1)	0.036(2)	0.0308(19)	0.0309(19)	0.0096(15)	0.0190(17)	0.0191(16)
C(m2)	0.032(2)	0.042(2)	0.0241(19)	−0.0030(16)	0.0027(16)	0.0193(18)
C(m3)	0.058(3)	0.029(2)	0.032(2)	0.0122(17)	0.022(2)	0.020(2)
C(m4)	0.0274(19)	0.039(2)	0.0275(19)	0.0011(16)	0.0090(16)	0.0149(17)
C(11)	0.048(3)	0.034(2)	0.040(2)	0.0154(18)	0.025(2)	0.0206(19)
C(21)	0.034(2)	0.064(3)	0.031(2)	−0.005(2)	−0.0019(19)	0.021(2)
C(31)	0.094(5)	0.033(2)	0.043(3)	0.016(2)	0.027(3)	0.015(3)
C(41)	0.027(2)	0.055(3)	0.032(2)	−0.004(2)	0.0034(17)	0.012(2)
C(12)	0.045(3)	0.033(2)	0.048(3)	0.0113(19)	0.029(2)	0.0122(19)
C(22)	0.040(3)	0.078(4)	0.054(3)	−0.004(3)	0.004(2)	0.036(3)
C(32)	0.121(7)	0.045(3)	0.057(4)	0.006(3)	0.051(4)	−0.009(4)
C(42)	0.034(3)	0.104(5)	0.043(3)	−0.002(3)	0.007(2)	0.034(3)

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

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

atom	x	y	z	U(eq)
H(b1)	−0.0039	−0.1526	0.3154	0.047
H(b2)	−0.1470	−0.0907	0.1287	0.047
H(b3)	−0.0178	0.3228	−0.0666	0.063
H(b4)	0.2104	0.5351	−0.0082	0.066
H(b5)	0.7734	0.7685	0.3680	0.046
H(b6)	0.9113	0.7117	0.5607	0.045
H(b7)	0.7837	0.2951	0.7552	0.050
H(b8)	0.5600	0.0789	0.6932	0.047
H(11a)	0.1856	−0.1600	0.4635	0.045
H(11b)	0.3611	−0.0939	0.5715	0.045
H(21a)	−0.1819	−0.0040	−0.0264	0.059
H(21b)	−0.1459	0.1247	−0.0821	0.059
H(31a)	0.4121	0.7051	0.1106	0.074
H(31b)	0.5895	0.7703	0.2155	0.074
H(41a)	0.9051	0.4971	0.7719	0.052
H(41b)	0.9440	0.6227	0.7126	0.052
H(12a)	0.1741	−0.1423	0.6509	0.061
H(12b)	0.1042	−0.0500	0.5746	0.061
H(12c)	0.2792	0.0119	0.6834	0.061
H(22a)	−0.3700	0.0785	−0.0411	0.090
H(22b)	−0.2315	0.2166	0.0413	0.090
H(22c)	−0.2637	0.0902	0.1003	0.090
H(32a)	0.6661	0.6668	0.0989	0.128
H(32b)	0.5877	0.7556	0.0242	0.128
H(32c)	0.4884	0.6006	−0.0060	0.128
H(42a)	1.1436	0.5546	0.7484	0.094
H(42b)	1.0415	0.5224	0.6033	0.094
H(42c)	1.0180	0.4083	0.6781	0.094

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

Table S7. Complete Crystallographic Details for [Fe(TPrP)(Cl)].

formula	$C_{32}H_{36}ClFeN_4$
FW, amu	567.95
a, Å	13.040(2)
b, Å	15.221(2)
c, Å	14.6681(9)
β, deg	109.997(11)
V, Å^3	2735.9(7)
space group	P2(1)/n
Z	4
D_c, g/cm^3	1.379
F(000)	1196
μ, mm^{-1}	0.678
power and current settings	50kV, 40mA
detector distance, mm	40
detector tilt angle, deg	−25
image time, sec	20
increment, deg	0.25
crystal dimensions, mm	0.35 × 0.33 × 0.30
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	130(2)
diffractometer	Enraf Nonius FAST
θ range for collected data, deg	2.25–29.94
index range	$-18 \leq h \leq 17$
	$-18 \leq k \leq 21$
	$-8 \leq l \leq 20$
total data collected	19425
absorption correction	None
unique data	7047 (R_{int} = 0.0544)
unique observed data [I > 2σ(I)]	6174
refinement method	Full-matrix least-sq
data/restraints/parameters	7047/0/347
goodness-of-fit (based on F^2)	1.052
max($\Delta\rho$), e/Å^3	0.949
min($\Delta\rho$), e/Å^3	−0.936
final R indices [I > 2σ(I)]	R_1 =0.0477 , wR_2 =0.1176
final R indices (all data)	R_1 = 0.0556, wR_2 = 0.1235

Table S8. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPrP)(Cl)][a]

atom	x	y	z	U(eq)
Fe(1)	0.44462(2)	0.16332(2)	0.61486(2)	0.0087(1)
Cl(1)	0.45108(4)	0.30989(3)	0.61265(3)	0.0179(1)
N(1)	0.30107(12)	0.13730(10)	0.63957(10)	0.0114(3)
N(2)	0.36154(11)	0.13041(9)	0.47291(10)	0.0108(3)
N(3)	0.58445(12)	0.12454(10)	0.59135(10)	0.0126(3)
N(4)	0.52419(12)	0.13165(9)	0.75846(10)	0.0109(3)
C(m1)	0.17364(14)	0.15512(11)	0.47112(12)	0.0117(3)
C(m2)	0.51424(14)	0.09674(11)	0.41438(12)	0.0127(3)
C(m3)	0.71386(14)	0.14100(12)	0.75929(12)	0.0135(3)
C(m4)	0.36868(15)	0.11137(11)	0.81684(11)	0.0137(3)
C(a1)	0.28625(14)	0.12531(12)	0.72754(12)	0.0142(3)
C(a2)	0.19830(14)	0.14848(11)	0.57141(12)	0.0129(3)
C(a3)	0.25083(13)	0.14293(11)	0.42630(11)	0.0118(3)
C(a4)	0.40433(14)	0.11106(11)	0.40129(11)	0.0124(3)
C(a5)	0.59776(14)	0.10498(12)	0.50415(12)	0.0136(3)
C(a6)	0.68813(13)	0.13036(12)	0.65902(12)	0.0132(3)
C(a7)	0.63603(14)	0.13540(11)	0.80463(12)	0.0129(3)
C(a8)	0.47972(14)	0.11620(11)	0.83008(11)	0.0126(3)
C(b1)	0.17224(15)	0.13001(14)	0.71390(13)	0.0193(4)
C(b2)	0.11807(15)	0.14577(13)	0.61836(13)	0.0179(3)
C(b3)	0.22455(14)	0.13294(12)	0.32331(12)	0.0148(3)
C(b4)	0.31836(15)	0.11117(12)	0.30843(12)	0.0160(3)
C(b5)	0.71212(15)	0.09721(14)	0.51830(13)	0.0198(4)
C(b6)	0.76764(15)	0.11557(14)	0.61293(13)	0.0199(4)
C(b7)	0.66166(15)	0.12425(12)	0.90733(12)	0.0165(3)
C(b8)	0.56590(15)	0.10997(12)	0.92251(12)	0.0159(3)
C(11)	0.05579(13)	0.16796(12)	0.40807(13)	0.0141(3)
C(12)	−0.00868(15)	0.08286(13)	0.37917(14)	0.0203(4)
C(13)	−0.12877(16)	0.10140(15)	0.32360(16)	0.0262(4)
C(21)	0.54426(15)	0.07472(12)	0.32610(12)	0.0145(3)
C(22)	0.56489(15)	0.15490(12)	0.27204(13)	0.0160(3)
C(23)	0.59004(16)	0.12751(14)	0.18184(13)	0.0199(4)
C(31)	0.83294(14)	0.14810(13)	0.82131(13)	0.0171(3)
C(32)	0.88980(15)	0.05922(14)	0.84855(14)	0.0210(4)

Table S8. Continued

atom	x	y	z	U(eq)
C(33)	1.01076(15)	0.06983(16)	0.90482(14)	0.0246(4)
C(41)	0.33527(16)	0.09100(13)	0.90427(12)	0.0171(3)
C(42)	0.32081(17)	0.17130(13)	0.96096(13)	0.0200(4)
C(43)	0.28739(17)	0.14550(15)	1.04700(14)	0.0236(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 S9. Bond Lengths for [Fe(TPrP)(Cl)][a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(2)	2.0536(14)	C(m4)–C(a1)	1.398(2)
Fe(1)–N(3)	2.0548(15)	C(m4)–C(41)	1.521(2)
Fe(1)–N(4)	2.0618(14)	C(a1)–C(b1)	1.432(3)
Fe(1)–N(1)	2.0632(15)	C(a2)–C(b2)	1.436(2)
Fe(1)–Cl(1)	2.2332(6)	C(a3)–C(b3)	1.438(2)
N(1)–C(a1)	1.381(2)	C(a4)–C(b4)	1.438(2)
N(1)–C(a2)	1.381(2)	C(a5)–C(b5)	1.438(2)
N(2)–C(a4)	1.379(2)	C(a6)–C(b6)	1.436(2)
N(2)–C(a3)	1.383(2)	C(a7)–C(b7)	1.437(2)
N(3)–C(a6)	1.380(2)	C(a8)–C(b8)	1.438(2)
N(3)–C(a5)	1.381(2)	C(b1)–C(b2)	1.358(3)
N(4)–C(a8)	1.383(2)	C(b3)–C(b4)	1.355(3)
N(4)–C(a7)	1.383(2)	C(b5)–C(b6)	1.357(3)
C(m1)–C(a3)	1.390(2)	C(b7)–C(b8)	1.359(3)
C(m1)–C(a2)	1.398(2)	C(11)–C(12)	1.523(3)
C(m1)–C(11)	1.511(2)	C(12)–C(13)	1.524(3)
C(m2)–C(a4)	1.397(2)	C(21)–C(22)	1.529(2)
C(m2)–C(a5)	1.398(2)	C(22)–C(23)	1.526(2)
C(m2)–C(21)	1.513(2)	C(31)–C(32)	1.529(3)
C(m3)–C(a7)	1.393(2)	C(32)–C(33)	1.518(3)
C(m3)–C(a6)	1.402(2)	C(41)–C(42)	1.526(3)
C(m3)–C(31)	1.511(2)	C(42)–C(43)	1.521(3)
C(m4)–C(a8)	1.395(3)		

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

Table S10. Bond Angles for [Fe(TPrP)(Cl)][a]

angle	degree	angle	degree
N(2)–Fe(1)–N(3)	87.16(6)	N(1)–C(a2)–C(m1)	125.99(16)
N(2)–Fe(1)–N(4)	152.31(6)	N(1)–C(a2)–C(b2)	109.57(15)
N(3)–Fe(1)–N(4)	86.50(6)	C(m1)–C(a2)–C(b2)	124.29(16)
N(2)–Fe(1)–N(1)	86.30(6)	N(2)–C(a3)–C(m1)	125.93(15)
N(3)–Fe(1)–N(1)	152.24(6)	N(2)–C(a3)–C(b3)	109.77(14)
N(4)–Fe(1)–N(1)	86.88(6)	C(m1)–C(a3)–C(b3)	124.04(15)
N(2)–Fe(1)–Cl(1)	103.79(4)	N(2)–C(a4)–C(m2)	126.30(14)
N(3)–Fe(1)–Cl(1)	104.15(4)	N(2)–C(a4)–C(b4)	109.50(15)
N(4)–Fe(1)–Cl(1)	103.89(4)	C(m2)–C(a4)–C(b4)	124.16(15)
N(1)–Fe(1)–Cl(1)	103.61(4)	N(3)–C(a5)–C(m2)	125.98(16)
C(a1)–N(1)–C(a2)	106.35(14)	N(3)–C(a5)–C(b5)	109.67(15)
C(a1)–N(1)–Fe(1)	127.95(11)	C(m2)–C(a5)–C(b5)	124.32(16)
C(a2)–N(1)–Fe(1)	124.28(11)	N(3)–C(a6)–C(m3)	125.90(16)
C(a4)–N(2)–C(a3)	106.18(13)	N(3)–C(a6)–C(b6)	109.81(15)
C(a4)–N(2)–Fe(1)	127.86(11)	(Cm3)–C(a6)–C(b6)	124.04(16)
C(a3)–N(2)–Fe(1)	124.56(11)	N(4)–C(a7)–C(m3)	125.95(15)
C(a6)–N(3)–C(a5)	106.12(14)	N(4)–C(a7)–C(b7)	109.67(15)
C(a6)–N(3)–Fe(1)	124.64(11)	C(m3)–C(a7)–C(b7)	124.14(16)
C(a5)–N(3)–Fe(1)	128.12(11)	N(4)–C(a8)–C(m4)	126.02(15)
C(a8)–N(4)–C(a7)	106.32(13)	N(4)–C(a8)–C(b8)	109.38(15)
C(a8)–N(4)–Fe(1)	128.36(11)	C(m4)–C(a8)–Cb8)	124.54(15)
C(a7)–N(4)–Fe(1)	124.65(11)	C(b2)–C(b1)–C(a1)	107.57(16)
C(a3)–C(m1)–C(a2)	123.01(15)	C(b1)–C(b2)–C(a2)	107.02(16)
C(a3)–C(m1)–C(11)	118.50(15)	C(b4)–C(b3)–C(a3)	106.92(15)
C(a2)–C(m1)–C(11)	118.24(16)	C(b3)–C(b4)–C(a4)	107.58(15)
C(a4)–C(m2)–C(a5)	123.21(15)	C(b6)–C(b5)–C(a5)	107.15(16)
C(a4)–C(m2)–C(21)	118.07(14)	C(b5)–C(b6)–C(a6)	107.17(16)
C(a5)–C(m2)–C(21)	118.67(15)	C(b8)–C(b7)–C(a7)	107.05(15)
C(a7)–C(m3)–C(a6)	122.80(15)	C(b7)–C(b8)–C(a8)	107.50(15)
C(a7)–C(m3)–C(31)	118.90(15)	C(m1)–C(11)–C(12)	114.17(15)
C(a6)–C(m3)–C(31)	117.90(16)	C(11)–C(12)–C(13)	111.09(16)
C(a8)–C(m4)–C(a1)	123.46(15)	C(m2)–C(21)–C(22)	114.21(15)
C(a8)–C(m4)–C(41)	118.44(15)	C(23)–C(22)–C(21)	111.09(15)
C(a1)–C(m4)–C(41)	118.10(16)	C(m3)–C(31)–C(32)	113.62(15)

Table S10. Continued

angle	degree	angle	degree
N(1)–C(a1)–C(m4)	125.97(16)	C(33)–C(32)–C(31)	111.64(17)
N(1)–C(a1)–C(b1)	109.46(15)	C(m4)–C(41)–C(42)	114.88(15)
C(m4)–C(a1)–C(b1)	124.57(16)	C(43)–C(42)–C(41)	111.67(17)

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

Table S11. Anisotropic Displacement Parameters (Å^2) for [Fe(TPrP)(Cl)][a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0126(1)	0.0075(1)	0.0051(1)	0.0004(1)	0.0021(1)	0.0000(1)
Cl(1)	0.0276(2)	0.0085(2)	0.0153(2)	0.0010(1)	0.0044(2)	−0.0014(2)
N(1)	0.0152(6)	0.0109(6)	0.0081(6)	0.0001(5)	0.0039(5)	−0.0007(5)
N(2)	0.0129(6)	0.0111(6)	0.0073(6)	−0.0004(5)	0.0020(5)	0.0004(5)
N(3)	0.0151(6)	0.0132(7)	0.0079(6)	0.0004(5)	0.0017(5)	0.0006(5)
N(4)	0.0162(6)	0.0091(6)	0.0069(6)	0.0008(5)	0.0031(5)	0.0002(5)
C(m1)	0.0123(7)	0.0092(7)	0.0115(7)	0.0008(5)	0.0016(6)	−0.0006(5)
C(m2)	0.0195(8)	0.0108(7)	0.0089(7)	−0.0001(5)	0.0063(6)	0.0008(6)
C(m3)	0.0158(7)	0.0111(7)	0.0102(7)	0.0007(6)	0.0003(6)	0.0005(6)
C(m4)	0.0233(8)	0.0117(8)	0.0074(7)	0.0009(5)	0.0070(6)	0.0006(6)
C(a1)	0.0193(8)	0.0141(8)	0.0107(7)	0.0000(6)	0.0070(6)	−0.0013(6)
C(a2)	0.0149(7)	0.0108(7)	0.0128(7)	−0.0005(6)	0.0046(6)	−0.0007(6)
C(a3)	0.0147(7)	0.0104(7)	0.0081(7)	0.0005(5)	0.0011(6)	−0.0011(6)
C(a4)	0.0182(8)	0.0120(7)	0.0065(7)	0.0007(5)	0.0035(6)	−0.0012(6)
C(a5)	0.0179(8)	0.0129(8)	0.0109(7)	0.0014(6)	0.0060(6)	0.0020(6)
C(a6)	0.0125(7)	0.0146(8)	0.0118(7)	0.0027(6)	0.0030(6)	0.0017(6)
C(a7)	0.0168(8)	0.0103(7)	0.0087(7)	−0.0006(6)	0.0005(6)	0.0013(6)
C(a8)	0.0213(8)	0.0090(7)	0.0071(7)	0.0003(5)	0.0045(6)	0.0009(6)
C(b1)	0.0200(8)	0.0253(10)	0.0157(8)	−0.0020(7)	0.0102(7)	−0.0018(7)
C(b2)	0.0149(8)	0.0232(9)	0.0168(8)	−0.0017(7)	0.0071(6)	−0.0003(7)
C(b3)	0.0175(8)	0.0156(8)	0.0088(7)	−0.0003(6)	0.0014(6)	−0.0028(6)
C(b4)	0.0207(8)	0.0187(9)	0.0075(7)	−0.0027(6)	0.0035(6)	−0.0026(7)
C(b5)	0.0189(8)	0.0278(10)	0.0144(8)	0.0027(7)	0.0079(7)	0.0048(7)
C(b6)	0.0167(8)	0.0268(10)	0.0167(8)	0.0035(7)	0.0062(7)	0.0030(7)
C(b7)	0.0206(8)	0.0181(9)	0.0075(7)	0.0007(6)	0.0007(6)	0.0045(7)
C(b8)	0.0253(9)	0.0146(8)	0.0062(7)	0.0021(6)	0.0035(6)	0.0049(7)
C(11)	0.0123(7)	0.0141(8)	0.0141(7)	0.0018(6)	0.0022(6)	0.0005(6)
C(12)	0.0174(8)	0.0167(9)	0.0227(9)	0.0014(7)	0.0018(7)	−0.0033(7)
C(13)	0.0165(8)	0.0285(11)	0.0298(10)	0.0026(8)	0.0029(8)	−0.0058(8)
C(21)	0.0218(8)	0.0142(8)	0.0096(7)	−0.0015(6)	0.0078(6)	0.0016(6)
C(22)	0.0221(8)	0.0152(8)	0.0127(8)	−0.0007(6)	0.0088(6)	−0.0015(6)
C(23)	0.0248(9)	0.0245(10)	0.0129(8)	−0.0002(7)	0.0095(7)	−0.0017(7)
C(31)	0.0141(8)	0.0192(9)	0.0141(8)	0.0000(6)	0.0000(6)	−0.0013(6)
C(32)	0.0185(8)	0.0228(10)	0.0177(8)	0.0010(7)	0.0007(7)	0.0029(7)

Table S11. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(33)	0.0151(8)	0.0358(12)	0.0220(9)	0.0023(8)	0.0052(7)	0.0051(8)
C(41)	0.0265(9)	0.0178(9)	0.0092(7)	0.0024(6)	0.0088(6)	−0.0012(7)
C(42)	0.0275(9)	0.0215(9)	0.0138(8)	0.0009(7)	0.0105(7)	0.0024(7)
C(43)	0.0235(9)	0.0367(12)	0.0141(8)	−0.0009(8)	0.0109(7)	−0.0003(8)

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

Table S11. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(TPrP)(Cl)][a]

atom	x	y	z	U(eq)
H(b1)	0.1403	0.1233	0.7628	0.023
H(b2)	0.0416	0.1535	0.5883	0.021
H(b3)	0.1547	0.1402	0.2749	0.018
H(b4)	0.3260	0.0983	0.2477	0.019
H(b5)	0.7430	0.0821	0.4704	0.024
H(b6)	0.8447	0.1182	0.6430	0.024
H(b7)	0.7322	0.1265	0.9555	0.020
H(b8)	0.5574	0.0981	0.9831	0.019
H(11a)	0.0535	0.1996	0.3484	0.017
H(11b)	0.0197	0.2055	0.4432	0.017
H(12a)	−0.0020	0.0484	0.4382	0.024
H(12b)	0.0222	0.0474	0.3382	0.024
H(13a)	−0.1586	0.1386	0.3631	0.039
H(13b)	−0.1691	0.0458	0.3092	0.039
H(13c)	−0.1358	0.1317	0.2628	0.039
H(21a)	0.4846	0.0396	0.2808	0.017
H(21b)	0.6107	0.0378	0.3467	0.017
H(22a)	0.4997	0.1933	0.2528	0.019
H(22b)	0.6270	0.1889	0.3157	0.019
H(23a)	0.6544	0.0893	0.2008	0.030
H(23b)	0.6045	0.1799	0.1493	0.030
H(23c)	0.5274	0.0958	0.1375	0.030
H(31a)	0.8388	0.1804	0.8815	0.020
H(31b)	0.8714	0.1829	0.7859	0.020
H(32a)	0.8554	0.0259	0.8884	0.025
H(32b)	0.8802	0.0251	0.7888	0.025
H(33a)	1.0440	0.1066	0.8676	0.037
H(33b)	1.0458	0.0120	0.9158	0.037
H(33c)	1.0205	0.0978	0.9674	0.037
H(41a)	0.3912	0.0523	0.9488	0.021
H(41b)	0.2657	0.0579	0.8819	0.021
H(42a)	0.3902	0.2045	0.9845	0.024
H(42b)	0.2644	0.2102	0.9173	0.024
H(43a)	0.2183	0.1131	1.0239	0.035

Table S11. Continued

atom	x	y	z	U(eq)
H(43b)	0.2782	0.1985	1.0813	0.035
H(43c)	0.3441	0.1083	1.0912	0.035

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

Table S13. Complete Crystallographic Details for [Fe(THexP)(Cl)].

formula	$C_{44}H_{60}ClFeN_4 \cdot 0.1CH_2Cl_2$
FW, amu	744.75
a, Å	10.246(7)
b, Å	12.834(4)
c, Å	17.420(15)
α, deg	69.74(3)
β, deg	87.52(4)
γ, deg	84.89(3)
V, Å^3	2140(2)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.156
F(000)	790
μ, mm^{-1}	0.460
power and current settings	50 kV and 40 mA
detector distance, mm	40
detector tilt angle, deg	−25
image time, sec	40
increment, deg	0.2
crystal dimensions, mm	0.77 × 0.33 × 0.10
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	130(2)
diffractometer	Enraf Nonius FAST
θ range for collected data, deg	2.34–29.86
index range	$-14 \leq h \leq 14$
	$-17 \leq k \leq 17$
	$-23 \leq l \leq 13$
total data collected	19908
absorption correction	DIFABS
relative transmission coefficients (I)	1.000 and 0.650
unique data	10732 (R_{int} = 0.082)
unique observed data [I > 2σ(I)]	6108
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	10732/115/540
goodness-of-fit (based on F^2)	1.026
max($\Delta\rho$), e/Å^3	1.174
min($\Delta\rho$), e/Å^3	−1.010
final R indices [I > 2σ(I)]	R_1 = 0.1024, wR_2 = 0.2659
final R indices (all data)	R_1 = 0.1647, wR_2 = 0.3239

Table S14. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(THexP)(Cl)][a]

atom	x	y	z	U(eq)
Fe	0.34162(7)	0.32158(6)	0.46190(4)	0.0370(2)
Cl	0.18944(13)	0.20416(11)	0.52345(9)	0.0492(4)
N(1)	0.4732(4)	0.2286(4)	0.4131(2)	0.0373(9)
N(2)	0.2707(4)	0.3998(4)	0.3452(3)	0.0407(9)
N(3)	0.2784(4)	0.4658(3)	0.4833(3)	0.0383(9)
N(4)	0.4768(4)	0.2933(4)	0.5520(3)	0.0401(9)
C(b1)	0.6186(5)	0.0848(5)	0.4074(3)	0.0447(12)
C(b2)	0.5647(6)	0.1319(5)	0.3341(4)	0.0509(13)
C(b3)	0.2054(7)	0.4314(5)	0.2143(4)	0.0574(15)
C(b4)	0.1262(6)	0.4999(5)	0.2432(4)	0.0562(15)
C(b5)	0.1369(7)	0.6142(5)	0.4870(4)	0.0591(16)
C(b6)	0.2238(7)	0.5921(5)	0.5483(4)	0.0552(15)
C(b7)	0.5674(6)	0.2830(7)	0.6721(4)	0.0627(17)
C(b8)	0.6148(7)	0.1917(6)	0.6556(4)	0.0639(18)
C(a1)	0.5629(5)	0.1458(4)	0.4577(3)	0.0382(10)
C(a2)	0.4705(5)	0.2198(5)	0.3364(3)	0.0449(12)
C(a3)	0.2945(6)	0.3676(5)	0.2778(3)	0.0469(12)
C(a4)	0.1670(5)	0.4810(4)	0.3240(3)	0.0420(11)
C(a5)	0.1727(6)	0.5370(5)	0.4455(3)	0.0454(12)
C(a6)	0.3109(6)	0.4965(4)	0.5481(3)	0.0453(12)
C(a7)	0.4792(5)	0.3468(5)	0.6081(3)	0.0449(12)
C(a8)	0.5623(5)	0.1991(5)	0.5800(3)	0.0440(11)
C(m1)	0.6006(5)	0.1283(4)	0.5372(3)	0.0427(11)
C(m2)	0.3896(7)	0.2854(6)	0.2718(4)	0.0567(15)
C(m3)	0.1147(5)	0.5410(5)	0.3733(4)	0.0474(12)
C(m4)	0.4059(5)	0.4444(4)	0.6064(3)	0.0411(11)
C(1)	0.6999(5)	0.0296(4)	0.5779(3)	0.0440(11)
C(2)	0.8415(5)	0.0648(5)	0.5681(3)	0.0479(12)
C(3)	0.9443(5)	−0.0298(5)	0.6052(4)	0.0565(15)
C(4)	0.9195(7)	−0.1043(6)	0.6915(4)	0.050(2)
C(5)	1.0367(9)	−0.1844(7)	0.7289(5)	0.060(2)
C(6)	1.0799(10)	−0.2642(7)	0.6854(6)	0.064(3)
C(41)	0.948(2)	−0.1527(12)	0.6325(14)	0.054(7)
C(51)	1.070(2)	−0.2169(17)	0.6770(13)	0.048(7)

Table S14. Continued

atom	x	y	z	U(eq)
C(61)	1.078(3)	−0.221(3)	0.7641(14)	0.070(9)
C(13)	0.0007(7)	0.6288(5)	0.3402(4)	0.0617(16)
C(14)	0.0436(9)	0.7394(5)	0.2850(5)	0.086(3)
C(15)	−0.0418(9)	0.8434(7)	0.2670(7)	0.108(3)
C(16)	−0.1654(9)	0.8406(12)	0.2331(8)	0.146(6)
C(17)	−0.2610(10)	0.9476(10)	0.2098(9)	0.127(4)
C(18)	−0.3741(13)	0.9332(12)	0.1655(12)	0.191(8)
C(19)	0.4234(6)	0.4916(5)	0.6738(3)	0.0504(13)
C(20)	0.3322(6)	0.4476(6)	0.7463(3)	0.0527(14)
C(21)	0.3475(6)	0.4997(6)	0.8115(3)	0.0576(15)
C(22)	0.2461(9)	0.4637(9)	0.8796(5)	0.097(3)
C(23)	0.2542(13)	0.5117(13)	0.9461(6)	0.140(5)
C(24)	0.223(3)	0.6318(15)	0.9235(13)	0.193(18)
C(240)	0.1246(18)	0.520(2)	0.9896(12)	0.083(8)
C(80)	0.4205(14)	0.2799(11)	0.1871(7)	0.046(3)
C(81)	0.3420(12)	0.1942(13)	0.1723(8)	0.060(3)
C(82)	0.3546(16)	0.1935(15)	0.0861(9)	0.085(5)
C(83)	0.2954(17)	0.0999(16)	0.0718(11)	0.103(6)
C(84)	0.153(2)	0.096(3)	0.0751(13)	0.132(11)
C(85)	0.063(2)	0.175(2)	0.0305(14)	0.124(9)
C(90)	0.3734(17)	0.2379(14)	0.2009(9)	0.062(4)
C(91)	0.4804(15)	0.2847(12)	0.1362(7)	0.066(3)
C(92)	0.4725(15)	0.2399(14)	0.0652(7)	0.070(4)
C(93)	0.5840(15)	0.2731(15)	0.0032(8)	0.081(5)
C(94)	0.5799(16)	0.2119(14)	−0.0598(9)	0.075(4)
C(95)	0.6990(19)	0.228(3)	−0.1136(12)	0.142(12)
Cl(1)	0.608(3)	0.296(2)	−0.0990(16)	0.153(8)
Cl(2)	0.746(4)	0.080(3)	−0.073(3)	0.27(2)
C(100)	0.741(4)	0.207(3)	−0.054(3)	0.044(11)

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

Table S15. Bond Lengths for [Fe(THexP)(Cl)][a]

bond	length (Å)	bond	length (Å)
Fe–N(4)	2.054(5)	C(4m)–C(19)	1.519(7)
Fe–N(3)	2.056(4)	C(1)–C(2)	1.543(7)
Fe–N(2)	2.063(5)	C(2)–C(3)	1.512(7)
Fe–N(1)	2.068(4)	C(3)–C(41)	1.479(14)
Fe–Cl	2.2375(18)	C(3)–C(4)	1.502(8)
N(1)–C(a1)	1.376(7)	C(4)–C(5)	1.520(9)
N(1)–C(a2)	1.381(6)	C(5)–C(6)	1.500(10)
N(2)–C(a3)	1.379(7)	C(41)–C(51)	1.515(14)
N(2)–C(a4)	1.386(7)	C(51)–C(61)	1.508(15)
N(3)–C(a6)	1.380(7)	C(13)–C(14)	1.504(9)
N(3)–C(a5)	1.382(7)	C(14)–C(15)	1.474(9)
N(4)–C(a7)	1.376(7)	C(15)–C(16)	1.428(11)
N(4)–C(a8)	1.382(7)	C(16)–C(17)	1.555(12)
C(b1)–C(b2)	1.330(8)	C(17)–C(18)	1.479(12)
C(b1)–C(a1)	1.434(7)	C(19)–C(20)	1.512(7)
C(b2)–C(a2)	1.429(8)	C(20)–C(21)	1.524(7)
C(b3)–C(b4)	1.353(9)	C(21)–C(22)	1.517(8)
C(b3)–C(a3)	1.434(8)	C(22)–C(23)	1.497(10)
C(b4)–C(a4)	1.418(8)	C(23)–C(24)	1.461(14)
C(b5)–C(b6)	1.357(9)	C(23)–C(240)	1.513(13)
C(b5)–C(a5)	1.431(8)	C(80)–C(81)	1.515(14)
C(b6)–C(a6)	1.453(8)	C(81)–C(82)	1.505(14)
C(b7)–C(b8)	1.346(9)	C(82)–C(83)	1.492(15)
C(b7)–C(a7)	1.433(9)	C(83)–C(84)	1.465(16)
C(b8)–C(a8)	1.412(8)	C(83)–CL2#1)	2.38(4)
C(a1)–C(m1)	1.391(8)	C(84)–C(85)	1.34(3)
C(a2)–C(m2)	1.401(9)	C(84)–CL2#1)	2.42(4)
C(a3)–C(m2)	1.399(8)	C(90)–C(91)	1.541(13)
C(a4)–C(m3)	1.401(8)	C(91)–C(92)	1.541(12)
C(a5)–C(m3)	1.397(8)	C(92)–C(93)	1.521(13)
C(a6)–C(m4)	1.388(8)	C(93)–C(94)	1.558(13)
C(a7)–C(m4)	1.394(8)	C(94)–C(95)	1.492(14)
C(a8)–C(m1)	1.385(7)	CL1)–C(100)	1.73(2)
C(m1)–C(1)	1.534(7)	CL1)–CL2)	2.889(19)

Table S15. Continued

bond	length (Å)	bond	length (Å)
C(m2)–C(80)	1.521(12)	CL2)–C(100)	1.76(2)
C(m2)–C(90)	1.576(17)	CL2)–C(83)#1)	2.38(4)
C(m3)–C(13)	1.530(8)	CL2)–C(84)#1)	2.42(4)

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

Table S16. Bond Angles for [Fe(THexP)(Cl)][a]

angle	degree	angle	degree
N(4)–Fe–N(3)	87.23(18)	C(a1)–C(m1)–C(1)	118.2(5)
N(4)–Fe–N(2)	153.32(17)	C(a3)–C(m2)–C(a2)	123.8(5)
N(3)–Fe–N(2)	86.41(17)	C(a3)–C(m2)–C(80)	117.4(7)
N(4)–Fe–N(1)	86.31(17)	C(a2)–C(m2)–C(80)	118.1(7)
N(3)–Fe–N(1)	152.14(17)	C(a3)–C(m2)–C(90)	116.8(8)
N(2)–Fe–N(1)	87.32(17)	C(a2)–C(m2)–C(90)	116.3(8)
N(4)–Fe–Cl	103.35(14)	C(80)–C(m2)–C(90)	27.1(5)
N(3)–Fe–Cl	103.99(13)	C(a5)–C(m3)–C(a4)	123.4(5)
N(2)–Fe–Cl	103.33(13)	C(a5)–C(m3)–C(13)	117.6(5)
N(1)–Fe–Cl	103.87(13)	C(a4)–C(m3)–C(13)	118.3(5)
C(a1)–N(1)–C(a2)	106.5(4)	C(a6)–C(m4)–C(a7)	122.2(5)
C(a1)–N(1)–Fe	124.9(3)	C(a6)–C(m4)–C(19)	118.4(5)
C(a2)–N(1)–Fe	127.3(4)	C(a7)–C(m4)–C(19)	119.2(5)
C(a3)–N(2)–C(a4)	105.7(4)	C(m1)–C(1)–C(2)	111.9(4)
C(a3)–N(2)–Fe	127.7(4)	C(3)–C(2)–C(1)	114.3(5)
C(a4)–N(2)–Fe	125.3(4)	C(41)–C(3)–C(4)	55.2(10)
C(a6)–N(3)–C(a5)	106.7(4)	C(41)–C(3)–C(2)	134.9(9)
C(a6)–N(3)–Fe	127.2(4)	C(4)–C(3)–C(2)	116.6(5)
C(a5)–N(3)–Fe	124.6(4)	C(3)–C(4)–C(5)	113.2(6)
C(a7)–N(4)–C(a8)	106.4(4)	C(6)–C(5)–C(4)	114.7(7)
C(a7)–N(4)–Fe	127.3(4)	C(3)–C(41)–C(51)	116.6(14)
C(a8)–N(4)–Fe	124.6(4)	C(61)–C(51)–C(41)	114.7(14)
C(b2)–C(b1)–C(a1)	106.8(5)	C(14)–C(13)–C(m3)	113.5(6)
C(b1)–C(b2)–C(a2)	109.0(5)	C(15)–C(14)–C(13)	122.3(8)
C(b4)–C(b3)–C(a3)	107.9(5)	C(16)–C(15)–C(14)	114.4(9)
C(b3)–C(b4)–C(a4)	106.8(5)	C(15)–C(16)–C(17)	118.3(11)
C(b6)–C(b5)–C(a5)	106.7(5)	C(18)–C(17)–C(16)	109.9(10)
C(b5)–C(b6)–C(a6)	107.9(5)	C(20)–C(19)–C(m4)	113.3(4)
C(b8)–C(b7)–C(a7)	107.8(5)	C(19)–C(20)–C(21)	112.4(5)
C(b7)–C(b8)–C(a8)	107.4(6)	C(22)–C(21)–C(20)	111.8(6)
N(1)–C(a1)–C(m1)	125.5(4)	C(23)–C(22)–C(21)	115.1(7)
N(1)–C(a1)–C(b1)	109.5(4)	C(24)–C(23)–C(22)	116.5(12)
C(m1)–C(a1)–C(b1)	124.9(5)	C(24)–C(23)–C(240)	77.1(15)
N(1)–C(a2)–C(m2)	126.2(5)	C(22)–C(23)–C(240)	113.3(11)

Table S16. Continued

angle	degree	angle	degree
N(1)–C(a2)–C(b2)	108.2(5)	C(81)–C(80)–C(m2)	110.2(10)
C(m2)–C(a2)–C(b2)	125.6(5)	C(82)–C(81)–C(80)	113.3(11)
N(2)–C(a3)–C(m2)	125.9(5)	C(83)–C(82)–C(81)	115.2(13)
N(2)–C(a3)–C(b3)	109.2(5)	C(84)–C(83)–C(82)	119.6(14)
C(m2)–C(a3)–C(b3)	124.9(5)	C(84)–C(83)–Cl(2)#1	73.6(17)
N(2)–C(a4)–C(m3)	124.9(5)	C(82)–C(83)–Cl(2)#1	163.0(17)
N(2)–C(a4)–C(b4)	110.5(5)	C(85)–C(84)–C(83)	128(2)
C(m3)–C(a4)–C(b4)	124.5(5)	C(85)–C(84)–Cl(2)#1	136.4(19)
N(3)–C(a5)–C(m3)	125.9(5)	C(83)–C(84)–Cl(2)#1	70.8(18)
N(3)–C(a5)–C(b5)	110.1(5)	C(91)–C(90)–C(2m)	106.9(12)
C(m3)–C(a5)–C(5b)	123.8(5)	C(92)–C(91)–C(90)	110.0(11)
N(3)–C(a6)–C(m4)	127.3(5)	C(93)–C(92)–C(91)	113.0(11)
N(3)–C(a6)–C(b6)	108.4(5)	C(92)–C(93)–C(94)	109.8(12)
C(m4)–C(a6)–C(b6)	124.2(5)	C(95)–C(94)–C(93)	111.5(13)
N(4)–C(a7)–C(m4)	127.0(5)	C(100)–Cl(1)–Cl(2)	34.5(9)
N(4)–C(a7)–C(b7)	108.6(5)	C(100)–Cl(2)–C(83)#1	164(3)
C(m4)–C(a7)–C(b7)	124.4(5)	C(100)–Cl(2)–C(84)#1	155(2)
N(4)–C(a8)–C(m1)	125.3(5)	C(83)#1–Cl(2)–C(84)#1	35.5(6)
N(4)–C(a8)–C(b8)	109.7(5)	C(100)–Cl(2)–Cl(1)	33.7(9)
C(m1)–C(a8)–C(b8)	124.8(5)	C(83)#1–Cl(2)–Cl(1)	139(2)
C(a8)–C(m1)–C(a1)	124.3(5)	C(84)#1–Cl(2)–Cl(1)	170(2)
C(a8)–C(m1)–C(1)	117.4(5)	Cl(1)–C(100)–Cl(2)	111.8(17)

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

Table S17. Anisotropic Displacement Parameters (Å^2) for [Fe(THexP)(Cl)]^a

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe	0.0371(4)	0.0322(4)	0.0419(4)	−0.0132(3)	0.0050(3)	−0.0048(3)
Cl	0.0433(7)	0.0357(6)	0.0673(9)	−0.0167(6)	0.0150(6)	−0.0081(5)
N(1)	0.038(2)	0.040(2)	0.036(2)	−0.0157(17)	0.0042(16)	−0.0050(17)
N(2)	0.036(2)	0.038(2)	0.050(2)	−0.0183(19)	0.0009(18)	−0.0031(17)
N(3)	0.042(2)	0.033(2)	0.041(2)	−0.0142(17)	0.0031(17)	−0.0077(17)
N(4)	0.040(2)	0.039(2)	0.042(2)	−0.0147(18)	0.0063(17)	−0.0053(18)
C(b1)	0.043(3)	0.041(3)	0.054(3)	−0.021(2)	0.003(2)	−0.001(2)
C(b2)	0.055(3)	0.053(3)	0.053(3)	−0.030(3)	0.006(3)	0.000(3)
C(b3)	0.067(4)	0.055(4)	0.053(3)	−0.022(3)	−0.014(3)	−0.001(3)
C(b4)	0.059(4)	0.046(3)	0.067(4)	−0.022(3)	−0.018(3)	−0.001(3)
C(b5)	0.077(4)	0.042(3)	0.054(3)	−0.016(3)	0.004(3)	0.014(3)
C(b6)	0.079(4)	0.038(3)	0.050(3)	−0.018(2)	0.005(3)	0.006(3)
C(b7)	0.057(4)	0.087(5)	0.057(4)	−0.042(4)	−0.010(3)	0.002(3)
C(b8)	0.062(4)	0.081(5)	0.047(3)	−0.027(3)	−0.008(3)	0.022(3)
C(a1)	0.040(2)	0.031(2)	0.040(2)	−0.0087(19)	0.004(2)	−0.0025(19)
C(a2)	0.048(3)	0.045(3)	0.046(3)	−0.021(2)	0.005(2)	−0.002(2)
C(a3)	0.052(3)	0.043(3)	0.047(3)	−0.017(2)	−0.008(2)	0.003(2)
C(a4)	0.040(3)	0.037(3)	0.050(3)	−0.015(2)	−0.010(2)	−0.005(2)
C(a5)	0.048(3)	0.041(3)	0.045(3)	−0.015(2)	0.004(2)	0.000(2)
C(a6)	0.056(3)	0.035(2)	0.049(3)	−0.019(2)	0.014(2)	−0.013(2)
C(a7)	0.040(3)	0.053(3)	0.042(3)	−0.016(2)	0.003(2)	−0.006(2)
C(a8)	0.041(3)	0.051(3)	0.040(3)	−0.018(2)	−0.003(2)	0.003(2)
C(m1)	0.042(3)	0.039(3)	0.044(3)	−0.010(2)	0.005(2)	−0.004(2)
C(m2)	0.064(4)	0.063(4)	0.045(3)	−0.023(3)	−0.003(3)	0.007(3)
C(m3)	0.043(3)	0.038(3)	0.061(3)	−0.016(2)	0.000(2)	−0.002(2)
C(m4)	0.038(2)	0.041(3)	0.048(3)	−0.019(2)	0.004(2)	−0.015(2)
C(1)	0.041(3)	0.040(3)	0.048(3)	−0.012(2)	0.003(2)	0.002(2)
C(2)	0.047(3)	0.043(3)	0.053(3)	−0.015(2)	0.005(2)	−0.004(2)
C(3)	0.043(3)	0.048(3)	0.068(4)	−0.008(3)	0.003(3)	0.003(2)
C(4)	0.054(4)	0.052(4)	0.043(4)	−0.014(3)	−0.002(3)	0.004(3)
C(5)	0.062(5)	0.065(5)	0.046(5)	−0.012(4)	−0.008(4)	0.009(4)
C(6)	0.076(6)	0.042(5)	0.063(5)	−0.004(4)	0.001(4)	0.009(4)
C(13)	0.060(4)	0.057(4)	0.066(4)	−0.022(3)	−0.008(3)	0.016(3)
C(14)	0.135(8)	0.048(4)	0.070(5)	−0.021(3)	−0.041(5)	0.034(4)

Table S17. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(15)	0.117(8)	0.080(6)	0.115(8)	−0.024(6)	0.011(6)	0.007(6)
C(16)	0.076(7)	0.250(19)	0.124(9)	−0.080(11)	−0.012(6)	−0.009(9)
C(17)	0.092(7)	0.126(10)	0.187(13)	−0.090(9)	−0.036(8)	0.032(7)
C(18)	0.123(11)	0.110(10)	0.30(2)	−0.007(12)	−0.091(13)	−0.002(8)
C(19)	0.058(3)	0.050(3)	0.052(3)	−0.026(3)	0.015(3)	−0.023(3)
C(20)	0.055(3)	0.061(4)	0.048(3)	−0.025(3)	0.010(3)	−0.016(3)
C(21)	0.060(4)	0.074(4)	0.045(3)	−0.029(3)	0.003(3)	−0.005(3)
C(22)	0.091(6)	0.155(10)	0.067(5)	−0.061(6)	0.029(4)	−0.041(6)
C(23)	0.146(11)	0.217(16)	0.103(8)	−0.111(10)	0.042(8)	−0.041(11)
C(24)	0.16(2)	0.30(4)	0.14(2)	−0.13(3)	−0.035(18)	0.09(3)
C(240)	0.094(17)	0.109(19)	0.050(11)	−0.034(12)	0.013(10)	−0.014(14)
C(80)	0.060(8)	0.041(7)	0.030(6)	−0.008(5)	0.006(5)	0.005(6)
C(81)	0.050(7)	0.078(9)	0.069(8)	−0.048(8)	−0.001(6)	−0.008(6)
C(82)	0.094(12)	0.104(13)	0.084(11)	−0.067(10)	−0.022(9)	0.009(10)
C(83)	0.122(17)	0.117(17)	0.086(12)	−0.056(12)	−0.017(11)	−0.004(13)
C(84)	0.16(2)	0.20(3)	0.088(14)	−0.094(18)	0.051(14)	−0.12(2)
C(85)	0.13(2)	0.12(2)	0.102(17)	−0.031(14)	0.042(15)	0.010(15)
C(90)	0.069(10)	0.054(9)	0.053(9)	−0.008(8)	0.011(7)	−0.008(7)
C(91)	0.080(10)	0.062(8)	0.055(8)	−0.017(6)	0.007(7)	−0.012(7)
C(92)	0.099(11)	0.080(10)	0.046(7)	−0.036(7)	0.004(7)	−0.032(8)
C(93)	0.090(11)	0.112(14)	0.049(8)	−0.036(8)	−0.003(7)	−0.015(10)
C(94)	0.101(12)	0.070(10)	0.064(9)	−0.029(8)	0.003(8)	−0.028(9)
C(95)	0.089(14)	0.29(4)	0.090(14)	−0.12(2)	0.018(11)	−0.022(18)

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

Table S18. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(THexP)(Cl)][a]

atom	x	y	z	U(eq)
H(b1)	0.6818	0.0227	0.4234	0.054
H(b2)	0.5855	0.1105	0.2877	0.061
H(b3)	0.2025	0.4264	0.1612	0.069
H(b4)	0.0567	0.5509	0.2148	0.067
H(b5)	0.0660	0.6702	0.4741	0.071
H(b6)	0.2270	0.6321	0.5849	0.066
H(b7)	0.5885	0.3017	0.7180	0.075
H(b8)	0.6729	0.1330	0.6886	0.077
H(1a)	0.6938	−0.0286	0.5532	0.053
H(1c)	0.6778	−0.0029	0.6369	0.053
H(2a)	0.8615	0.0997	0.5091	0.057
H(2c)	0.8471	0.1219	0.5939	0.057
H(3a)	0.9527	−0.0764	0.5704	0.083
H(3c)	1.0280	0.0023	0.6039	0.083
H(4a)	0.8440	−0.1478	0.6922	0.060
H(4c)	0.8956	−0.0576	0.7256	0.060
H(5a)	1.1111	−0.1405	0.7296	0.072
H(5c)	1.0148	−0.2277	0.7864	0.072
H(6a)	1.1563	−0.3119	0.7128	0.097
H(6c)	1.1033	−0.2224	0.6286	0.097
H(6d)	1.0084	−0.3105	0.6863	0.097
H(41a)	0.9373	−0.1742	0.5839	0.065
H(41b)	0.8712	−0.1767	0.6691	0.065
H(51a)	1.0726	−0.2943	0.6770	0.058
H(51b)	1.1476	−0.1828	0.6462	0.058
H(61a)	1.1594	−0.2638	0.7884	0.105
H(61b)	1.0029	−0.2562	0.7958	0.105
H(61c)	1.0784	−0.1447	0.7649	0.105
H(13a)	−0.0583	0.6008	0.3095	0.074
H(13b)	−0.0500	0.6397	0.3869	0.074
H(14a)	0.1251	0.7515	0.3083	0.103
H(14b)	0.0682	0.7310	0.2318	0.103
H(15a)	−0.0576	0.8599	0.3182	0.129
H(15b)	0.0047	0.9051	0.2282	0.129

Table S18. Continued

atom	x	y	z	U(eq)
H(16a)	−0.2113	0.7794	0.2729	0.175
H(16b)	−0.1481	0.8208	0.1833	0.175
H(17a)	−0.2921	0.9623	0.2599	0.152
H(17b)	−0.2148	1.0122	0.1748	0.152
H(18d)	−0.4497	0.9817	0.1725	0.286
H(18e)	−0.3958	0.8554	0.1875	0.286
H(18f)	−0.3519	0.9530	0.1072	0.286
H(19a)	0.5150	0.4735	0.6928	0.061
H(19b)	0.4081	0.5738	0.6510	0.061
H(20a)	0.3500	0.3658	0.7708	0.063
H(20b)	0.2405	0.4630	0.7272	0.063
H(21a)	0.4363	0.4777	0.8349	0.069
H(21b)	0.3386	0.5818	0.7859	0.069
H(22a)	0.1579	0.4850	0.8554	0.117
H(22b)	0.2556	0.3814	0.9044	0.117
H(23a)	H0.1900	0.4751	0.9892	0.168
H(23b)	H0.3408	0.4938	0.9679	0.168
H(24a)	0.2331	0.6540	0.9713	0.290
H(24b)	0.1329	0.6509	0.9043	0.290
H(24c)	0.2832	0.6710	0.8798	0.290
H(24d)	0.0980	0.4444	1.0193	0.124
H(24e)	0.0579	0.5609	0.9493	0.124
H(24f)	0.1339	0.5585	1.0283	0.124
H(80a)	0.3989	0.3539	0.1451	0.055
H(80b)	0.5152	0.2596	0.1823	0.055
H(81a)	0.3715	0.1193	0.2105	0.071
H(81b)	0.2484	0.2093	0.1846	0.071
H(82a)	0.3129	0.2646	0.0489	0.102
H(82b)	0.4488	0.1905	0.0711	0.102
H(83a)	0.3257	0.0993	0.0172	0.123
H(83b)	0.3326	0.0297	0.1125	0.123
H(84a)	0.1362	0.0273	0.0652	0.159
H(84b)	0.1271	0.0839	0.1329	0.159
H(85a)	−0.0245	0.1488	0.0448	0.186
H(85b)	0.0809	0.1884	−0.0278	0.186
H(85c)	0.0689	0.2438	0.0418	0.186

Table S18. Continued

atom	x	y	z	U(eq)
H(90a)	0.3840	0.1554	0.2223	0.074
H(90b)	0.2854	0.2616	0.1766	0.074
H(91a)	0.4685	0.3671	0.1150	0.080
H(91b)	0.5678	0.2624	0.1616	0.080
H(92a)	0.4742	0.1576	0.0879	0.084
H(92b)	0.3881	0.2685	0.0371	0.084
H(93a)	0.6690	0.2531	0.0317	0.097
H(93b)	0.5756	0.3547	−0.0257	0.097
H(94a)	0.5733	0.1314	−0.0302	0.090
H(94b)	0.5010	0.2409	−0.0940	0.090
H(95a)	0.6932	0.1888	−0.1526	0.213
H(95b)	0.7771	0.1977	−0.0801	0.213
H(95c)	0.7051	0.3075	−0.1436	0.213

[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.