

Supporting Information

Table S1. Complete Crystallographic Details for $[\text{K}(222)][\text{Fe}(\text{TpivPP})(\text{NO}_3)] \cdot \text{C}_6\text{H}_5\text{Cl}$.

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for $[\text{K}(222)][\text{Fe}(\text{TpivPP})(\text{NO}_3)] \cdot \text{C}_6\text{H}_5\text{Cl}$.

Table S3. Bond Lengths for $[\text{K}(222)][\text{Fe}(\text{TpivPP})(\text{NO}_3)] \cdot \text{C}_6\text{H}_5\text{Cl}$.

Table S4. Bond Angles for $[\text{K}(222)][\text{Fe}(\text{TpivPP})(\text{NO}_3)] \cdot \text{C}_6\text{H}_5\text{Cl}$.

Table S5. Anisotropic Displacement Parameters for $[\text{K}(222)][\text{Fe}(\text{TpivPP})(\text{NO}_3)] \cdot \text{C}_6\text{H}_5\text{Cl}$.

Table S6. Hydrogen Coordinates and Isotropic Displacement Parameters for $[\text{K}(222)][\text{Fe}(\text{TpivPP})(\text{NO}_3)] \cdot \text{C}_6\text{H}_5\text{Cl}$.

S1. Crystallographic details for $[\text{K}(222)][\text{Fe}(\text{TpivPP})(\text{NO}_3)] \cdot \text{C}_6\text{H}_5\text{Cl}$

formula	$\text{FeKClO}_{13}\text{N}_{11}\text{C}_{88}\text{H}_{105}$
FW	1655.28
a , Å	17.888(5)
b , Å	21.500(9)
c , Å	22.514(11)
β , deg	100.32(3)
V , Å ³	8519
Z	4
space group	$P2_1/n$
D_c , g/cm ³	1.29
μ , mm ⁻¹	0.321
crystal dimens, mm	$0.81 \times 0.53 \times 0.21$
absorption correction	none
λ , Å	0.71073
T , K	118 K
diffractometer	Enraf-Nonius CAD-4
total data colld	19627
unique data	19485
unique obsd data [$F_o > 3 \sigma(\text{F})$]	10231
refinement method	full-matrix on F
variables	514
obs. data/variable	20.1
GOF	1.88
final R indices [$I > 2 \sigma(\text{I})$]	$R_1 = 0.074$, $wR_2 = 0.093$

**Table S2. Fractional Coordinates of
[K(222)][Fe(NO₃)TpiVPP]·C₆H₅Cl**

atom	x	y	z
Fe	0.45742(4)	0.07511(3)	0.77636(3)
O(11)	0.49325(22)	0.06542(17)	0.69441(17)
N(11)	0.50657(25)	0.01162(21)	0.67398(20)
O(12)	0.49213(26)	-0.03490(18)	0.70163(20)
O(13)	0.53209(26)	0.00876(20)	0.62672(18)
O(1)	0.14756(27)	-0.05319(22)	0.55803(27)
O(2)	0.51154(26)	0.30431(20)	0.55860(20)
O(3)	0.88866(22)	0.08413(23)	0.81930(20)
O(4)	0.60788(26)	-0.25289(19)	0.76686(22)
N(1)	0.37385(21)	0.00924(17)	0.77477(17)
N(2)	0.37180(21)	0.14065(17)	0.74919(17)
N(3)	0.52488(21)	0.15033(17)	0.80931(18)
N(4)	0.52906(22)	0.01970(17)	0.83585(18)
N(5)	0.20637(25)	0.02616(20)	0.61170(19)
N(6)	0.4897(3)	0.26172(21)	0.64426(24)
N(7)	0.76632(23)	0.08640(20)	0.83334(20)
N(8)	0.52844(24)	-0.17068(18)	0.76026(19)
C(a1)	0.29839(27)	0.01438(21)	0.75026(20)
C(a2)	0.38530(28)	-0.05192(21)	0.79024(22)
C(a3)	0.29606(29)	0.12810(22)	0.72839(22)
C(a4)	0.38105(28)	0.20247(21)	0.73743(22)
C(a5)	0.51623(28)	0.21126(22)	0.78989(23)
C(a6)	0.59527(28)	0.14836(22)	0.84610(23)
C(a7)	0.59866(28)	0.03548(22)	0.87066(22)
C(a8)	0.52129(26)	-0.04220(20)	0.84501(21)
C(b1)	0.26198(27)	-0.04551(22)	0.74949(22)
C(b2)	0.31598(26)	-0.08667(21)	0.77299(22)
C(b3)	0.25822(28)	0.18363(23)	0.70202(24)
C(b4)	0.31150(29)	0.22888(22)	0.70701(24)

Table S2. - continued

C(b5)	0.58199(27)	0.24716(21)	0.81273(25)
C(b6)	0.6309(3)	0.20928(23)	0.84836(26)
C(b7)	0.63508(28)	-0.01936(23)	0.90070(24)
C(b8)	0.58608(28)	-0.06731(22)	0.88358(24)
C(m1)	0.26067(28)	0.07048(21)	0.72908(21)
C(m2)	0.45019(27)	0.23534(21)	0.75492(24)
C(m3)	0.62927(28)	0.09607(21)	0.87619(22)
C(m4)	0.45454(25)	-0.07653(21)	0.82186(21)
C(1)	0.17722(27)	0.06649(20)	0.70471(23)
C(2)	0.15146(29)	0.04334(23)	0.64674(24)
C(3)	0.0737(3)	0.03913(24)	0.62414(25)
C(4)	0.02227(29)	0.05765(24)	0.65994(28)
C(5)	0.04673(29)	0.08109(23)	0.71691(26)
C(6)	0.12384(29)	0.08525(21)	0.73913(24)
C(7)	0.2040(4)	-0.02146(26)	0.57226(29)
C(8)	0.2780(4)	-0.03458(26)	0.54961(27)
C(9)	0.3335(4)	0.0197(3)	0.5557(4)
C(10)	0.3169(4)	-0.0890(3)	0.5869(3)
C(11)	0.2573(5)	-0.0532(4)	0.4833(3)
C(12)	0.45258(28)	0.30093(23)	0.73367(25)
C(13)	0.4719(3)	0.31309(25)	0.67731(28)
C(14)	0.4775(3)	0.37471(27)	0.6589(3)
C(15)	0.4630(3)	0.42270(25)	0.6951(3)
C(16)	0.4439(3)	0.41151(24)	0.7510(3)
C(17)	0.43770(29)	0.35051(24)	0.76942(26)
C(18)	0.5098(3)	0.25866(27)	0.58953(27)
C(19)	0.5288(3)	0.19371(27)	0.56916(25)
C(20)	0.5893(3)	0.16258(27)	0.61687(27)
C(21)	0.5580(4)	0.1991(3)	0.51069(28)
C(22)	0.4560(4)	0.1541(3)	0.5591(3)

Table S2. - continued

C(23)	0.70436(28)	0.10792(22)	0.91710(24)
C(24)	0.77254(29)	0.10562(23)	0.89362(25)
C(25)	0.8398(3)	0.12571(26)	0.92985(28)
C(26)	0.8398(3)	0.14720(26)	0.98681(28)
C(27)	0.7735(4)	0.14939(26)	1.01002(26)
C(28)	0.7067(3)	0.12934(24)	0.97497(25)
C(29)	0.8213(3)	0.07783(25)	0.79970(27)
C(30)	0.7935(3)	0.06061(24)	0.73374(26)
C(31)	0.8352(4)	0.00156(29)	0.7210(3)
C(32)	0.8155(4)	0.11393(29)	0.6953(3)
C(33)	0.7073(3)	0.05000(27)	0.71709(27)
C(34)	0.45251(26)	-0.14428(21)	0.83597(22)
C(35)	0.48649(26)	-0.18959(21)	0.80511(22)
C(36)	0.47670(29)	-0.25256(21)	0.81690(23)
C(37)	0.43524(29)	-0.27032(22)	0.85985(25)
C(38)	0.40243(28)	-0.22589(24)	0.89174(24)
C(39)	0.41188(27)	-0.16399(22)	0.87977(22)
C(40)	0.5873(3)	-0.20315(24)	0.74326(26)
C(41)	0.6248(3)	-0.17480(25)	0.69412(27)
C(42)	0.6874(5)	-0.2194(3)	0.6830(4)
C(43)	0.6610(4)	-0.11268(29)	0.7160(3)
C(44)	0.5669(4)	-0.1652(3)	0.63683(28)
K	0.74705(6)	-0.15046(5)	0.04080(5)
O(5)	0.73298(19)	-0.02124(16)	0.05656(15)
O(6)	0.61006(20)	-0.10208(17)	0.06484(17)
O(7)	0.68094(20)	-0.21048(17)	-0.06833(17)
O(8)	0.81228(20)	-0.13705(19)	-0.06187(16)
O(9)	0.88372(18)	-0.17167(15)	0.12390(16)
O(10)	0.76108(20)	-0.25624(16)	0.11597(16)

Table S2. - Continued

N(9)	0.88480(23)	-0.06552(19)	0.04132(19)
N(10)	0.61126(26)	-0.23488(21)	0.04018(21)
C(45)	0.8599(3)	-0.00078(23)	0.04563(24)
C(46)	0.8022(3)	0.00682(23)	0.08600(23)
C(47)	0.6729(3)	-0.00585(25)	0.08683(25)
C(48)	0.6022(3)	-0.03667(26)	0.05731(25)
C(49)	0.5426(3)	-0.13508(28)	0.04467(27)
C(50)	0.5528(3)	-0.2011(3)	0.06532(29)
C(51)	0.5819(3)	-0.25278(26)	-0.02246(28)
C(52)	0.6436(3)	-0.26702(25)	-0.05797(27)
C(53)	0.7351(3)	-0.2202(3)	-0.10627(27)
C(54)	0.7707(3)	-0.1601(3)	-0.11754(25)
C(55)	0.8542(3)	-0.08253(28)	-0.06940(25)
C(56)	0.9148(3)	-0.07455(26)	-0.01417(26)
C(57)	0.94298(29)	-0.08039(24)	0.09430(25)
C(58)	0.95099(28)	-0.14931(24)	0.10585(25)
C(59)	0.8915(3)	-0.23415(23)	0.14515(25)
C(60)	0.8214(3)	-0.25358(25)	0.16626(24)
C(61)	0.6923(3)	-0.27684(28)	0.13299(26)
C(62)	0.6348(3)	-0.28979(28)	0.07688(29)
Cl	0.23957(15)	0.17970(12)	-0.45298(20)
C(63)	0.1747(5)	0.1470(3)	0.4874(4)
C(64)	0.1059(4)	0.1302(3)	0.5014(4)
C(65)	0.0511(8)	0.1007(5)	0.4581(6)
C(66)	0.0655(13)	0.0947(6)	0.4029(10)
C(67)	0.1408(16)	0.1126(7)	0.3919(5)
C(68)	0.1989(10)	0.1410(6)	0.4375(7)

Table S3. Bond Distance in [K(222)] [Fe(NO₃)TpivPP] · C₆H₅Cl ^a

type	length , Å	type	length , Å
Fe-N(1)	2.055(4)	C(23)-C(28)	1.375(7)
Fe-N(2)	2.091(4)	C(24)-N(7)	1.404(7)
Fe-N(3)	2.074(4)	C(24)-C(25)	1.395(7)
Fe-N(4)	2.059(4)	C(25)-C(26)	1.363(9)
Fe-O11	2.069(4)	C(26)-C(27)	1.380(9)
O(11)-N(11)	1.283(6)	C(27)-C(28)	1.377(8)
N(11)-O(12)	1.230(6)	C(29)-N(7)	1.357(7)
N(11)-O(13)	1.232(6)	C(29)-O(3)	1.214(6)
N(1)-C(a1)	1.368(6)	C(29)-C(30)	1.525(8)
N(1)-C(a2)	1.366(6)	C(30)-C(31)	1.525(8)
N(2)-C(a3)	1.379(6)	C(30)-C(32)	1.529(8)
N(2)-C(a4)	1.371(6)	C(30)-C(33)	1.537(8)
N(3)-C(a5)	1.381(6)	C(34)-C(35)	1.397(6)
N(3)-C(a6)	1.378(6)	C(34)-C(39)	1.392(7)
N(4)-C(a7)	1.389(6)	C(35)-N(8)	1.421(6)
N(4)-C(a8)	1.358(6)	C(35)-C(36)	1.397(6)
C(a1)-C(b1)	1.442(6)	C(36)-C(37)	1.374(7)
C(a1)-C(m1)	1.422(6)	C(37)-C(38)	1.387(7)
C(a2)-C(b2)	1.440(7)	C(38)-C(39)	1.374(7)
C(a2)-C(m4)	1.416(7)	C(40)-N(8)	1.373(6)
C(a3)-C(b3)	1.446(7)	C(40)-O(4)	1.222(6)
C(a3)-C(m1)	1.393(7)	C(40)-C(41)	1.521(8)
C(a4)-C(b4)	1.426(7)	C(41)-C(42)	1.528(8)
C(a4)-C(m2)	1.418(7)	C(41)-C(43)	1.527(8)
C(a5)-C(b5)	1.424(7)	C(41)-C(44)	1.517(9)
C(a5)-C(m2)	1.397(7)	K-O(5)	2.818(4)
C(a6)-C(b6)	1.454(7)	K-O(6)	2.803(4)
C(a6)-C(m3)	1.395(7)	K-O(7)	2.839(4)
C(a7)-C(b7)	1.454(7)	K-O(8)	2.785(4)
C(a7)-C(m3)	1.410(7)	K-O(9)	2.837(4)
C(a8)-C(b8)	1.424(7)	K-O(10)	2.819(4)
C(a8)-C(m4)	1.421(7)	K-N(9)	3.065(4)
C(b1)-C(b2)	1.346(7)	K-N(10)	3.030(5)
C(b3)-C(b4)	1.352(7)	C(45)-N(9)	1.470(6)
C(b5)-C(b6)	1.349(7)	C(45)-C(46)	1.502(7)

Table S3.- continued

C(b7)-C(b8)	1.363(7)	C(46)-O(5)	1.429(6)
C(m1)-C(1)	1.498(5)	O(5)-C(47)	1.411(6)
C(m2)-C(12)	1.492(5)	C(47)-C(48)	1.476(8)
C(m3)-C(23)	1.508(5)	C(48)-O(6)	1.421(6)
C(m4)-C(34)	1.493(5)	O(6)-C(49)	1.403(7)
C(1)-C(2)	1.396(7)	C(49)-C(50)	1.494(8)
C(1)-C(6)	1.393(7)	C(50)-N(10)	1.467(7)
C(2)-C(3)	1.396(7)	N(10)-C(51)	1.465(7)
C(2)-N(5)	1.415(6)	C(51)-C(52)	1.505(8)
C(3)-C(4)	1.386(8)	C(52)-O(7)	1.426(7)
C(4)-C(5)	1.374(8)	O(7)-C(53)	1.417(7)
C(5)-C(6)	1.383(7)	C(53)-C(54)	1.482(9)
C(7)-N(5)	1.351(7)	C(54)-O(8)	1.427(6)
C(7)-O(1)	1.213(7)	O(8)-C(55)	1.418(7)
C(7)-C(8)	1.527(8)	C(55)-C(56)	1.505(8)
C(8)-C(9)	1.522(9)	C(56)-N(9)	1.458(7)
C(8)-C(10)	1.532(9)	N(9)-C(57)	1.471(7)
C(8)-C(11)	1.525(9)	C(57)-C(58)	1.507(7)
C(12)-C(13)	1.398(8)	C(58)-O(9)	1.421(6)
C(12)-C(17)	1.390(7)	O(9)-C(59)	1.424(6)
C(13)-N(6)	1.400(7)	C(59)-C(60)	1.479(8)
C(13)-C(14)	1.397(7)	C(60)-O(10)	1.418(6)
C(14)-C(15)	1.369(9)	O(10)-C(61)	1.422(6)
C(15)-C(16)	1.383(9)	C(61)-C(62)	1.506(8)
C(16)-C(17)	1.386(7)	C(62)-N(10)	1.459(7)
C(18)-N(6)	1.346(7)	Cl-C(63)	1.757(9)
C(18)-O(2)	1.207(6)	C(63)-C(64)	1.371(11)
C(18)-C(19)	1.527(8)	C(64)-C(65)	1.403(14)
C(19)-C(20)	1.535(8)	C(65)-C(66)	1.320(28)
C(19)-C(21)	1.506(8)	C(66)-C(67)	1.46(3)
C(19)-C(22)	1.538(8)	C(67)-C(68)	1.456(26)
C(23)-C(24)	1.414(7)	C(68)-C(63)	1.280(12)

a Numbers in parentheses are the estimated standard deviation in the least significant digit(s).

Table S4. Bond Angles (deg) in [K(222)] [Fe(NO₃)TpivotPP]·C₆H₅Cl

angle	value	angle	value
N(1)FeN(2)	88.10(14)	C(27)C(26)C(25)	120.8(5)
N(1)FeN(3)	156.70(16)	C(26)C(27)C(28)	119.2(5)
N(1)FeN(4)	88.78(15)	C(23)C(28)C(27)	121.6(5)
N(2)FeN(3)	85.86(14)	C(29)N(7)C(24)	129.8(5)
N(2)FeN(4)	156.67(15)	O(3)C(29)N(7)	123.6(5)
N(3)FeN(4)	87.94(15)	O(3)C(29)C(30)	120.6(5)
O(11)FeN(1)	104.81(16)	N(7)C(29)C(30)	115.8(5)
O(11)FeN(2)	87.74(15)	C(31)C(30)C(29)	107.5(5)
O(11)FeN(3)	98.29(15)	C(32)C(30)C(29)	107.3(4)
O(11)FeN(4)	105.41(15)	C(33)C(30)C(29)	114.3(5)
FeN(1)C(a1)	127.8(3)	C(31)C(30)C(32)	109.5(5)
FeN(1)C(a2)	125.41(15)	C(31)C(30)C(33)	109.5(5)
FeN(2)C(a3)	126.25(29)	C(32)C(30)C(33)	108.7(5)
FeN(2)C(a4)	127.0(3)	C(39)C(34)C(35)	118.0(4)
FeN(3)C(a5)	127.0(3)	C(39)C(34)C(m4)	118.8(4)
FeN(3)C(a6)	127.0(3)	C(m4)C(34)C(35)	123.0(4)
FeN(4)C(a7)	127.7(4)	C(36)C(35)C(34)	120.8(4)
FeN(4)C(a8)	128.0(3)	C(36)C(35)N(8)	123.0(4)
FeO(11)N(11)	121.2(3)	C(34)C(35)N(8)	119.1(4)
O(11)N(11)O(12)	118.8(4)	C(37)C(36)C(35)	120.3(5)
O(11)N(11)O(13)	118.4(4)	C(36)C(37)C(38)	120.3(4)
O(12)N(11)O(13)	122.7(5)	C(39)C(38)C(37)	119.2(5)
C(a1)N(1)C(a2)	105.6(4)	C(34)C(39)C(38)	122.1(5)
C(a3)N(2)C(a4)	105.6(4)	C(40)N(8)C(35)	125.5(4)
C(a5)N(3)C(a6)	104.9(4)	O(4)C(40)N(8)	120.7(5)
C(a7)N(4)C(a8)	105.0(4)	O(4)C(40)C(41)	121.9(5)
N(1)C(a1)C(b1)	110.1(4)	N(8)C(40)C(41)	117.3(5)
N(1)C(a1)C(m1)	125.3(4)	C(42)C(41)C(40)	107.4(5)
C(b1)C(a1)C(m1)	124.6(4)	C(43)C(41)C(40)	109.4(5)
N(1)C(a2)C(b2)	110.4(4)	C(44)C(41)C(40)	110.5(5)
N(1)C(a2)C(m4)	124.4(4)	C(42)C(41)C(43)	108.7(5)
C(b2)C(a2)C(m4)	125.1(4)	C(42)C(41)C(44)	110.8(6)

Table S4. - continued

N(2)C(a3)C(b3)	109.7(4)	C(43)C(41)C(44)	109.9(5)
N(2)C(a3)C(m1)	126.3(4)	O(5)KO(6)	60.6(1)
C(b3)C(a3)C(m1)	124.0(5)	O(5)KO(7)	121.6(1)
N(2)C(a4)C(b4)	110.7(4)	O(5)KO(8)	93.6(1)
N(2)C(a4)C(m2)	124.0(4)	O(5)KO(9)	99.3(1)
C(b4)C(a4)C(m2)	125.3(4)	O(5)KO(10)	136.1(1)
N(3)C(a5)C(b5)	111.2(4)	O(5)KN(9)	60.1(1)
N(3)C(a5)C(m2)	124.4(4)	O(5)KN(10)	120.1(1)
C(b5)C(a5)C(m2)	124.3(4)	O(6)KO(7)	95.3(1)
N(3)C(a6)C(b6)	109.9(4)	O(6)KO(8)	129.3(1)
N(3)C(a6)C(m3)	126.1(4)	O(6)KO(9)	127.8(1)
C(b6)C(a6)C(m3)	124.0(5)	O(6)KO(10)	99.8(1)
N(4)C(a7)C(b7)	110.2(4)	O(6)KN(9)	120.5(1)
N(4)C(a7)C(m3)	124.7(4)	O(6)KN(10)	59.7(1)
C(b7)C(a7)C(m3)	125.0(5)	O(7)KO(8)	60.0(1)
N(4)C(a8)C(b8)	111.7(4)	O(7)KO(9)	132.4(1)
N(4)C(a8)C(m4)	123.7(4)	O(7)KO(10)	97.5(1)
C(b8)C(a8)C(m4)	124.4(4)	O(7)KN(9)	118.9(1)
C(b2)C(b1)C(a1)	106.9(4)	O(7)KN(10)	61.0(1)
C(b1)C(b2)C(a2)	106.7(4)	O(8)KO(9)	97.1(1)
C(b4)C(b3)C(a3)	106.8(4)	O(8)KO(10)	125.2(1)
C(b3)C(b4)C(a4)	107.1(4)	O(8)KN(9)	59.0(1)
C(b6)C(b5)C(a5)	107.1(4)	O(8)KN(10)	120.9(1)
C(b5)C(b6)C(a6)	106.8(4)	O(9)KO(10)	60.1(1)
C(b8)C(b7)C(a7)	105.7(4)	O(9)KN(9)	59.7(1)
C(b7)C(b8)C(a8)	107.3(4)	O(9)KN(10)	120.1(1)
C(a3)C(m1)C(a1)	124.7(4)	O(10)KN(9)	119.6(1)
C(a3)C(m1)C(1)	118.2(4)	O(10)KN(10)	60.3(1)
C(a1)C(m1)C(1)	117.1(4)	N(9)KN(10)	179.8(1)
C(a5)C(m2)C(a4)	125.4(4)	N(9)C(45)C(46)	113.1(4)
C(a5)C(m2)C(12)	117.4(4)	C(45)C(46)O(5)	107.8(4)
C(a4)C(m2)C(12)	117.1(4)	C(46)O(5)C(47)	110.4(4)
C(a7)C(m3)C(a6)	125.0(5)	KO(5)C(46)	112.7(3)
C(a7)C(m3)C(23)	120.0(4)	KO(5)C(47)	112.6(3)

Table S4. - continued

C(a6)C(m3)C(23)	115.0(4)	O(5)C(47)C(48)	110.0(4)
C(a8)C(m4)C(a2)	126.3(4)	C(47)C(48)O(6)	109.4(4)
C(a8)C(m4)C(34)	118.7(4)	C(48)O(6)C(49)	113.7(4)
C(a2)C(m4)C(34)	114.8(3)	KO(6)C(48)	114.5(3)
C(6)C(1)C(2)	118.6(5)	KO(6)C(49)	149.2(4)
C(6)C(1)C(m1)	121.2(5)	O(6)C(49)C(50)	109.2(4)
C(2)C(1)C(m1)	120.2(4)	C(49)C(50)N(10)	113.9(5)
C(3)C(2)C(1)	120.3(5)	KN(10)C(50)	109.1(3)
C(3)C(2)N(5)	121.7(5)	KN(10)C(51)	108.1(3)
C(1)C(2)N(5)	117.9(4)	KN(10)C(62)	109.4(3)
C(4)C(3)C(2)	119.4(5)	C(50)N(10)C(51)	110.1(4)
C(5)C(4)C(3)	121.0(5)	C(50)N(10)C(62)	109.6(5)
C(4)C(5)C(6)	119.4(5)	C(51)N(10)C(62)	110.5(5)
C(1)C(6)C(5)	121.2(5)	N(10)C(51)C(52)	113.2(4)
C(7)N(5)C(2)	128.4(5)	C(51)C(52)O(7)	108.8(4)
O(1)C(7)N(5)	121.7(6)	C(52)O(7)C(53)	111.3(4)
O(1)C(7)C(8)	122.6(5)	KO(7)C(52)	112.4(3)
N(5)C(7)C(8)	115.6(5)	KO(7)C(53)	111.4(3)
C(9)C(8)C(7)	114.7(5)	O(7)C(53)C(54)	109.6(5)
C(10)C(8)C(7)	107.0(5)	C(53)C(54)O(8)	108.9(5)
C(11)C(8)C(7)	107.5(6)	C(54)O(8)C(55)	112.7(4)
C(9)C(8)C(10)	108.1(6)	KO(8)C(54)	117.6(3)
C(9)C(8)C(11)	109.3(6)	KO(8)C(55)	119.6(3)
C(10)C(8)C(11)	110.1(5)	O(8)C(55)C(56)	108.3(5)
C(17)C(12)C(13)	119.1(5)	C(55)C(56)N(9)	113.7(4)
C(17)C(12)C(m2)	121.3(5)	C(56)N(9)C(57)	110.5(4)
C(13)C(12)C(m2)	119.6(5)	C(56)N(9)C(45)	110.2(4)
C(14)C(13)C(12)	119.3(6)	C(45)N(9)C(57)	109.3(4)
C(14)C(13)N(6)	123.7(6)	KN(9)C(56)	109.6(3)
C(12)C(13)N(6)	116.8(5)	KN(9)C(57)	109.0(3)
C(15)C(14)C(13)	120.4(6)	KN(9)C(45)	108.2(3)
C(14)C(15)C(16)	121.0(5)	C(58)C(57)N(9)	112.7(4)
C(17)C(16)C(15)	118.8(5)	C(57)C(58)O(9)	108.8(4)
C(16)C(17)C(12)	121.3(5)	C(58)O(9)C(59)	112.2(4)

Table S4. - continued

C(18)N(6)C(13)	130.4(5)	KO(9)C(58)	115.5(3)
O(2)C(18)N(6)	121.8(6)	KO(9)C(59)	113.2(3)
O(2)C(18)C(19)	122.7(6)	O(9)C(59)C(60)	109.7(4)
N(6)C(18)C(19)	115.5(5)	C(59)C(60)O(10)	108.8(4)
C(20)C(19)C(18)	110.8(5)	C(60)O(10)C(61)	111.6(4)
C(21)C(19)C(18)	108.8(5)	KO(10)C(60)	114.8(3)
C(22)C(19)C(18)	108.5(5)	KO(10)C(61)	115.1(3)
C(20)C(19)C(21)	109.5(5)	O(10)C(61)C(62)	109.0(5)
C(20)C(19)C(22)	109.5(5)	C(61)C(62)N(10)	114.2(5)
C(21)C(19)C(22)	109.3(5)	C(64)C(63)Cl	115.3(7)
C(28)C(23)C(24)	118.9(5)	C(68)C(63)C(64)	129(1)
C(28)C(23)C(m3)	120.5(5)	ClC(63)C(68)	115(1)
C(24)C(23)C(m3)	119.9(5)	C(63)C(64)C(65)	120(1)
C(23)C(24)C(25)	118.8(5)	C(64)C(65)C(66)	118(2)
C(23)C(24)N(7)	116.6(5)	C(65)C(66)C(67)	118(1)
C(25)C(24)N(7)	124.5(5)	C(66)C(67)C(68)	124(1)
C(26)C(25)C(24)	120.7(6)	C(67)C(68)C(63)	110(2)

Table S5. Anisotropic Thermal Parameters (in Square Angstroms)

Atom	B(11)	B(22)	B(33)	B(12)	B(13)	B(23)
Fe	1.674(28)	1.120(25)	2.37(3)	0.024(23)	0.247(22)	0.265(24)
O(11)	4.06(19)	2.42(17)	2.99(18)	0.24(14)	1.60(15)	0.27(14)
N(11)	2.79(21)	2.81(21)	2.58(21)	0.58(17)	0.51(17)	0.35(17)
O(12)	6.13(25)	2.32(18)	4.51(22)	1.12(17)	2.76(20)	0.97(16)
O(13)	5.95(25)	3.82(21)	2.89(19)	0.63(18)	2.24(18)	0.45(16)
O(1)	4.25(24)	3.87(23)	9.6(4)	-0.92(19)	1.52(24)	-3.88(24)
O(2)	5.05(24)	3.58(21)	4.40(23)	-0.06(18)	1.53(19)	2.19(18)
O(3)	1.58(17)	6.70(28)	4.29(22)	-0.14(17)	0.07(15)	-0.22(20)
O(4)	5.43(25)	2.67(19)	5.97(26)	1.84(17)	3.29(21)	1.38(18)
N(1)	1.65(16)	0.95(15)	2.04(17)	0.20(12)	-0.01(13)	0.28(13)
N(2)	1.73(17)	1.23(16)	1.90(17)	-0.44(13)	-0.05(14)	-0.15(13)
N(3)	1.52(16)	1.24(15)	2.47(18)	0.21(13)	0.38(14)	0.36(14)
N(4)	1.66(17)	1.19(16)	2.50(19)	-0.27(13)	0.60(14)	-0.09(14)
N(5)	2.89(21)	2.14(19)	2.30(19)	-0.23(16)	0.27(16)	-0.27(16)
N(6)	6.1(3)	1.56(19)	3.58(24)	0.08(19)	1.96(23)	0.91(18)
N(7)	1.47(17)	2.67(20)	2.75(21)	-0.34(15)	-0.08(15)	0.23(16)
N(8)	2.88(20)	0.98(15)	2.20(19)	0.34(14)	0.50(16)	0.08(14)
C(a1)	2.21(21)	1.50(19)	1.21(18)	-0.05(16)	0.47(16)	0.06(15)
C(a2)	2.37(22)	1.00(17)	2.16(21)	-0.21(16)	0.59(17)	-0.35(16)
C(a3)	2.62(23)	1.46(19)	1.83(21)	0.45(17)	0.62(18)	0.13(16)
C(a4)	2.46(23)	1.31(19)	2.09(21)	0.59(16)	0.40(18)	0.39(16)
C(a5)	2.22(22)	1.32(19)	2.58(23)	0.20(16)	0.66(18)	0.40(17)
C(a6)	2.44(23)	1.48(20)	2.71(23)	0.07(17)	0.85(19)	0.19(18)
C(a7)	2.46(23)	1.59(20)	2.12(22)	0.48(17)	0.82(18)	0.51(17)
C(a8)	1.72(20)	1.16(18)	1.70(20)	0.76(15)	0.16(16)	0.39(15)
C(b1)	1.92(21)	1.47(19)	2.23(21)	-0.33(16)	0.21(17)	-0.09(16)
C(b2)	1.76(20)	1.26(19)	2.03(21)	-0.07(15)	-0.10(16)	-0.26(16)
C(b3)	2.28(22)	1.82(21)	2.82(24)	0.58(18)	0.30(19)	0.35(18)
C(b4)	2.44(23)	1.34(20)	3.17(25)	0.31(17)	0.18(19)	0.35(18)
C(b5)	1.66(21)	1.18(19)	3.80(27)	-0.68(16)	-0.48(19)	0.36(18)
C(b6)	2.69(24)	1.66(21)	3.30(26)	-0.16(18)	0.04(20)	0.39(19)
C(b7)	2.00(21)	1.68(20)	3.03(24)	0.31(17)	0.45(18)	0.40(18)
C(b8)	2.22(21)	1.42(19)	2.89(23)	0.57(17)	0.85(18)	0.40(18)
C(m1)	2.64(22)	1.33(18)	1.49(19)	0.31(17)	0.44(16)	0.14(16)
C(m2)	1.98(21)	1.14(18)	3.05(24)	-0.14(16)	0.50(18)	0.10(17)
C(m3)	2.64(22)	1.23(19)	2.07(21)	0.26(16)	0.98(18)	0.31(16)
C(m4)	1.51(18)	1.17(17)	2.10(20)	0.08(15)	0.47(15)	-0.19(16)
C(1)	1.92(20)	0.74(17)	2.68(23)	0.23(15)	0.09(17)	0.32(16)
C(2)	2.37(23)	1.57(20)	2.60(24)	0.11(17)	0.38(19)	-0.06(18)
C(3)	2.67(25)	2.02(22)	2.75(25)	-0.21(19)	-0.40(20)	0.00(19)
C(4)	1.61(22)	1.86(22)	4.4(3)	-0.01(17)	-0.28(21)	0.29(21)
C(5)	2.23(22)	1.41(20)	3.79(28)	0.28(18)	0.81(20)	0.32(20)
C(6)	2.70(23)	0.99(19)	2.74(23)	0.17(17)	0.58(19)	0.21(17)
C(7)	3.41(29)	1.89(24)	4.5(3)	0.23(21)	-0.06(24)	-0.75(22)
C(8)	4.6(3)	1.91(23)	3.18(27)	0.18(22)	0.78(24)	-0.36(20)
C(9)	4.8(4)	3.01(29)	6.9(4)	0.02(26)	2.7(3)	-1.07(29)
C(10)	5.0(4)	3.7(3)	5.4(4)	1.41(27)	1.8(3)	0.35(28)
C(11)	6.9(5)	4.6(4)	3.9(3)	-0.3(3)	1.2(3)	-0.88(29)
C(12)	1.82(22)	1.51(20)	3.12(25)	0.03(16)	-0.06(19)	0.50(18)
C(13)	2.73(25)	1.76(23)	4.3(3)	0.01(19)	0.25(23)	0.82(21)
C(14)	3.43(28)	2.13(24)	4.6(3)	-0.27(21)	0.64(25)	1.34(23)
C(15)	3.18(26)	1.33(22)	5.3(3)	-0.33(20)	0.06(24)	1.44(23)
C(16)	2.20(23)	1.33(21)	4.9(3)	0.05(17)	-0.35(22)	0.17(20)
C(17)	2.10(22)	1.70(21)	3.60(27)	-0.33(17)	0.15(20)	0.33(19)
C(18)	2.35(24)	3.03(26)	3.19(27)	-0.37(20)	0.39(21)	1.50(22)

Table S5. - Continued

C(19)	2.76(25)	3.23(26)	2.44(25)	-0.25(21)	0.07(20)	0.62(21)
C(20)	3.13(26)	3.09(27)	3.29(27)	0.35(21)	1.12(22)	0.91(22)
C(21)	5.2(4)	4.7(3)	2.84(29)	-0.31(28)	1.25(26)	0.33(25)
C(22)	4.5(3)	3.4(3)	5.1(4)	-0.87(26)	0.83(29)	0.22(27)
C(23)	2.14(22)	1.00(18)	2.85(24)	-0.38(16)	-0.29(19)	0.48(17)
C(24)	2.04(22)	1.64(20)	2.90(25)	-0.38(17)	-0.11(19)	0.48(19)
C(25)	2.30(24)	2.44(24)	4.0(3)	-0.51(20)	-0.11(22)	0.58(22)
C(26)	3.21(28)	1.98(23)	3.8(3)	-0.72(20)	-1.12(23)	0.33(22)
C(27)	4.1(3)	2.14(23)	2.61(25)	-0.38(22)	-0.28(22)	0.16(20)
C(28)	2.89(25)	1.73(21)	2.96(26)	-0.02(19)	0.06(21)	0.04(19)
C(29)	2.11(24)	2.36(23)	3.69(28)	0.12(20)	0.19(20)	0.64(22)
C(30)	2.40(23)	1.89(22)	3.44(27)	-0.42(18)	0.52(20)	0.07(19)
C(31)	3.15(29)	2.87(28)	5.7(4)	-0.04(22)	0.66(26)	-0.57(26)
C(32)	3.8(3)	3.03(28)	4.3(3)	-1.04(23)	0.84(26)	0.20(24)
C(33)	2.95(26)	2.84(25)	3.33(27)	-0.57(21)	0.31(22)	-0.20(22)
C(34)	1.51(19)	1.15(18)	2.27(22)	-0.14(15)	-0.16(16)	-0.13(16)
C(35)	1.49(20)	1.46(19)	1.98(21)	-0.03(15)	-0.14(17)	0.01(16)
C(36)	2.47(22)	0.94(18)	2.24(22)	-0.22(16)	-0.24(18)	-0.31(16)
C(37)	2.42(23)	1.07(19)	2.98(25)	-0.32(17)	-0.47(19)	0.14(18)
C(38)	1.79(21)	1.97(22)	2.79(25)	-0.21(17)	-0.12(18)	0.75(19)
C(39)	1.92(21)	1.40(19)	2.11(21)	0.11(16)	0.18(17)	0.01(16)
C(40)	2.92(25)	1.64(22)	3.16(26)	0.19(19)	0.65(21)	-0.62(19)
C(41)	3.64(28)	1.83(22)	3.44(28)	-0.16(20)	1.52(23)	-0.40(20)
C(42)	6.8(5)	3.6(3)	7.1(5)	1.4(3)	4.3(4)	0.6(3)
C(43)	4.0(3)	3.21(28)	4.0(3)	-0.98(24)	0.81(26)	0.02(24)
C(44)	4.8(3)	5.2(4)	2.72(28)	-1.81(29)	1.01(25)	-0.24(26)
K	2.05(4)	1.80(4)	2.38(5)	0.21(4)	0.10(4)	-0.31(4)
O(5)	2.74(16)	1.97(15)	2.22(15)	0.52(12)	0.84(13)	-0.45(12)
O(6)	2.35(16)	2.42(16)	3.43(18)	0.08(13)	0.35(14)	-0.35(14)
O(7)	2.78(17)	2.29(16)	3.09(18)	0.18(13)	0.37(14)	-1.02(14)
O(8)	2.45(17)	4.06(20)	2.21(16)	-0.36(14)	0.34(13)	-0.46(14)
O(9)	1.77(14)	1.73(14)	3.06(17)	0.21(12)	0.08(12)	-0.15(13)
O(10)	2.43(16)	2.53(16)	2.51(16)	-0.44(13)	0.10(13)	0.33(13)
N(9)	2.32(18)	1.79(18)	2.38(19)	-0.01(14)	0.38(15)	-0.52(15)
N(10)	2.77(21)	2.45(20)	3.15(22)	-0.21(16)	0.29(17)	0.11(17)
C(45)	3.24(26)	1.69(21)	2.46(23)	-0.28(18)	0.12(20)	-0.23(18)
C(46)	3.33(26)	1.58(20)	2.13(22)	0.20(18)	-0.06(19)	-0.20(17)
C(47)	3.63(27)	2.33(23)	3.04(26)	0.42(20)	1.50(22)	-0.61(20)
C(48)	2.97(26)	2.79(25)	2.86(25)	1.17(20)	1.17(21)	-0.05(20)
C(49)	1.98(23)	3.90(29)	3.57(28)	0.48(21)	0.54(21)	-0.22(23)
C(50)	2.28(25)	4.1(3)	4.2(3)	-0.86(22)	0.79(22)	-0.25(25)
C(51)	2.46(25)	2.46(24)	4.1(3)	-0.45(20)	-0.39(22)	-0.07(22)
C(52)	3.50(28)	2.07(23)	3.34(27)	0.13(20)	-0.54(22)	-0.72(20)
C(53)	3.15(27)	4.3(3)	3.07(27)	0.88(24)	0.19(22)	-1.76(24)
C(54)	3.10(27)	5.0(3)	2.12(24)	0.20(24)	0.44(20)	-1.35(23)
C(55)	2.89(24)	3.53(27)	2.56(24)	0.23(21)	1.08(20)	-0.27(21)
C(56)	2.49(23)	2.61(24)	3.46(26)	0.02(20)	0.68(20)	-0.41(21)
C(57)	2.05(22)	2.22(22)	3.13(25)	-0.37(18)	-0.25(19)	-0.47(20)
C(58)	1.88(21)	2.18(22)	3.09(25)	-0.13(18)	-0.21(19)	-0.32(19)
C(59)	2.59(24)	1.80(21)	2.92(25)	0.19(18)	-0.31(20)	0.02(19)
C(60)	3.25(26)	2.34(23)	2.33(24)	-0.45(20)	-0.03(20)	0.11(19)
C(61)	3.08(26)	3.33(27)	2.89(26)	-0.84(21)	0.16(21)	0.68(22)
C(62)	3.41(29)	2.80(26)	4.3(3)	-0.73(22)	0.29(24)	1.02(23)
Cl	6.09(13)	5.03(12)	23.3(4)	0.92(10)	-2.51(18)	-3.70(17)
C(63)	5.4(4)	2.9(3)	8.9(6)	0.2(3)	0.7(4)	-0.2(3)
C(64)	4.7(4)	3.2(3)	7.4(5)	1.10(28)	0.4(4)	0.4(3)

Table S5. - continued

C(65)	11.0(8)	5.2(5)	10.9(8)	2.2(5)	-5.9(8)	0.7(6)
C(66)	23.9(20)	2.7(5)	21.0(20)	2.0(8)	-17.05(18)	-1.4(8)
C(67)	43.(3)	7.6(9)	2.3(5)	11.5(14)	1.2(10)	-0.1(5)
C(68)	23.7(15)	7.9(7)	10.8(8)	10.1(9)	12.6(10)	6.3(7)

- a. The estimated standard deviations of the least significant digits are given in parentheses. The B(ij)'s are related to the dimensionless beta(ij)'s employed during refinement as $B(ij) = 4\beta(ij)/a(i)*a(j)^*$.

Table S6. Fractional Coordinates and Isotropic Thermal Parameters for the Fixed Atoms

atom	x	y	z	Biso
H(b1)	0.2098	-0.0542	0.7352	2.35
H(b2)	0.3096	-0.1302	0.7774	2.14
H(b3)	0.2060	0.1877	0.6848	2.77
H(b4)	0.3043	0.2705	0.6929	2.72
H(b5)	0.5898	0.2899	0.8046	2.37
H(b6)	0.6794	0.2203	0.8707	3.05
H(b7)	0.6829	-0.0216	0.9268	2.74
H(b8)	0.5938	-0.1096	0.8950	2.52
H(3)	0.0562	0.0236	0.5845	3.19
H(4)	-0.0306	0.0540	0.6449	3.07
H(5)	0.0110	0.0942	0.7408	2.79
H(6)	0.1405	0.1013	0.7784	2.56
H(14)	0.4907	0.3832	0.6208	3.85
H(15)	0.4663	0.4643	0.6816	3.23
H(16)	0.4348	0.4451	0.7764	3.18
H(17)	0.4232	0.3424	0.8073	3.01
H(25)	0.8859	0.1246	0.9147	3.48
H(26)	0.8860	0.1605	1.0111	3.59
H(27)	0.7737	0.1646	1.0494	3.74
H(28)	0.6612	0.1306	0.9911	3.22
H(36)	0.4989	-0.2833	0.7951	2.19
H(37)	0.4290	-0.3132	0.8678	2.56
H(38)	0.3736	-0.2382	0.9214	2.66
H(39)	0.3901	-0.1337	0.9022	2.33
H(N5)	0.2482	0.0502	0.6161	3.11
H(N6)	0.4870	0.2249	0.6627	3.68
H(N7)	0.7187	0.0789	0.8141	2.81
H(N8)	0.5149	-0.1344	0.7412	2.35
H(9a)	0.3114	0.0543	0.5331	5.53
H(9b)	0.3785	0.0080	0.5414	5.53
H(9c)	0.3473	0.0316	0.5969	5.53
H(10a)	0.3296	-0.0776	0.6282	5.66
H(10b)	0.3618	-0.1006	0.5730	5.66
H(10c)	0.2837	-0.1239	0.5836	5.66
H(11a)	0.2219	-0.0866	0.4787	6.31
H(11b)	0.3018	-0.0669	0.4690	6.31
H(11c)	0.2362	-0.0193	0.4595	6.31
H(20a)	0.5715	0.1588	0.6540	3.81
H(20b)	0.6346	0.1866	0.6234	3.81
H(20c)	0.6008	0.1222	0.6039	3.81
H(21a)	0.6032	0.2234	0.5164	5.28
H(21b)	0.5212	0.2183	0.4808	5.28
H(21c)	0.5693	0.1590	0.4967	5.28
H(22a)	0.4182	0.1732	0.5297	5.30
H(22b)	0.4370	0.1505	0.5957	5.30
H(22c)	0.4662	0.1139	0.5455	5.30
H(31a)	0.8217	-0.0319	0.7445	4.88
H(31b)	0.8883	0.0078	0.7305	4.88
H(31c)	0.8218	-0.0092	0.6794	4.88
H(32a)	0.8684	0.1214	0.7048	4.60
H(32b)	0.7894	0.1510	0.7028	4.60
H(32c)	0.8021	0.1041	0.6536	4.60
H(33a)	0.6808	0.0865	0.7250	3.90
H(33b)	0.6924	0.0168	0.7403	3.90
H(33c)	0.6934	0.0399	0.6756	3.90
H(42a)	0.6665	-0.2582	0.6694	5.98
H(42b)	0.7229	-0.2252	0.7194	5.98

Table S6. - continued

H(43a)	0.6972	-0.1184	0.7518	4.70
H(43b)	0.6230	-0.0845	0.7242	4.70
H(43c)	0.6856	-0.0949	0.6860	4.70
H(44a)	0.5281	-0.1375	0.6442	4.94
H(44b)	0.5442	-0.2036	0.6229	4.94
H(44c)	0.5906	-0.1479	0.6060	4.94
H(45a)	0.8377	0.0131	0.0062	3.04
H(45b)	0.9027	0.0240	0.0609	3.04
H(46a)	0.7942	0.0497	0.0925	2.94
H(46b)	0.8196	-0.0133	0.1235	2.94
H(47a)	0.6657	0.0378	0.0856	3.38
H(47b)	0.6853	-0.0194	0.1276	3.38
H(48a)	0.5927	-0.0270	0.0154	3.32
H(48b)	0.5610	-0.0228	0.0752	3.32
H(49a)	0.5309	-0.1338	0.0018	3.87
H(49b)	0.5023	-0.1166	0.0608	3.87
H(50a)	0.5058	-0.2221	0.0538	4.20
H(50b)	0.5667	-0.2011	0.1081	4.20
H(51a)	0.5520	-0.2194	-0.0418	3.71
H(51b)	0.5508	-0.2886	-0.0224	3.71
H(52a)	0.6218	-0.2853	-0.0956	3.73
H(52b)	0.6790	-0.2951	-0.0358	3.73
H(53a)	0.7106	-0.2372	-0.1437	3.94
H(53b)	0.7733	-0.2480	-0.0873	3.94
H(54a)	0.7325	-0.1310	-0.1338	3.87
H(54b)	0.8044	-0.1660	-0.1454	3.87
H(55a)	0.8213	-0.0476	-0.0739	3.61
H(55b)	0.8771	-0.0867	-0.1041	3.61
H(56a)	0.9456	-0.1109	-0.0096	3.59
H(56b)	0.9447	-0.0395	-0.0201	3.59
H(57a)	0.9903	-0.0647	0.0877	3.05
H(57b)	0.9292	-0.0611	0.1287	3.05
H(58a)	0.9932	-0.1567	0.1371	2.99
H(58b)	0.9582	-0.1699	0.0700	2.99
H(59a)	0.9335	-0.2367	0.1776	3.17
H(59b)	0.9001	-0.2607	0.1132	3.17
H(60a)	0.8095	-0.2243	0.1948	3.31
H(60b)	0.8287	-0.2935	0.1846	3.31
H(61a)	0.6732	-0.2452	0.1559	3.89
H(61b)	0.7012	-0.3136	0.1564	3.89
H(62a)	0.6562	-0.3188	0.0529	4.29
H(62b)	0.5908	-0.3074	0.0886	4.29