Supporting Information

Calix[4]pyrrole Schiff base macrocycles.
Novel binucleating ligands for μ-oxo iron complexes.

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Figure S1. UV-Vis spectra of the free base form of **1** (– – –), the HCl salt of **1** (---) and of the μ-oxo bis iron complex, **6** (—) in CH_2Cl_2.

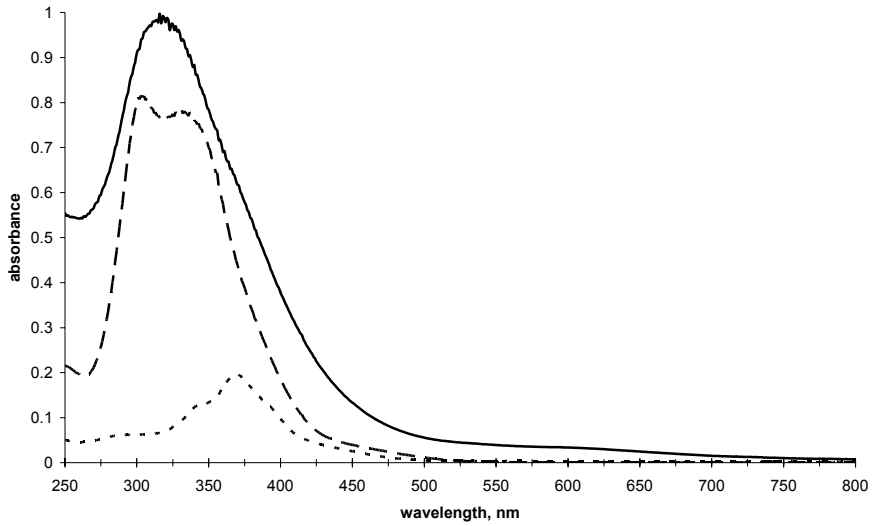

Figure S2. UV-Vis spectra of the free base form of **2** (– – –), the HCl salt of **2** (---), the μ-oxo bis iron complex, **7** (—) in CH_2Cl_2, and the μ-oxo bis iron bis Cl complex, **9** (– -- –) in CH_2Cl_2.

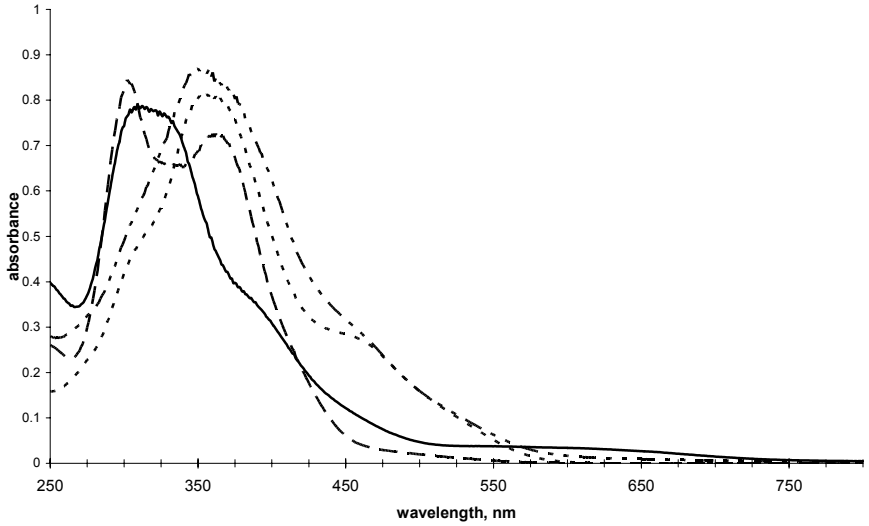

Figure S3. UV-Vis spectra of the free base form of **4** (– – –), the HCl salt of **4** (---) and of the μ-oxo bis iron complex, **8** (—) in CH_2Cl_2.

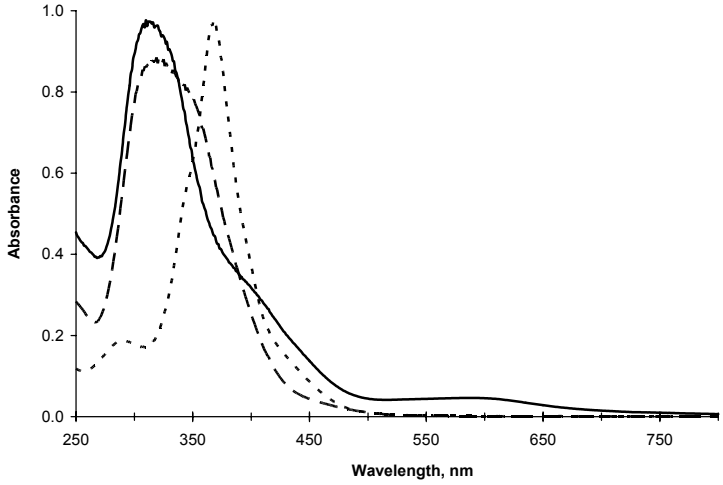

Figure S4. UV-Vis spectra of the free base form of **3** (– – –), the HCl salt of **3** (---) and of the μ-oxo bis iron complex, **10** (—) in CH_2Cl_2.

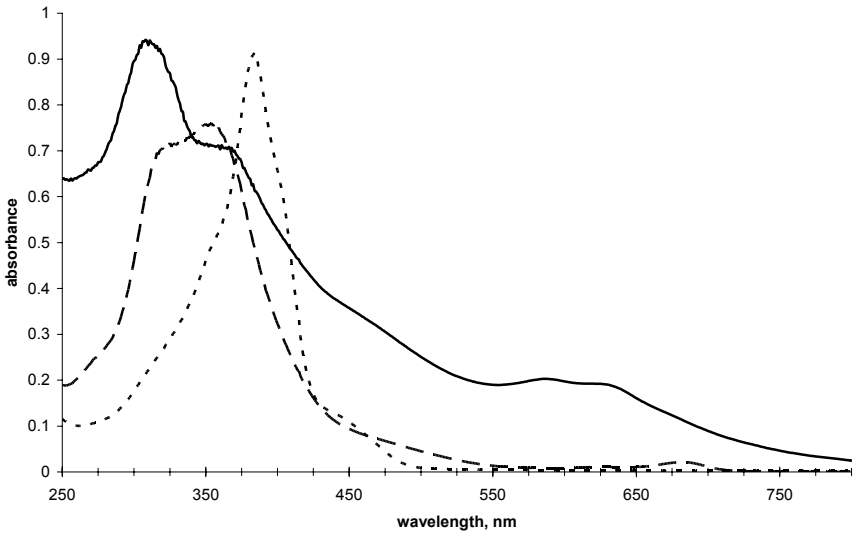

Figure SA1. View of **6** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. The methyl hydrogen atoms have been removed for clarity. The complex lies on a crystallographic mirror plane of symmetry at y = ¼. The crystallographic mirror bisects the two phenyl rings and passes through the bridging oxide ion, O1. Atoms related by x, ½ - y, z have labels appended by a '.

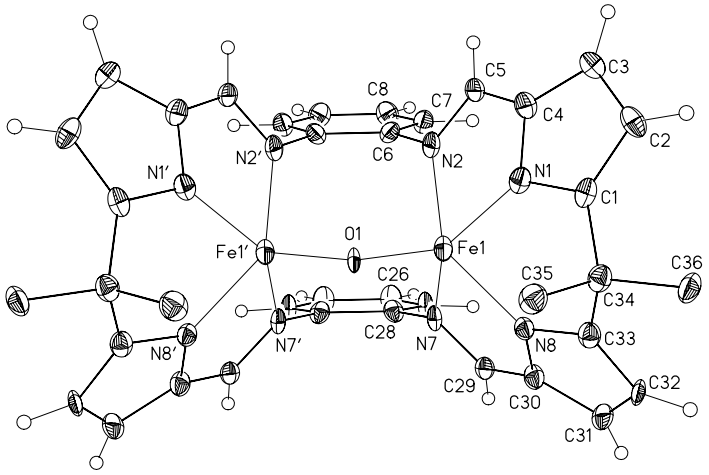

Figure SA2. Unit cell packing diagram for **6**. The view is approximately down the **c** axis. The methylene chloride solvate molecules lie on the crystallographic mirror planes perpendicular to the **b** axis.

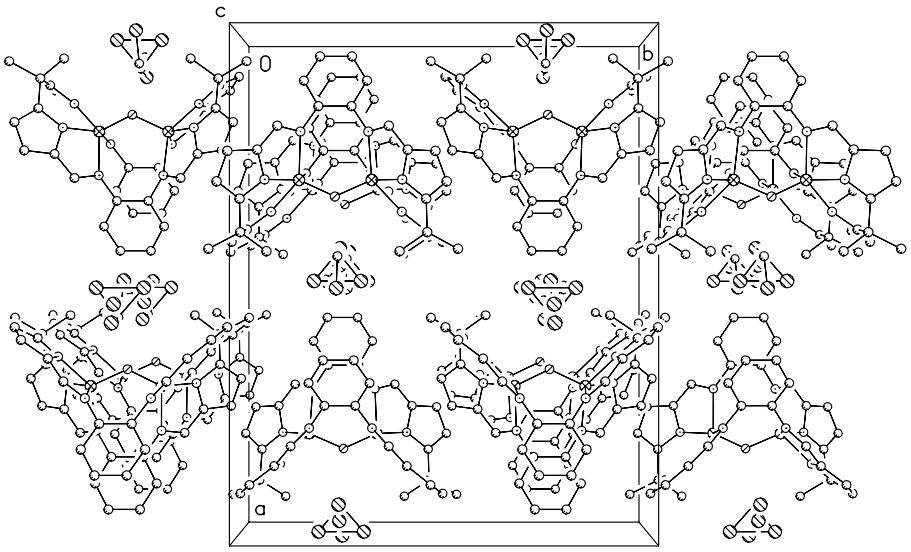

Table SA1. Crystal data and structure refinement for **6**.

Empirical formula	C39 H34 Cl2 Fe2 N8 O	
Formula weight	813.34	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 22.9779(13) Å	α= 90°.
	b = 18.8198(9) Å	β= 90°.
	c = 8.2504(4) Å	γ = 90°.
Volume	3567.8(3) $Å^3$	
Z	4	
Density (calculated)	1.514 Mg/m^3	
Absorption coefficient	1.008 mm^{-1}	
F(000)	1672	
Crystal size	0.27 x 0.20 x 0.04 mm	
Theta range for data collection	3.04 to 24.99°.	
Index ranges	-27<=h<=27, -22<=k<=22, -9<=l<=9	
Reflections collected	5899	
Independent reflections	3233 [R(int) = 0.0770]	
Completeness to theta = 24.99°	99.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3233 / 43 / 264	
Goodness-of-fit on F^2	1.834	
Final R indices [I>2sigma(I)]	R1 = 0.0694, wR2 = 0.1295	
R indices (all data)	R1 = 0.1318, wR2 = 0.1380	
Largest diff. peak and hole	0.989 and -0.521 $e.Å^{-3}$	

Table SA2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe1	3029(1)	1664(1)	1244(1)	28(1)
O1	3350(2)	2500	1718(6)	22(1)
O1A	2810(30)	2500	1510(80)	22
N1	3615(2)	982(2)	280(6)	30(1)
N2	2851(2)	1740(2)	-1289(6)	29(1)
N7	2143(2)	1727(2)	2166(5)	27(1)
N8	3056(2)	943(2)	3052(5)	25(1)
C1	3962(2)	448(3)	889(7)	30(2)
C2	4182(2)	33(3)	-375(7)	34(2)
C3	3957(2)	324(3)	-1854(7)	35(2)
C4	3600(2)	898(3)	-1385(7)	31(1)
C5	3183(2)	1325(3)	-2202(7)	30(1)
C6	2389(2)	2129(3)	-2064(6)	27(1)
C7	1930(2)	1772(3)	-2775(6)	32(1)
C8	1474(2)	2136(3)	-3470(7)	36(2)
C26	670(2)	2129(3)	634(7)	39(2)
C27	1150(2)	1774(3)	1160(7)	31(1)
C28	1648(2)	2121(3)	1635(7)	28(1)

C29	2069(2)	1243(3)	3294(6)	26(1)
C30	2524(2)	813(3)	3782(7)	29(1)
C31	2569(2)	190(3)	4715(7)	34(2)
C32	3119(2)	-60(3)	4503(6)	28(1)
C33	3418(2)	401(3)	3459(6)	28(1)
C34	4030(2)	379(3)	2722(7)	30(1)
C35	4389(2)	1002(3)	3370(7)	37(2)
C36	4343(2)	-316(3)	3180(7)	35(2)
C1A	4458(6)	2500	-601(14)	65(7)
Cl1	4631(5)	2500	-2614(13)	175(6)
Cl2	5073(3)	2500	544(10)	105(2)
C1B	4374(7)	2500	-1205(16)	109(11)
Cl1B	4286(4)	2500	-3268(9)	91(2)
Cl2B	4935(4)	3049(6)	-676(14)	115(3)

Table SA3. Bond lengths [Å] and angles [°] **6**.

Fe1-O1A	1.67(2)	C8-H8	0.96
Fe1-O1	1.780(2)	C26-C27	1.361(7)
Fe1-N8	2.018(4)	C26-C26#1	1.397(11)
Fe1-N1	2.024(5)	C26-H26	0.96
Fe1-N2	2.135(5)	C27-C28	1.375(6)
Fe1-N7	2.176(4)	C27-H27	0.95
O1-Fe1#1	1.780(2)	C28-C28#1	1.427(10)
O1A-Fe1#1	1.67(2)	C29-C30	1.383(7)
N1-C1	1.377(6)	C29-H29	0.95
N1-C4	1.383(7)	C30-C31	1.406(7)
N2-C5	1.328(6)	C31-C32	1.360(7)
N2-C6	1.439(6)	C31-H31	0.95
N7-C29	1.313(6)	C32-C33	1.403(7)
N7-C28	1.427(6)	C32-H32	0.96
N8-C33	1.359(6)	C33-C34	1.532(7)
N8-C30	1.384(6)	C34-C35	1.529(7)
C1-C2	1.398(7)	C34-C36	1.541(7)
C1-C34	1.525(7)	C35-H35A	0.96
C2-C3	1.434(7)	C35-H35B	0.96
C2-H2	0.96	C35-H35C	0.96
C3-C4	1.410(7)	C36-H36A	0.96
C3-H3	0.96	C36-H36B	0.96
C4-C5	1.421(7)	C36-H36C	0.96
C5-H5	0.96	C1A-Cl2	1.699(9)
C6-C7	1.382(7)	C1A-Cl1	1.708(9)
C6-C6#1	1.395(10)	C1B-Cl2B#1	1.709(9)
C7-C8	1.377(7)	C1B-Cl2B	1.709(9)
C7-H7	0.96	C1B-Cl1B	1.714(10)
C8-C8#1	1.369(11)	Cl2B-Cl2B#1	2.07(2)
O1A-Fe1-N8	123(2)	O1-Fe1-N2	103.64(19)
O1-Fe1-N8	114.82(19)	N8-Fe1-N2	140.74(16)
O1A-Fe1-N1	149(2)	N1-Fe1-N2	77.60(17)
O1-Fe1-N1	111.82(19)	O1A-Fe1-N7	67(2)
N8-Fe1-N1	81.00(17)	O1-Fe1-N7	105.25(18)
O1A-Fe1-N2	90(2)	N8-Fe1-N7	78.82(17)

N1-Fe1-N7	142.54(17)	C27-C26-H26	120.3
N2-Fe1-N7	99.12(16)	C26#1-C26-H26	120.3
Fe1-O1-Fe1#1	124.1(3)	C26-C27-C28	122.2(5)
Fe1-O1A-Fe1#1	141(4)	C26-C27-H27	118.9
C1-N1-C4	107.1(5)	C28-C27-H27	118.9
C1-N1-Fe1	134.8(4)	C27-C28-N7	120.3(4)
C4-N1-Fe1	116.5(3)	C27-C28-C28#1	118.3(3)
C5-N2-C6	118.2(5)	N7-C28-C28#1	121.3(3)
C5-N2-Fe1	113.9(4)	N7-C29-C30	120.9(5)
C6-N2-Fe1	127.7(3)	N7-C29-H29	119.5
C29-N7-C28	118.3(4)	C30-C29-H29	119.5
C29-N7-Fe1	109.4(3)	C29-C30-N8	115.9(5)
C28-N7-Fe1	131.8(3)	C29-C30-C31	134.7(5)
C33-N8-C30	107.5(4)	N8-C30-C31	108.7(5)
C33-N8-Fe1	134.9(4)	C32-C31-C30	106.7(5)
C30-N8-Fe1	114.5(3)	C32-C31-H31	126.7
N1-C1-C2	110.1(5)	C30-C31-H31	126.7
N1-C1-C34	118.9(5)	C31-C32-C33	108.6(5)
C2-C1-C34	130.9(5)	C31-C32-H32	126.6
C1-C2-C3	106.9(5)	C33-C32-H32	124.7
C1-C2-H2	127.2	N8-C33-C32	108.4(4)
C3-C2-H2	125.8	N8-C33-C34	119.0(5)
C4-C3-C2	105.6(5)	C32-C33-C34	132.5(5)
C4-C3-H3	126.5	C1-C34-C35	109.7(5)
C2-C3-H3	127.9	C1-C34-C33	107.3(4)
N1-C4-C3	110.2(5)	C35-C34-C33	109.6(5)
N1-C4-C5	115.1(5)	C1-C34-C36	111.3(5)
C3-C4-C5	134.0(6)	C35-C34-C36	108.3(4)
N2-C5-C4	116.9(5)	C33-C34-C36	110.7(5)
N2-C5-H5	121.0	C34-C35-H35A	109.1
C4-C5-H5	122.1	C34-C35-H35B	111.2
C7-C6-C6#1	119.2(3)	H35A-C35-H35B	109.5
C7-C6-N2	120.2(5)	C34-C35-H35C	108.0
C6#1-C6-N2	120.6(3)	H35A-C35-H35C	109.5
C8-C7-C6	121.0(5)	H35B-C35-H35C	109.5
C8-C7-H7	120.1	C34-C36-H36A	110.5
C6-C7-H7	119.0	C34-C36-H36B	108.4
C8#1-C8-C7	119.9(3)	H36A-C36-H36B	109.5
C8#1-C8-H8	119.3	C34-C36-H36C	109.5
C7-C8-H8	120.8	H36A-C36-H36C	109.5
C27-C26-C26#1	119.4(3)	H36B-C36-H36C	109.5

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Table SA4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe1	32(1)	18(1)	35(1)	0(1)	0(1)	0(1)
O1	24(3)	8(3)	33(4)	0	1(2)	0
N1	34(3)	23(3)	34(3)	3(2)	-3(2)	-3(2)
N2	33(2)	17(2)	37(3)	0(2)	-3(2)	-5(2)

N7	31(2)	13(2)	37(3)	-2(2)	-4(2)	-1(2)
N8	29(3)	19(3)	26(3)	-3(2)	-1(2)	-1(2)
C1	29(3)	22(3)	39(4)	6(3)	-6(3)	-3(3)
C2	23(3)	32(4)	47(4)	-12(3)	0(3)	4(3)
C3	36(3)	32(4)	36(4)	-7(3)	3(3)	5(3)
C4	32(3)	26(3)	34(4)	-5(3)	-3(3)	-1(3)
C5	37(3)	20(3)	32(4)	-5(3)	3(3)	-8(3)
C6	31(3)	24(3)	24(3)	5(3)	-3(2)	-3(3)
C7	37(3)	26(3)	34(4)	3(3)	-2(3)	0(3)
C8	33(3)	35(3)	41(4)	-6(3)	-4(3)	-3(3)
C26	28(3)	33(4)	56(4)	-2(3)	-7(3)	-3(3)
C27	31(3)	15(3)	47(4)	-1(3)	-8(3)	1(3)
C28	23(3)	25(3)	34(4)	-3(3)	4(2)	3(2)
C29	27(3)	21(3)	30(4)	-3(3)	-1(2)	-9(3)
C30	31(3)	21(3)	35(4)	-2(3)	1(3)	-3(3)
C31	44(4)	22(4)	36(4)	3(3)	1(3)	-12(3)
C32	42(4)	11(3)	31(3)	7(3)	-6(3)	3(3)
C33	29(3)	25(3)	31(4)	-1(3)	-6(3)	-1(3)
C34	32(3)	25(3)	33(4)	2(3)	-3(3)	-4(3)
C35	40(3)	33(4)	36(4)	1(3)	-4(3)	-8(3)
C36	35(3)	27(3)	42(4)	14(3)	5(3)	9(3)
C1A	63(10)	63(11)	69(10)	0	12(8)	0
Cl1	165(8)	210(9)	150(9)	0	19(7)	0
Cl2	65(4)	130(6)	120(6)	0	8(4)	0
C1B	115(13)	110(14)	102(13)	0	17(10)	0
Cl1B	111(5)	61(4)	101(6)	0	63(4)	0
Cl2B	68(5)	125(7)	152(8)	-32(6)	16(5)	-13(5)

Table SA5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6**.

	x	y	z	U(eq)
H2	4430	-376	-286	41
H3	4033	169	-2943	42
H5	3143	1320	-3360	36
H7	1932	1262	-2776	39
H8	1154	1887	-3956	44
H26	333	1872	276	47
H27	1140	1270	1201	38
H29	1697	1188	3782	31
H31	2273	-16	5366	41
H32	3281	-483	4970	34
H35A	4196	1439	3102	55
H35B	4437	971	4524	55
H35C	4763	989	2856	55
H36A	4381	-355	4336	52
H36B	4117	-708	2780	52
H36C	4722	-325	2691	52

Table SA6. Torsion angles [°] for **6**.

N8-Fe1-O1-Fe1#1	-135.3(3)	Fe1-N1-C1-C34	-12.1(7)
N1-Fe1-O1-Fe1#1	134.8(3)	N1-C1-C2-C3	-0.4(6)
N2-Fe1-O1-Fe1#1	52.9(3)	C34-C1-C2-C3	177.3(5)
N7-Fe1-O1-Fe1#1	-50.7(4)	C1-C2-C3-C4	-1.0(6)
Fe1#1-O1-O1A-Fe1	159(3)	C1-N1-C4-C3	-2.3(6)
Fe1-O1-O1A-Fe1#1	-159(3)	Fe1-N1-C4-C3	-169.8(3)
N8-Fe1-O1A-Fe1#1	124(6)	C1-N1-C4-C5	169.6(4)
N1-Fe1-O1A-Fe1#1	-11(10)	Fe1-N1-C4-C5	2.0(6)
N2-Fe1-O1A-Fe1#1	-78(6)	C2-C3-C4-N1	2.0(6)
N7-Fe1-O1A-Fe1#1	-177(7)	C2-C3-C4-C5	-167.7(6)
O1A-Fe1-N1-C1	126(4)	C6-N2-C5-C4	-174.4(4)
O1-Fe1-N1-C1	95.5(5)	Fe1-N2-C5-C4	0.1(6)
N8-Fe1-N1-C1	-17.7(5)	N1-C4-C5-N2	-1.3(7)
N2-Fe1-N1-C1	-164.6(5)	C3-C4-C5-N2	168.0(6)
N7-Fe1-N1-C1	-75.8(6)	C5-N2-C6-C7	64.7(6)
O1A-Fe1-N1-C4	-71(4)	Fe1-N2-C6-C7	-109.0(5)
O1-Fe1-N1-C4	-101.3(4)	C5-N2-C6-C6#1	-117.3(4)
N8-Fe1-N1-C4	145.4(4)	Fe1-N2-C6-C6#1	69.0(4)
N2-Fe1-N1-C4	-1.4(4)	C6#1-C6-C7-C8	-0.4(6)
N7-Fe1-N1-C4	87.4(5)	N2-C6-C7-C8	177.6(5)
O1A-Fe1-N2-C5	152(2)	C6-C7-C8-C8#1	0.4(6)
O1-Fe1-N2-C5	110.5(4)	C26#1-C26-C27-C28	-2.7(7)
N8-Fe1-N2-C5	-57.8(4)	C26-C27-C28-N7	-179.5(5)
N1-Fe1-N2-C5	0.7(3)	C26-C27-C28-C28#1	2.7(7)
N7-Fe1-N2-C5	-141.3(3)	C29-N7-C28-C27	-51.3(7)
O1A-Fe1-N2-C6	-35(2)	Fe1-N7-C28-C27	119.6(5)
O1-Fe1-N2-C6	-75.6(4)	C29-N7-C28-C28#1	126.5(4)
N8-Fe1-N2-C6	116.1(4)	Fe1-N7-C28-C28#1	-62.7(5)
N1-Fe1-N2-C6	174.6(4)	C28-N7-C29-C30	175.7(5)
N7-Fe1-N2-C6	32.6(4)	Fe1-N7-C29-C30	2.9(6)
O1A-Fe1-N7-C29	-138(2)	N7-C29-C30-N8	2.1(8)
O1-Fe1-N7-C29	-117.7(4)	N7-C29-C30-C31	-167.3(6)
N8-Fe1-N7-C29	-4.8(3)	C33-N8-C30-C29	-169.6(5)
N1-Fe1-N7-C29	53.9(5)	Fe1-N8-C30-C29	-6.5(6)
N2-Fe1-N7-C29	135.3(3)	C33-N8-C30-C31	2.4(6)
O1A-Fe1-N7-C28	50(2)	Fe1-N8-C30-C31	165.6(4)
O1-Fe1-N7-C28	70.8(5)	C29-C30-C31-C32	168.2(6)
N8-Fe1-N7-C28	-176.3(5)	N8-C30-C31-C32	-1.7(6)
N1-Fe1-N7-C28	-117.6(5)	C30-C31-C32-C33	0.3(6)
N2-Fe1-N7-C28	-36.1(4)	C30-N8-C33-C32	-2.2(6)
O1A-Fe1-N8-C33	-144(3)	Fe1-N8-C33-C32	-160.3(4)
O1-Fe1-N8-C33	-95.3(5)	C30-N8-C33-C34	175.9(5)
N1-Fe1-N8-C33	14.7(5)	Fe1-N8-C33-C34	17.9(7)
N2-Fe1-N8-C33	72.2(5)	C31-C32-C33-N8	1.2(6)
N7-Fe1-N8-C33	163.0(5)	C31-C32-C33-C34	-176.6(6)
O1A-Fe1-N8-C30	59(3)	N1-C1-C34-C35	-70.0(6)
O1-Fe1-N8-C30	107.8(4)	C2-C1-C34-C35	112.5(6)
N1-Fe1-N8-C30	-142.3(4)	N1-C1-C34-C33	49.0(6)
N2-Fe1-N8-C30	-84.8(4)	C2-C1-C34-C33	-128.5(6)
N7-Fe1-N8-C30	6.0(4)	N1-C1-C34-C36	170.2(4)
C4-N1-C1-C2	1.6(6)	C2-C1-C34-C36	-7.3(8)
Fe1-N1-C1-C2	165.9(4)	N8-C33-C34-C1	-52.0(6)
C4-N1-C1-C34	-176.4(4)	C32-C33-C34-C1	125.7(6)

N8-C33-C34-C35	67.1(6)
C32-C33-C34-C35	-115.3(7)
N8-C33-C34-C36	-173.6(4)
C32-C33-C34-C36	4.1(9)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Figure SB1. View of **7** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. Most hydrogen atoms have been removed for clarity.

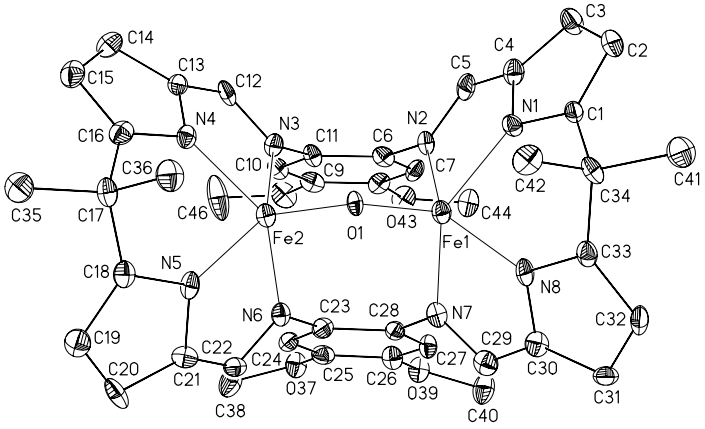

Figure SB2. Unit cell packing diagram for **7**. The view is approximately down the **b** axis. The dashed lines are indicative of close C-H···O and Cl contacts involving the methylene chloride solvate molecules. The geometry of these interactions are listed in Table 7.

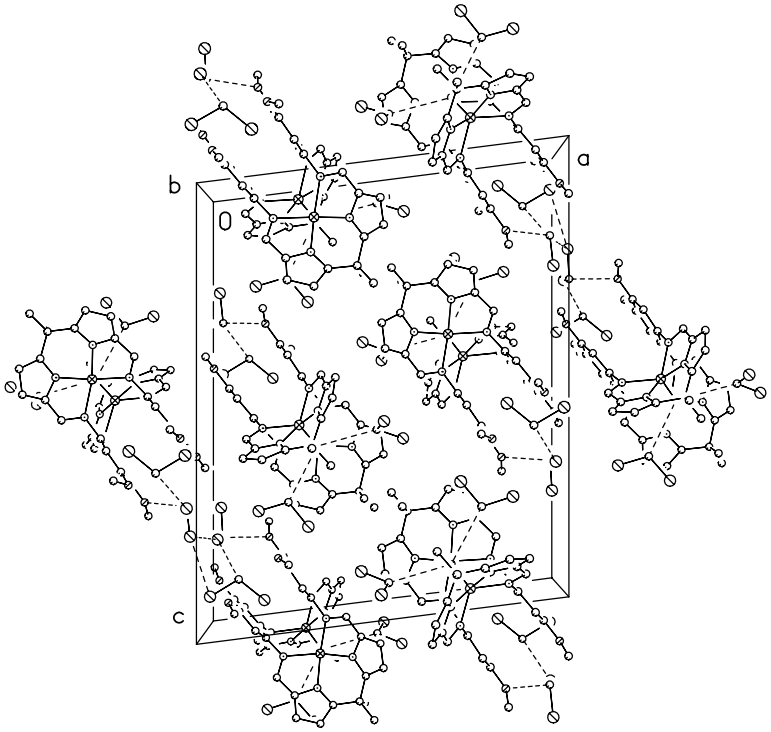

Table SB1. Crystal data and structure refinement for **7**.

Empirical formula	C46 H48 Cl8 Fe2 N8 O5	
Formula weight	1188.22	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 19.3235(11) Å	α= 90°.
	b = 11.4123(6) Å	β= 97.258(2)°.
	c = 23.7326(15) Å	γ = 90°.
Volume	5191.7(5) Å^3	
Z	4	
Density (calculated)	1.520 Mg/m^3	
Absorption coefficient	1.023 mm^{-1}	
F(000)	2432	
Crystal size	0.29 x 0.24 x 0.03 mm	
Theta range for data collection	2.99 to 23.75°.	
Index ranges	-21<=h<=21, -12<=k<=12, -26<=l<=26	
Reflections collected	13705	
Independent reflections	7506 [R(int) = 0.0982]	
Completeness to theta = 23.75°	95.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7506 / 0 / 623	
Goodness-of-fit on F^2	1.227	
Final R indices [I>2sigma(I)]	R1 = 0.0733, wR2 = 0.1426	
R indices (all data)	R1 = 0.1639, wR2 = 0.1674	
Extinction coefficient	1.6(2)x10^{-6}	
Largest diff. peak and hole	0.469 and -0.836 e.Å^{-3}	

Table SB2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe1	2691(1)	7033(1)	5545(1)	25(1)
Fe2	3161(1)	4595(1)	6079(1)	24(1)
O1	3178(2)	6167(4)	6078(2)	21(1)
N1	2203(3)	8350(5)	5900(3)	24(2)
N2	1656(3)	6383(5)	5517(3)	25(2)
N3	2085(3)	4166(5)	6011(3)	27(2)
N4	3089(3)	3884(5)	6846(3)	24(2)
N5	4121(3)	3860(5)	6217(3)	25(2)
N6	3340(3)	4160(5)	5242(3)	24(2)
N7	2949(3)	6412(5)	4750(3)	26(2)
N8	3235(3)	8393(5)	5278(3)	27(2)
C1	2370(4)	9484(6)	6038(3)	22(2)
C2	1760(4)	10053(7)	6180(3)	36(2)
C3	1223(4)	9235(7)	6112(3)	36(2)
C4	1509(4)	8202(6)	5935(3)	30(2)
C5	1235(4)	7119(7)	5710(3)	31(2)
C6	1377(4)	5291(6)	5271(3)	26(2)
C7	908(4)	5315(7)	4773(3)	30(2)
C8	647(4)	4296(7)	4522(3)	29(2)
C9	836(4)	3217(7)	4773(4)	33(2)

C10	1302(4)	3183(6)	5274(3)	29(2)
C11	1575(4)	4227(6)	5524(3)	25(2)
C12	1914(4)	3626(6)	6461(4)	30(2)
C13	2437(4)	3442(6)	6923(3)	26(2)
C14	2495(4)	2715(7)	7409(3)	36(2)
C15	3199(4)	2707(7)	7615(3)	35(2)
C16	3556(4)	3422(6)	7262(3)	29(2)
C17	4327(4)	3658(6)	7272(3)	28(2)
C18	4509(4)	3405(6)	6677(3)	26(2)
C19	5024(4)	2698(7)	6500(4)	34(2)
C20	4934(4)	2683(6)	5916(4)	36(2)
C21	4370(4)	3408(6)	5738(3)	26(2)
C22	3936(4)	3595(6)	5238(3)	26(2)
C23	2895(4)	4258(6)	4708(3)	28(2)
C24	2667(4)	3234(6)	4423(3)	28(2)
C25	2261(4)	3277(7)	3911(4)	33(2)
C26	2089(4)	4381(7)	3654(3)	31(2)
C27	2325(4)	5386(6)	3930(3)	29(2)
C28	2725(4)	5336(6)	4458(3)	24(2)
C29	3298(4)	7177(7)	4486(3)	32(2)
C30	3457(4)	8274(6)	4753(4)	29(2)
C31	3721(4)	9342(7)	4594(3)	28(2)
C32	3648(4)	10125(7)	5031(3)	31(2)
C33	3340(4)	9523(6)	5452(3)	27(2)
C34	3109(4)	9922(6)	6007(3)	28(2)
C35	4756(4)	2914(7)	7704(3)	37(2)
C36	4475(4)	4960(6)	7418(3)	36(2)
O37	1989(3)	2320(4)	3607(2)	37(1)
C38	2317(5)	1227(7)	3756(4)	51(3)
O39	1671(3)	4345(4)	3139(2)	36(1)
C40	1631(5)	5379(7)	2800(3)	50(3)
C41	3124(4)	11266(6)	6058(4)	39(2)
C42	3597(4)	9404(7)	6506(3)	33(2)
O43	210(3)	4226(5)	4023(2)	40(2)
C44	22(4)	5278(7)	3735(3)	40(2)
O45	556(3)	2234(5)	4496(2)	42(2)
C46	772(5)	1119(7)	4723(5)	82(4)
C1A	4839(4)	6575(8)	5870(4)	59(3)
Cl1A	5035(1)	8033(2)	5696(1)	49(1)
Cl2A	5571(1)	5785(2)	6154(1)	53(1)
C1B	391(5)	2355(7)	2965(4)	63(3)
Cl1B	309(2)	832(2)	2953(1)	71(1)
Cl2B	321(2)	2924(2)	2274(1)	79(1)
C1C	2386(5)	6681(9)	7247(4)	72(3)
Cl1C	2945(2)	7031(3)	7843(2)	120(1)
Cl2C	1548(2)	6385(3)	7369(1)	82(1)
C1D	-1001(5)	3473(12)	1163(5)	97(4)
Cl1D	-213(2)	3284(3)	861(2)	97(1)
Cl2D	-1712(2)	3510(3)	622(2)	103(1)

Table SB3. Bond lengths [Å] and angles [°] for **7**.

Fe1-O1	1.777(4)	C17-C36	1.544(10)
Fe1-N1	2.015(6)	C18-C19	1.387(10)
Fe1-N8	2.021(6)	C19-C20	1.374(11)
Fe1-N2	2.126(6)	C19-H19	0.96
Fe1-N7	2.134(6)	C20-C21	1.392(10)
Fe2-O1	1.794(4)	C20-H20	0.96
Fe2-N4	2.014(6)	C21-C22	1.380(10)
Fe2-N5	2.025(6)	C22-H22	0.96
Fe2-N6	2.118(6)	C23-C28	1.387(10)
Fe2-N3	2.124(6)	C23-C24	1.393(10)
N1-C1	1.364(9)	C24-C25	1.362(10)
N1-C4	1.364(9)	C24-H24	0.96
N2-C5	1.293(9)	C25-O37	1.376(9)
N2-C6	1.452(9)	C25-C26	1.421(10)
N3-C12	1.310(9)	C26-C27	1.370(10)
N3-C11	1.423(9)	C26-O39	1.378(8)
N4-C16	1.357(9)	C27-C28	1.388(10)
N4-C13	1.390(9)	C27-H27	0.96
N5-C18	1.347(9)	C29-C30	1.419(10)
N5-C21	1.389(9)	C29-H29	0.96
N6-C22	1.322(8)	C30-C31	1.392(10)
N6-C23	1.443(9)	C31-C32	1.389(10)
N7-C29	1.308(9)	C31-H31	0.96
N7-C28	1.449(9)	C32-C33	1.406(10)
N8-C33	1.362(9)	C32-H32	0.96
N8-C30	1.374(10)	C33-C34	1.513(11)
C1-C2	1.423(10)	C34-C42	1.536(10)
C1-C34	1.523(10)	C34-C41	1.539(10)
C2-C3	1.390(10)	C35-H35A	0.96
C2-H2	0.96	C35-H35B	0.96
C3-C4	1.389(10)	C35-H35C	0.96
C3-H3	0.96	C36-H36A	0.96
C4-C5	1.421(10)	C36-H36B	0.96
C5-H5	0.96	C36-H36C	0.96
C6-C11	1.387(10)	O37-C38	1.425(9)
C6-C7	1.395(10)	C38-H38A	0.96
C7-C8	1.373(10)	C38-H38B	0.96
C7-H7	0.96	C38-H38C	0.96
C8-O43	1.367(8)	O39-C40	1.425(8)
C8-C9	1.396(10)	C40-H40A	0.96
C9-O45	1.376(8)	C40-H40B	0.96
C9-C10	1.400(10)	C40-H40C	0.96
C10-C11	1.403(9)	C41-H41A	0.96
C10-H10	0.96	C41-H41B	0.96
C12-C13	1.410(10)	C41-H41C	0.96
C12-H12	0.96	C42-H42A	0.96
C13-C14	1.416(10)	C42-H42B	0.96
C14-C15	1.386(10)	C42-H42C	0.96
C14-H14	0.96	O43-C44	1.407(8)
C15-C16	1.410(10)	C44-H44A	0.96
C15-H15	0.96	C44-H44B	0.96
C16-C17	1.511(10)	C44-H44C	0.96
C17-C35	1.499(10)	O45-C46	1.424(9)
C17-C18	1.524(11)	C46-H46A	0.96

C46-H46B	0.96	C1B-H1BB	0.96
C46-H46C	0.96	C1C-Cl2C	1.714(10)
C1A-Cl2A	1.739(9)	C1C-Cl1C	1.715(10)
C1A-Cl1A	1.767(9)	C1C-H1CA	0.96
C1A-H1AA	0.96	C1C-H1CB	0.96
C1A-H1AB	0.96	C1D-Cl2D	1.758(10)
C1B-Cl1B	1.745(9)	C1D-Cl1D	1.777(11)
C1B-Cl2B	1.753(10)	C1D-H1DA	0.96
C1B-H1BA	0.96	C1D-H1DB	0.96

O1-Fe1-N1	110.5(2)	N1-C1-C34	119.7(6)
O1-Fe1-N8	113.6(2)	C2-C1-C34	132.2(7)
N1-Fe1-N8	81.3(2)	C3-C2-C1	107.2(7)
O1-Fe1-N2	103.9(2)	C3-C2-H2	127.0
N1-Fe1-N2	77.6(2)	C1-C2-H2	125.9
N8-Fe1-N2	141.4(2)	C4-C3-C2	106.6(7)
O1-Fe1-N7	106.5(2)	C4-C3-H3	126.3
N1-Fe1-N7	142.3(2)	C2-C3-H3	127.1
N8-Fe1-N7	77.8(3)	N1-C4-C3	110.2(6)
N2-Fe1-N7	100.4(2)	N1-C4-C5	114.0(7)
O1-Fe2-N4	114.1(2)	C3-C4-C5	135.1(8)
O1-Fe2-N5	113.5(2)	N2-C5-C4	118.5(7)
N4-Fe2-N5	81.6(3)	N2-C5-H5	121.0
O1-Fe2-N6	103.2(2)	C4-C5-H5	120.5
N4-Fe2-N6	142.3(2)	C11-C6-C7	119.9(7)
N5-Fe2-N6	78.5(2)	C11-C6-N2	120.6(6)
O1-Fe2-N3	104.4(2)	C7-C6-N2	119.5(6)
N4-Fe2-N3	78.3(3)	C8-C7-C6	120.9(7)
N5-Fe2-N3	141.8(2)	C8-C7-H7	119.7
N6-Fe2-N3	98.6(2)	C6-C7-H7	119.4
Fe1-O1-Fe2	123.3(3)	O43-C8-C7	125.3(7)
C1-N1-C4	108.0(6)	O43-C8-C9	114.6(7)
C1-N1-Fe1	134.3(5)	C7-C8-C9	120.0(7)
C4-N1-Fe1	116.7(5)	O45-C9-C8	116.7(7)
C5-N2-C6	118.8(6)	O45-C9-C10	123.8(7)
C5-N2-Fe1	113.2(5)	C8-C9-C10	119.5(7)
C6-N2-Fe1	127.8(5)	C9-C10-C11	120.2(7)
C12-N3-C11	117.8(7)	C9-C10-H10	119.8
C12-N3-Fe2	113.1(5)	C11-C10-H10	120.1
C11-N3-Fe2	128.4(5)	C6-C11-C10	119.5(7)
C16-N4-C13	107.1(6)	C6-C11-N3	121.4(6)
C16-N4-Fe2	134.3(5)	C10-C11-N3	119.1(6)
C13-N4-Fe2	115.6(5)	N3-C12-C13	118.3(7)
C18-N5-C21	107.8(6)	N3-C12-H12	120.8
C18-N5-Fe2	134.1(6)	C13-C12-H12	120.9
C21-N5-Fe2	115.2(5)	N4-C13-C12	114.6(7)
C22-N6-C23	117.0(6)	N4-C13-C14	109.9(7)
C22-N6-Fe2	111.5(5)	C12-C13-C14	134.2(8)
C23-N6-Fe2	131.0(5)	C15-C14-C13	105.2(7)
C29-N7-C28	118.6(7)	C15-C14-H14	127.6
C29-N7-Fe1	113.2(5)	C13-C14-H14	127.2
C28-N7-Fe1	127.9(5)	C14-C15-C16	108.7(7)
C33-N8-C30	108.5(6)	C14-C15-H15	126.2
C33-N8-Fe1	134.0(6)	C16-C15-H15	125.1
C30-N8-Fe1	116.3(5)	N4-C16-C15	109.0(7)
N1-C1-C2	108.1(6)	N4-C16-C17	120.3(7)

C15-C16-C17	130.5(7)	C33-C34-C42	109.6(6)
C35-C17-C16	111.7(7)	C1-C34-C42	109.0(6)
C35-C17-C18	110.7(6)	C33-C34-C41	111.3(7)
C16-C17-C18	107.2(6)	C1-C34-C41	109.4(6)
C35-C17-C36	108.7(6)	C42-C34-C41	108.6(6)
C16-C17-C36	109.2(6)	C17-C35-H35A	110.1
C18-C17-C36	109.3(6)	C17-C35-H35B	108.9
N5-C18-C19	109.0(7)	H35A-C35-H35B	109.5
N5-C18-C17	120.5(7)	C17-C35-H35C	109.5
C19-C18-C17	130.5(7)	H35A-C35-H35C	109.5
C20-C19-C18	108.1(7)	H35B-C35-H35C	109.5
C20-C19-H19	126.4	C17-C36-H36A	109.1
C18-C19-H19	125.5	C17-C36-H36B	109.8
C19-C20-C21	107.0(8)	H36A-C36-H36B	109.5
C19-C20-H20	126.9	C17-C36-H36C	109.5
C21-C20-H20	126.1	H36A-C36-H36C	109.5
C22-C21-N5	114.3(7)	H36B-C36-H36C	109.5
C22-C21-C20	136.1(8)	C25-O37-C38	115.9(6)
N5-C21-C20	108.1(7)	O37-C38-H38A	110.0
N6-C22-C21	120.3(7)	O37-C38-H38B	108.9
N6-C22-H22	119.8	H38A-C38-H38B	109.5
C21-C22-H22	119.9	O37-C38-H38C	109.6
C28-C23-C24	119.6(7)	H38A-C38-H38C	109.5
C28-C23-N6	121.8(6)	H38B-C38-H38C	109.5
C24-C23-N6	118.5(6)	C26-O39-C40	117.3(6)
C25-C24-C23	120.9(7)	O39-C40-H40A	109.4
C25-C24-H24	119.1	O39-C40-H40B	109.4
C23-C24-H24	120.0	H40A-C40-H40B	109.5
C24-C25-O37	125.3(7)	O39-C40-H40C	109.6
C24-C25-C26	119.5(7)	H40A-C40-H40C	109.5
O37-C25-C26	115.2(7)	H40B-C40-H40C	109.5
C27-C26-O39	124.9(7)	C34-C41-H41A	110.2
C27-C26-C25	119.4(7)	C34-C41-H41B	108.6
O39-C26-C25	115.7(7)	H41A-C41-H41B	109.5
C26-C27-C28	120.7(7)	C34-C41-H41C	109.6
C26-C27-H27	120.4	H41A-C41-H41C	109.5
C28-C27-H27	118.9	H41B-C41-H41C	109.5
C23-C28-C27	119.8(7)	C34-C42-H42A	109.7
C23-C28-N7	120.5(6)	C34-C42-H42B	109.5
C27-C28-N7	119.7(6)	H42A-C42-H42B	109.5
N7-C29-C30	118.1(8)	C34-C42-H42C	109.2
N7-C29-H29	121.6	H42A-C42-H42C	109.5
C30-C29-H29	120.3	H42B-C42-H42C	109.5
N8-C30-C31	109.0(6)	C8-O43-C44	117.6(6)
N8-C30-C29	114.6(7)	O43-C44-H44A	108.7
C31-C30-C29	135.9(8)	O43-C44-H44B	109.4
C32-C31-C30	106.6(7)	H44A-C44-H44B	109.5
C32-C31-H31	127.4	O43-C44-H44C	110.3
C30-C31-H31	126.0	H44A-C44-H44C	109.5
C31-C32-C33	107.9(7)	H44B-C44-H44C	109.5
C31-C32-H32	126.6	C9-O45-C46	117.9(6)
C33-C32-H32	125.5	O45-C46-H46A	109.9
N8-C33-C32	107.9(7)	O45-C46-H46B	109.5
N8-C33-C34	120.0(7)	H46A-C46-H46B	109.5
C32-C33-C34	132.0(7)	O45-C46-H46C	108.9
C33-C34-C1	108.9(6)	H46A-C46-H46C	109.5

H46B-C46-H46C	109.5	Cl2C-C1C-Cl1C	114.6(6)
Cl2A-C1A-Cl1A	113.0(5)	Cl2C-C1C-H1CA	108.5
Cl2A-C1A-H1AA	109.2	Cl1C-C1C-H1CA	109.0
Cl1A-C1A-H1AA	108.9	Cl2C-C1C-H1CB	108.2
Cl2A-C1A-H1AB	108.7	Cl1C-C1C-H1CB	108.3
Cl1A-C1A-H1AB	108.7	H1CA-C1C-H1CB	108.1
H1AA-C1A-H1AB	108.3	Cl2D-C1D-Cl1D	109.8(7)
Cl1B-C1B-Cl2B	111.0(5)	Cl2D-C1D-H1DA	109.6
Cl1B-C1B-H1BA	109.1	Cl1D-C1D-H1DA	109.9
Cl2B-C1B-H1BA	109.4	Cl2D-C1D-H1DB	109.7
Cl1B-C1B-H1BB	109.2	Cl1D-C1D-H1DB	109.2
Cl2B-C1B-H1BB	109.7	H1DA-C1D-H1DB	108.6
H1BA-C1B-H1BB	108.4		

Table SB4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe1	23(1)	20(1)	30(1)	0(1)	0(1)	-1(1)
Fe2	24(1)	20(1)	28(1)	0(1)	-1(1)	0(1)
O1	23(3)	17(3)	22(3)	2(2)	-6(2)	4(2)
N1	16(4)	22(4)	34(4)	0(3)	4(3)	1(3)
N2	27(4)	17(4)	30(4)	2(3)	-1(3)	2(3)
N3	28(4)	23(4)	28(4)	4(3)	2(3)	-2(3)
N4	30(4)	16(3)	25(4)	0(3)	1(3)	-2(3)
N5	20(4)	25(4)	25(4)	6(3)	-11(3)	-3(3)
N6	23(4)	19(4)	29(4)	0(3)	-1(3)	-3(3)
N7	26(4)	23(4)	28(4)	-3(3)	-5(3)	0(3)
N8	29(4)	13(4)	36(5)	-2(3)	-2(3)	-2(3)
C1	27(5)	19(4)	22(5)	1(3)	3(4)	5(4)
C2	44(6)	22(5)	42(6)	-3(4)	9(5)	3(4)
C3	29(5)	27(5)	52(6)	-1(4)	7(4)	4(4)
C4	28(5)	25(5)	38(6)	3(4)	0(4)	-2(4)
C5	27(5)	30(5)	34(5)	13(4)	-5(4)	2(4)
C6	14(4)	28(5)	36(5)	-4(4)	2(4)	-3(4)
C7	25(5)	31(5)	34(6)	13(4)	5(4)	-3(4)
C8	19(5)	36(6)	32(6)	2(4)	-1(4)	-9(4)
C9	24(5)	35(5)	40(6)	-11(4)	5(4)	-6(4)
C10	21(5)	23(5)	43(6)	-4(4)	4(4)	-5(4)
C11	16(4)	21(5)	35(5)	-1(4)	-2(4)	0(4)
C12	24(5)	16(4)	50(6)	2(4)	4(5)	6(4)
C13	30(5)	19(4)	31(5)	2(4)	10(4)	0(4)
C14	38(6)	38(5)	33(6)	6(4)	8(5)	-8(4)
C15	50(6)	31(5)	23(5)	-2(4)	0(5)	2(4)
C16	37(5)	27(5)	22(5)	-3(4)	3(4)	-3(4)
C17	30(5)	19(4)	34(6)	2(4)	-3(4)	1(4)
C18	28(5)	19(4)	30(6)	0(4)	-2(4)	-5(4)
C19	22(5)	38(5)	41(6)	5(4)	-2(4)	-4(4)
C20	20(5)	26(5)	61(7)	-4(4)	-4(5)	9(4)
C21	24(5)	31(5)	20(5)	-10(4)	0(4)	-4(4)
C22	30(5)	19(4)	30(6)	-6(4)	13(4)	-5(4)

C23	31(5)	27(5)	27(5)	-1(4)	6(4)	-2(4)
C24	32(5)	26(5)	27(5)	2(4)	8(4)	-1(4)
C25	36(5)	32(5)	31(6)	-7(4)	10(5)	-1(4)
C26	22(5)	33(5)	36(6)	0(4)	-7(4)	-2(4)
C27	36(5)	21(5)	28(5)	0(4)	-1(4)	0(4)
C28	28(5)	22(5)	23(5)	-2(4)	6(4)	0(4)
C29	26(5)	39(5)	29(5)	1(4)	-4(4)	5(4)
C30	31(5)	25(5)	30(6)	-6(4)	0(4)	-5(4)
C31	28(5)	32(5)	27(5)	-3(4)	12(4)	0(4)
C32	27(5)	18(5)	46(6)	10(4)	0(4)	0(4)
C33	19(4)	23(5)	37(6)	5(4)	0(4)	3(4)
C34	29(5)	19(4)	37(6)	-8(4)	1(4)	5(4)
C35	38(5)	46(5)	25(5)	-3(4)	-6(4)	4(4)
C36	40(5)	26(5)	40(6)	-4(4)	1(5)	-4(4)
O37	49(4)	26(3)	33(4)	-6(3)	-3(3)	-5(3)
C38	84(8)	29(5)	40(6)	-2(4)	5(5)	-12(5)
O39	41(4)	31(3)	32(4)	-2(3)	-6(3)	-4(3)
C40	70(7)	40(6)	36(6)	6(5)	-8(5)	-3(5)
C41	44(6)	31(5)	40(6)	-8(4)	5(5)	-5(4)
C42	23(5)	37(5)	36(6)	-2(4)	-3(4)	-11(4)
O43	32(3)	46(4)	38(4)	1(3)	-6(3)	-7(3)
C44	42(5)	36(5)	39(6)	3(4)	-12(4)	-9(4)
O45	37(3)	38(4)	47(4)	-17(3)	-7(3)	-8(3)
C46	95(9)	24(6)	111(10)	-11(6)	-46(8)	6(6)
C1A	39(6)	69(7)	73(8)	-10(6)	19(5)	-23(5)
Cl1A	48(2)	59(2)	41(2)	0(1)	5(1)	13(1)
Cl2A	65(2)	43(1)	53(2)	4(1)	13(1)	-6(1)
C1B	58(7)	45(6)	85(9)	-16(6)	1(6)	3(5)
Cl1B	84(2)	52(2)	76(2)	-8(1)	7(2)	-9(2)
Cl2B	78(2)	62(2)	91(2)	9(2)	-19(2)	0(2)
C1C	76(8)	78(8)	64(8)	-29(6)	18(6)	-6(6)
Cl1C	90(2)	146(3)	112(3)	-56(2)	-34(2)	52(2)
Cl2C	71(2)	90(2)	90(2)	-5(2)	25(2)	-6(2)
C1D	51(7)	152(12)	84(10)	-11(8)	-8(7)	-2(8)
Cl1D	80(2)	70(2)	143(3)	14(2)	20(2)	2(2)
Cl2D	79(2)	84(2)	139(3)	-31(2)	-6(2)	-9(2)

Table SB5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **7**.

	x	y	z	U(eq)
H2	1730	10852	6300	43
H3	746	9355	6172	43
H5	749	6939	5706	37
H7	762	6057	4607	36
H10	1436	2443	5447	35
H12	1444	3366	6476	36
H14	2123	2322	7566	43
H15	3413	2284	7940	42
H19	5371	2277	6745	41
H20	5212	2266	5674	44

H22	4068	3313	4886	31
H24	2798	2485	4587	33
H27	2217	6139	3760	34
H29	3435	7016	4119	39
H31	3908	9499	4246	34
H32	3784	10935	5047	37
H35A	4671	2099	7622	56
H35B	5241	3084	7692	56
H35C	4637	3089	8075	56
H36A	4965	5108	7422	54
H36B	4215	5450	7138	54
H36C	4340	5129	7785	54
H38A	2094	614	3523	77
H38B	2800	1276	3699	77
H38C	2285	1058	4148	77
H40A	1326	5243	2455	75
H40B	1451	6011	3006	75
H40C	2087	5580	2711	75
H41A	3588	11553	6042	58
H41B	2815	11589	5748	58
H41C	2971	11496	6411	58
H42A	4065	9678	6492	49
H42B	3444	9643	6858	49
H42C	3588	8565	6480	49
H44A	-282	5099	3394	61
H44B	-219	5774	3973	61
H44C	429	5675	3639	61
H46A	545	508	4491	122
H46B	1269	1044	4733	122
H46C	650	1057	5101	122
H1AA	4623	6188	5534	71
H1AB	4512	6590	6143	71
H1BA	837	2562	3166	76
H1BB	33	2684	3162	76
H1CA	2564	6010	7069	86
H1CB	2373	7327	6987	86
H1DA	-983	4190	1375	117
H1DB	-1056	2833	1416	117

Table SB6. Torsion angles [°] for **7**.

N1-Fe1-O1-Fe2	133.9(3)	O1-Fe1-N1-C4	-101.5(5)
N8-Fe1-O1-Fe2	-136.8(3)	N8-Fe1-N1-C4	146.4(6)
N2-Fe1-O1-Fe2	52.2(4)	N2-Fe1-N1-C4	-1.1(5)
N7-Fe1-O1-Fe2	-53.2(4)	N7-Fe1-N1-C4	89.8(6)
N4-Fe2-O1-Fe1	-136.4(3)	O1-Fe1-N2-C5	110.6(5)
N5-Fe2-O1-Fe1	132.6(3)	N1-Fe1-N2-C5	2.2(5)
N6-Fe2-O1-Fe1	49.6(4)	N8-Fe1-N2-C5	-56.1(7)
N3-Fe2-O1-Fe1	-53.0(4)	N7-Fe1-N2-C5	-139.4(5)
O1-Fe1-N1-C1	92.0(7)	O1-Fe1-N2-C6	-74.7(6)
N8-Fe1-N1-C1	-20.0(7)	N1-Fe1-N2-C6	176.9(6)
N2-Fe1-N1-C1	-167.6(7)	N8-Fe1-N2-C6	118.6(6)
N7-Fe1-N1-C1	-76.7(8)	N7-Fe1-N2-C6	35.3(6)

O1-Fe2-N3-C12	-115.3(5)	Fe1-N1-C4-C3	-171.6(5)
N4-Fe2-N3-C12	-3.1(5)	C1-N1-C4-C5	169.9(6)
N5-Fe2-N3-C12	56.5(7)	Fe1-N1-C4-C5	0.0(9)
N6-Fe2-N3-C12	138.7(5)	C2-C3-C4-N1	1.0(9)
O1-Fe2-N3-C11	75.2(6)	C2-C3-C4-C5	-168.1(9)
N4-Fe2-N3-C11	-172.6(6)	C6-N2-C5-C4	-178.1(7)
N5-Fe2-N3-C11	-113.1(6)	Fe1-N2-C5-C4	-2.9(9)
N6-Fe2-N3-C11	-30.8(6)	N1-C4-C5-N2	2.0(10)
O1-Fe2-N4-C16	-98.2(7)	C3-C4-C5-N2	170.9(8)
N5-Fe2-N4-C16	13.8(7)	C5-N2-C6-C11	-115.2(8)
N6-Fe2-N4-C16	72.3(8)	Fe1-N2-C6-C11	70.3(9)
N3-Fe2-N4-C16	161.1(7)	C5-N2-C6-C7	65.2(10)
O1-Fe2-N4-C13	104.3(5)	Fe1-N2-C6-C7	-109.2(7)
N5-Fe2-N4-C13	-143.7(5)	C11-C6-C7-C8	-1.1(12)
N6-Fe2-N4-C13	-85.2(6)	N2-C6-C7-C8	178.5(7)
N3-Fe2-N4-C13	3.6(5)	C6-C7-C8-O43	-177.0(7)
O1-Fe2-N5-C18	98.8(7)	C6-C7-C8-C9	1.5(12)
N4-Fe2-N5-C18	-13.8(7)	O43-C8-C9-O45	-1.1(11)
N6-Fe2-N5-C18	-161.7(7)	C7-C8-C9-O45	-179.8(7)
N3-Fe2-N5-C18	-72.4(8)	O43-C8-C9-C10	177.7(7)
O1-Fe2-N5-C21	-103.4(5)	C7-C8-C9-C10	-1.1(12)
N4-Fe2-N5-C21	143.9(5)	O45-C9-C10-C11	178.8(7)
N6-Fe2-N5-C21	-3.9(5)	C8-C9-C10-C11	0.1(12)
N3-Fe2-N5-C21	85.3(6)	C7-C6-C11-C10	0.1(11)
O1-Fe2-N6-C22	115.4(5)	N2-C6-C11-C10	-179.4(7)
N4-Fe2-N6-C22	-55.8(6)	C7-C6-C11-N3	176.0(7)
N5-Fe2-N6-C22	3.7(5)	N2-C6-C11-N3	-3.5(11)
N3-Fe2-N6-C22	-137.6(5)	C9-C10-C11-C6	0.4(12)
O1-Fe2-N6-C23	-72.6(6)	C9-C10-C11-N3	-175.7(7)
N4-Fe2-N6-C23	116.3(6)	C12-N3-C11-C6	125.4(8)
N5-Fe2-N6-C23	175.7(6)	Fe2-N3-C11-C6	-65.5(9)
N3-Fe2-N6-C23	34.5(6)	C12-N3-C11-C10	-58.7(10)
O1-Fe1-N7-C29	-112.7(5)	Fe2-N3-C11-C10	110.4(7)
N1-Fe1-N7-C29	56.2(7)	C11-N3-C12-C13	172.9(6)
N8-Fe1-N7-C29	-1.4(5)	Fe2-N3-C12-C13	2.1(8)
N2-Fe1-N7-C29	139.3(5)	C16-N4-C13-C12	-167.0(6)
O1-Fe1-N7-C28	74.2(6)	Fe2-N4-C13-C12	-3.7(8)
N1-Fe1-N7-C28	-116.8(6)	C16-N4-C13-C14	1.8(8)
N8-Fe1-N7-C28	-174.5(6)	Fe2-N4-C13-C14	165.2(5)
N2-Fe1-N7-C28	-33.8(6)	N3-C12-C13-N4	0.9(10)
O1-Fe1-N8-C33	-88.8(7)	N3-C12-C13-C14	-164.4(8)
N1-Fe1-N8-C33	19.9(7)	N4-C13-C14-C15	-1.4(9)
N2-Fe1-N8-C33	77.1(8)	C12-C13-C14-C15	164.4(8)
N7-Fe1-N8-C33	168.4(7)	C13-C14-C15-C16	0.5(9)
O1-Fe1-N8-C30	105.1(5)	C13-N4-C16-C15	-1.5(8)
N1-Fe1-N8-C30	-146.2(5)	Fe2-N4-C16-C15	-160.3(5)
N2-Fe1-N8-C30	-89.0(6)	C13-N4-C16-C17	175.3(6)
N7-Fe1-N8-C30	2.3(5)	Fe2-N4-C16-C17	16.4(10)
C4-N1-C1-C2	1.8(8)	C14-C15-C16-N4	0.6(9)
Fe1-N1-C1-C2	169.1(5)	C14-C15-C16-C17	-175.7(8)
C4-N1-C1-C34	-177.0(6)	N4-C16-C17-C35	-170.5(7)
Fe1-N1-C1-C34	-9.7(11)	C15-C16-C17-C35	5.4(11)
N1-C1-C2-C3	-1.1(9)	N4-C16-C17-C18	-49.1(9)
C34-C1-C2-C3	177.4(8)	C15-C16-C17-C18	126.8(8)
C1-C2-C3-C4	0.1(9)	N4-C16-C17-C36	69.3(9)
C1-N1-C4-C3	-1.8(9)	C15-C16-C17-C36	-114.8(9)

C21-N5-C18-C19	2.3(8)
Fe2-N5-C18-C19	161.2(5)
C21-N5-C18-C17	-175.0(6)
Fe2-N5-C18-C17	-16.1(10)
C35-C17-C18-N5	171.1(6)
C16-C17-C18-N5	49.0(8)
C36-C17-C18-N5	-69.2(8)
C35-C17-C18-C19	-5.6(11)
C16-C17-C18-C19	-127.6(8)
C36-C17-C18-C19	114.1(8)
N5-C18-C19-C20	-2.2(9)
C17-C18-C19-C20	174.7(7)
C18-C19-C20-C21	1.2(9)
C18-N5-C21-C22	167.0(6)
Fe2-N5-C21-C22	3.6(8)
C18-N5-C21-C20	-1.5(8)
Fe2-N5-C21-C20	-164.9(5)
C19-C20-C21-C22	-164.7(9)
C19-C20-C21-N5	0.1(8)
C23-N6-C22-C21	-176.3(6)
Fe2-N6-C22-C21	-3.0(8)
N5-C21-C22-N6	-0.3(10)
C20-C21-C22-N6	163.9(8)
C22-N6-C23-C28	-117.6(8)
Fe2-N6-C23-C28	70.7(9)
C22-N6-C23-C24	58.8(9)
Fe2-N6-C23-C24	-112.9(7)
C28-C23-C24-C25	-1.9(12)
N6-C23-C24-C25	-178.4(7)
C23-C24-C25-O37	-177.6(7)
C23-C24-C25-C26	2.3(12)
C24-C25-C26-C27	-1.1(12)
O37-C25-C26-C27	178.8(7)
C24-C25-C26-O39	-179.4(7)
O37-C25-C26-O39	0.5(10)
O39-C26-C27-C28	177.6(7)
C25-C26-C27-C28	-0.5(12)
C24-C23-C28-C27	0.3(11)
N6-C23-C28-C27	176.6(7)
C24-C23-C28-N7	179.2(7)
N6-C23-C28-N7	-4.5(11)
C26-C27-C28-C23	0.9(12)
C26-C27-C28-N7	-178.0(7)
C29-N7-C28-C23	125.9(8)
Fe1-N7-C28-C23	-61.4(9)
C29-N7-C28-C27	-55.3(10)
Fe1-N7-C28-C27	117.5(7)
C28-N7-C29-C30	174.1(6)
Fe1-N7-C29-C30	0.3(8)
C33-N8-C30-C31	1.1(8)
Fe1-N8-C30-C31	170.6(5)
C33-N8-C30-C29	-172.4(6)
Fe1-N8-C30-C29	-2.9(8)
N7-C29-C30-N8	1.7(10)
N7-C29-C30-C31	-169.5(8)
N8-C30-C31-C32	-0.7(9)
C29-C30-C31-C32	170.8(9)
C30-C31-C32-C33	0.0(8)
C30-N8-C33-C32	-1.1(8)
Fe1-N8-C33-C32	-167.9(5)
C30-N8-C33-C34	177.0(6)
Fe1-N8-C33-C34	10.2(10)
C31-C32-C33-N8	0.7(8)
C31-C32-C33-C34	-177.1(7)
N8-C33-C34-C1	-46.6(9)
C32-C33-C34-C1	131.0(8)
N8-C33-C34-C42	72.6(8)
C32-C33-C34-C42	-109.8(9)
N8-C33-C34-C41	-167.2(6)
C32-C33-C34-C41	10.3(11)
N1-C1-C34-C33	46.3(9)
C2-C1-C34-C33	-132.1(8)
N1-C1-C34-C42	-73.2(8)
C2-C1-C34-C42	108.4(9)
N1-C1-C34-C41	168.2(7)
C2-C1-C34-C41	-10.2(12)
C24-C25-O37-C38	-19.0(11)
C26-C25-O37-C38	161.1(7)
C27-C26-O39-C40	17.4(11)
C25-C26-O39-C40	-164.4(7)
C7-C8-O43-C44	1.3(11)
C9-C8-O43-C44	-177.3(7)
C8-C9-O45-C46	176.3(8)
C10-C9-O45-C46	-2.4(12)

Table SB7. Hydrogen bonds for **7** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C1B-H1BA...O37	0.96	2.35	3.266(11)	158.6
C1B-H1BA...O39	0.96	2.60	3.344(10)	134.4
C1B-H1BB...O43	0.96	2.68	3.348(11)	126.8
C1A-H1AB...O1	0.96	2.61	3.341(10)	133.4
C1C-H1CA...O1	0.96	2.77	3.385(11)	122.6
C1D-H1DA...Cl1B#1	0.96	2.69	3.568(12)	152.7

Symmetry transformations used to generate equivalent atoms:
#1 -x,y+1/2,-z+1/2

Figure SC1. View of **8** showing a partial atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. The hydrogen atoms have been removed for clarity.

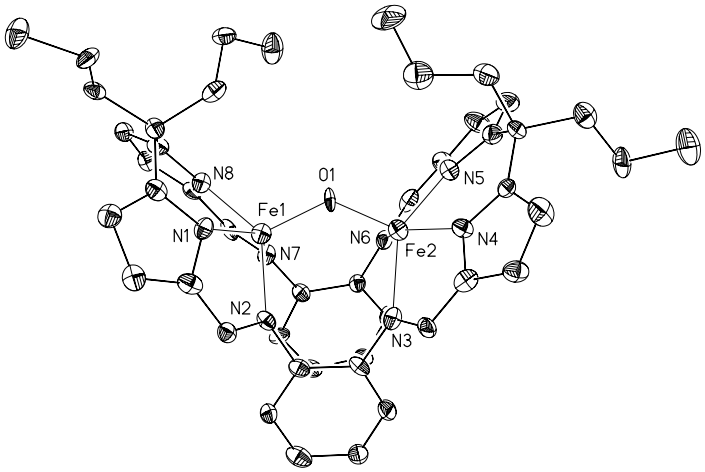

Figure SC2. View of the ligand in **8** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. The hydrogen atoms have been removed for clarity.

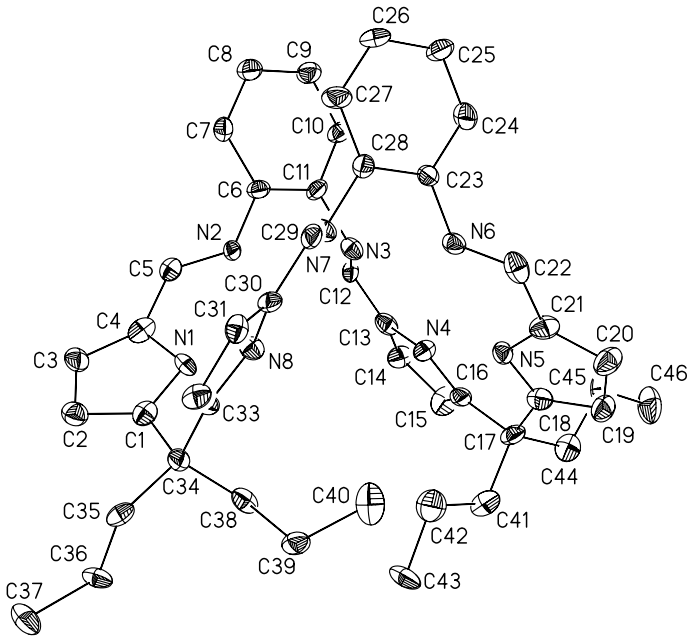

Figure SC3. Unit cell packing diagram for **8**. The view is approximately down the **b** axis.

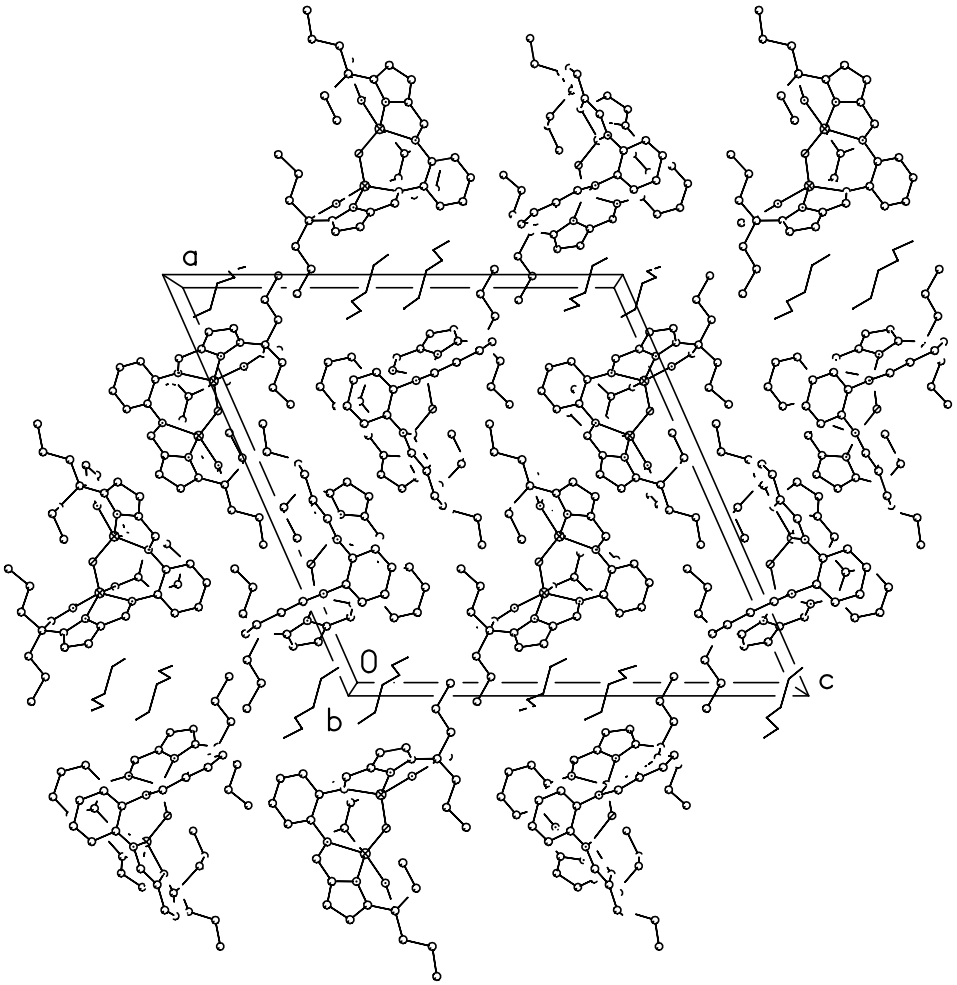

Table SC1. Crystal data and structure refinement for **8**.

Empirical formula	C52 H62 Fe2 N8 O	
Formula weight	926.80	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 23.7941(10) Å	α= 90°.
	b = 8.8588(5) Å	β= 113.805(2)°.
	c = 23.7874(14) Å	γ = 90.000(2)°.
Volume	4587.5(4) $Å^3$	
Z	4	
Density (calculated)	1.342 Mg/m^3	
Absorption coefficient	0.681 mm^{-1}	
F(000)	1960	
Crystal size	0.35 x 0.06 x 0.02 mm	
Theta range for data collection	2.96 to 24.78°.	
Index ranges	0<=h<=27, 0<=k<=10, -28<=l<=25	
Reflections collected	7559	
Independent reflections	7559 [R(int) = 0.0000]	
Completeness to theta = 24.78°	95.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7559 / 0 / 569	
Goodness-of-fit on F^2	0.985	
Final R indices [I>2sigma(I)]	R1 = 0.0839, wR2 = 0.1042	
R indices (all data)	R1 = 0.3412, wR2 = 0.1498	
Extinction coefficient	2.5(2)x10^{-6}	
Largest diff. peak and hole	0.482 and -0.649 e.$Å^{-3}$	

Table SC2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe1	3747(1)	4956(1)	6151(1)	35(1)
Fe2	2355(1)	4735(1)	5249(1)	38(1)
O1	3124(2)	5308(5)	5438(2)	35(2)
N1	4492(3)	4236(8)	6025(3)	32(2)
N2	3733(4)	2634(7)	6315(3)	28(2)
N3	2472(3)	2406(7)	5515(4)	34(2)
N4	1964(3)	3712(8)	4427(3)	34(2)
N5	1756(3)	6349(7)	4780(4)	32(2)
N6	2169(3)	5795(8)	5955(4)	33(2)
N7	3427(4)	5713(7)	6828(3)	33(2)
N8	4298(3)	6718(7)	6530(3)	31(2)
C1	5000(5)	4940(10)	6045(4)	34(2)
C2	5496(4)	3942(11)	6162(4)	41(3)
C3	5255(5)	2534(11)	6232(4)	40(3)
C4	4657(5)	2741(10)	6167(4)	38(3)
C5	4224(5)	1935(9)	6319(4)	32(3)
C6	3310(5)	1812(9)	6489(5)	33(3)
C7	3526(4)	1156(9)	7066(4)	34(3)
C8	3113(5)	399(9)	7258(4)	47(3)

C9	2494(4)	317(10)	6866(4)	44(3)
C10	2302(5)	976(9)	6299(4)	44(3)
C11	2699(5)	1727(10)	6104(5)	34(3)
C12	2306(4)	1536(10)	5036(5)	38(3)
C13	2038(4)	2154(10)	4448(5)	37(3)
C14	1767(4)	1629(10)	3831(5)	42(3)
C15	1528(5)	2884(11)	3457(5)	54(3)
C16	1649(4)	4144(11)	3835(5)	36(3)
C17	1458(5)	5781(10)	3658(5)	40(3)
C18	1423(5)	6707(11)	4186(5)	40(3)
C19	1101(4)	8052(10)	4157(5)	47(3)
C20	1199(5)	8436(10)	4746(5)	53(3)
C21	1599(5)	7382(12)	5116(5)	44(3)
C22	1828(4)	7034(10)	5743(5)	45(3)
C23	2324(4)	5266(9)	6567(4)	30(2)
C24	1858(4)	4810(10)	6742(4)	41(3)
C25	1996(5)	4231(9)	7309(5)	42(3)
C26	2596(5)	4058(9)	7726(4)	45(3)
C27	3065(5)	4555(9)	7564(4)	43(3)
C28	2936(4)	5170(10)	6999(4)	33(2)
C29	3761(4)	6826(10)	7168(4)	36(3)
C30	4253(5)	7412(10)	7027(5)	32(2)
C31	4729(4)	8435(9)	7296(4)	32(3)
C32	5079(4)	8384(9)	6951(4)	34(3)
C33	4811(5)	7307(10)	6487(5)	36(3)
C34	4986(4)	6690(9)	5979(4)	33(3)
C35	5619(4)	7323(8)	6054(4)	33(3)
C36	5806(4)	6957(9)	5510(4)	38(3)
C37	6483(4)	7264(9)	5684(4)	52(3)
C38	4470(4)	7101(8)	5339(4)	36(3)
C39	4320(4)	8814(8)	5235(4)	40(3)
C40	3710(4)	9208(9)	5266(4)	62(3)
C41	1920(5)	6527(10)	3429(4)	55(3)
C42	2555(5)	6756(10)	3893(5)	67(3)
C43	2983(4)	7504(10)	3641(5)	75(4)
C44	830(5)	5801(9)	3106(4)	48(3)
C45	302(4)	5099(11)	3223(4)	57(3)
C46	-305(4)	5134(11)	2663(4)	81(3)
C1A	-746(5)	-1203(11)	3480(5)	94(4)
C2A	-586(6)	122(16)	3885(6)	149(7)
C3A	-385(8)	1398(14)	3785(8)	216(12)
C4A	-191(5)	2715(12)	4217(6)	80(4)
C5A	477(7)	2597(16)	4655(7)	123(6)
C6A	701(6)	3715(14)	5086(6)	135(7)

Table SC3. Bond lengths [Å] and angles [°] for **8**.

Fe1-O1	1.772(5)	Fe2-N5	2.009(7)
Fe1-N8	2.004(7)	Fe2-N4	2.010(7)
Fe1-N1	2.017(7)	Fe2-N6	2.122(7)
Fe1-N2	2.096(6)	Fe2-N3	2.143(7)
Fe1-N7	2.149(7)	N1-C1	1.344(9)
Fe2-O1	1.772(5)	N1-C4	1.384(9)

N2-C5	1.318(9)	C17-C41	1.557(11)
N2-C6	1.433(10)	C18-C19	1.404(11)
N3-C12	1.299(10)	C19-C20	1.367(11)
N3-C11	1.417(10)	C20-C21	1.370(12)
N4-C16	1.356(10)	C21-C22	1.400(12)
N4-C13	1.389(9)	C23-C24	1.390(10)
N5-C18	1.349(10)	C23-C28	1.406(10)
N5-C21	1.362(10)	C24-C25	1.354(10)
N6-C22	1.336(9)	C25-C26	1.381(11)
N6-C23	1.430(9)	C26-C27	1.391(11)
N7-C29	1.318(9)	C27-C28	1.366(10)
N7-C28	1.464(10)	C29-C30	1.438(11)
N8-C33	1.367(10)	C30-C31	1.390(11)
N8-C30	1.375(10)	C31-C32	1.385(10)
C1-C2	1.409(10)	C32-C33	1.403(11)
C1-C34	1.558(11)	C33-C34	1.531(11)
C2-C3	1.411(10)	C34-C35	1.547(10)
C3-C4	1.380(12)	C34-C38	1.564(11)
C4-C5	1.416(12)	C35-C36	1.563(10)
C6-C11	1.373(11)	C36-C37	1.519(10)
C6-C7	1.385(11)	C38-C39	1.556(9)
C7-C8	1.408(10)	C39-C40	1.525(10)
C8-C9	1.391(11)	C41-C42	1.482(11)
C9-C10	1.368(10)	C42-C43	1.528(11)
C10-C11	1.378(11)	C44-C45	1.524(10)
C12-C13	1.394(11)	C45-C46	1.520(10)
C13-C14	1.422(11)	C1A-C2A	1.467(11)
C14-C15	1.394(10)	C2A-C3A	1.287(13)
C15-C16	1.390(11)	C3A-C4A	1.499(14)
C16-C17	1.527(11)	C4A-C5A	1.512(14)
C17-C18	1.531(12)	C5A-C6A	1.369(14)
C17-C44	1.541(12)		

O1-Fe1-N8	115.9(3)	C4-N1-Fe1	116.5(7)
O1-Fe1-N1	111.1(3)	C5-N2-C6	118.9(7)
N8-Fe1-N1	81.9(3)	C5-N2-Fe1	112.4(6)
O1-Fe1-N2	106.3(3)	C6-N2-Fe1	128.2(6)
N8-Fe1-N2	137.5(3)	C12-N3-C11	118.4(8)
N1-Fe1-N2	78.4(3)	C12-N3-Fe2	110.8(7)
O1-Fe1-N7	104.4(3)	C11-N3-Fe2	130.8(6)
N8-Fe1-N7	77.5(3)	C16-N4-C13	109.1(8)
N1-Fe1-N7	144.0(3)	C16-N4-Fe2	136.7(7)
N2-Fe1-N7	97.4(3)	C13-N4-Fe2	114.3(6)
O1-Fe2-N5	111.4(3)	C18-N5-C21	105.8(8)
O1-Fe2-N4	113.6(3)	C18-N5-Fe2	137.2(7)
N5-Fe2-N4	80.5(3)	C21-N5-Fe2	117.0(7)
O1-Fe2-N6	101.3(3)	C22-N6-C23	121.4(8)
N5-Fe2-N6	78.3(3)	C22-N6-Fe2	110.7(6)
N4-Fe2-N6	143.8(3)	C23-N6-Fe2	127.7(6)
O1-Fe2-N3	101.7(3)	C29-N7-C28	115.2(8)
N5-Fe2-N3	145.9(3)	C29-N7-Fe1	112.7(6)
N4-Fe2-N3	78.9(3)	C28-N7-Fe1	132.0(6)
N6-Fe2-N3	103.7(3)	C33-N8-C30	106.0(8)
Fe1-O1-Fe2	124.9(3)	C33-N8-Fe1	134.8(7)
C1-N1-C4	105.8(8)	C30-N8-Fe1	118.1(7)
C1-N1-Fe1	132.9(6)	N1-C1-C2	112.7(8)

N1-C1-C34	118.4(9)	C20-C21-C22	134.8(11)
C2-C1-C34	128.8(9)	N6-C22-C21	119.9(9)
C1-C2-C3	103.3(8)	C24-C23-C28	118.7(8)
C4-C3-C2	108.6(9)	C24-C23-N6	119.4(8)
C3-C4-N1	109.4(9)	C28-C23-N6	121.9(8)
C3-C4-C5	136.8(10)	C25-C24-C23	120.4(9)
N1-C4-C5	112.4(10)	C24-C25-C26	121.5(10)
N2-C5-C4	119.7(8)	C25-C26-C27	118.6(9)
C11-C6-C7	120.5(9)	C28-C27-C26	120.8(9)
C11-C6-N2	121.0(9)	C27-C28-C23	119.8(9)
C7-C6-N2	118.5(10)	C27-C28-N7	121.1(8)
C6-C7-C8	119.5(9)	C23-C28-N7	119.1(8)
C9-C8-C7	119.7(9)	N7-C29-C30	118.2(9)
C10-C9-C8	118.8(9)	N8-C30-C31	110.8(9)
C9-C10-C11	122.4(10)	N8-C30-C29	113.2(9)
C6-C11-C10	119.1(9)	C31-C30-C29	135.8(10)
C6-C11-N3	121.0(9)	C32-C31-C30	106.2(9)
C10-C11-N3	119.9(10)	C31-C32-C33	107.3(9)
N3-C12-C13	120.1(9)	N8-C33-C32	109.7(8)
N4-C13-C12	115.2(9)	N8-C33-C34	117.3(9)
N4-C13-C14	106.9(8)	C32-C33-C34	133.0(10)
C12-C13-C14	137.7(10)	C33-C34-C35	110.0(8)
C15-C14-C13	107.2(8)	C33-C34-C1	106.1(7)
C16-C15-C14	107.6(9)	C35-C34-C1	111.6(7)
N4-C16-C15	109.2(8)	C33-C34-C38	109.1(7)
N4-C16-C17	122.3(9)	C35-C34-C38	112.0(7)
C15-C16-C17	128.5(10)	C1-C34-C38	107.8(7)
C16-C17-C18	112.9(9)	C34-C35-C36	114.7(7)
C16-C17-C44	109.0(7)	C37-C36-C35	111.3(7)
C18-C17-C44	109.8(8)	C39-C38-C34	114.9(7)
C16-C17-C41	109.0(8)	C40-C39-C38	112.1(7)
C18-C17-C41	109.8(8)	C42-C41-C17	116.7(9)
C44-C17-C41	106.1(8)	C41-C42-C43	114.1(9)
N5-C18-C19	109.3(9)	C45-C44-C17	115.3(8)
N5-C18-C17	122.0(9)	C46-C45-C44	113.2(8)
C19-C18-C17	128.5(10)	C3A-C2A-C1A	126.8(13)
C20-C19-C18	107.2(9)	C2A-C3A-C4A	126.2(14)
C19-C20-C21	106.0(9)	C3A-C4A-C5A	111.5(12)
N5-C21-C20	111.4(9)	C6A-C5A-C4A	116.7(12)
N5-C21-C22	113.3(10)		

Table SC4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe1	35(1)	37(1)	33(1)	-2(1)	15(1)	-1(1)
Fe2	38(1)	41(1)	33(1)	2(1)	11(1)	2(1)
O1	11(4)	50(4)	31(4)	-1(3)	-4(3)	2(3)
N1	26(5)	40(5)	38(6)	-3(4)	20(5)	-1(4)
N2	28(6)	33(5)	26(5)	4(4)	14(5)	11(4)
N3	29(6)	42(5)	33(6)	-9(5)	14(5)	-6(4)

N4	42(6)	31(5)	29(6)	2(4)	14(5)	3(4)
N5	32(6)	36(5)	30(6)	-2(5)	15(5)	7(4)
N6	26(5)	43(5)	28(6)	-1(4)	11(5)	-5(4)
N7	31(6)	44(5)	28(6)	-6(4)	15(5)	-5(4)
N8	33(6)	36(5)	25(6)	-7(4)	13(5)	-2(4)
C1	41(7)	33(6)	26(6)	-4(5)	11(5)	3(7)
C2	43(8)	47(7)	39(7)	-1(5)	21(6)	-1(6)
C3	39(8)	53(7)	33(7)	-4(5)	20(7)	5(6)
C4	56(9)	26(7)	29(7)	-4(5)	13(7)	4(6)
C5	34(7)	30(6)	26(7)	-4(5)	7(6)	-1(6)
C6	40(8)	35(6)	26(7)	5(5)	17(7)	3(6)
C7	25(7)	35(6)	37(8)	2(5)	8(6)	3(5)
C8	59(8)	51(7)	41(8)	13(6)	29(7)	17(6)
C9	36(7)	52(7)	41(8)	13(6)	14(6)	-5(6)
C10	39(8)	57(7)	28(7)	13(6)	4(6)	-6(6)
C11	39(8)	38(6)	24(7)	9(5)	9(7)	11(6)
C12	21(7)	46(7)	43(8)	17(6)	10(7)	7(5)
C13	41(8)	33(7)	47(9)	-9(6)	28(7)	-1(6)
C14	58(8)	31(6)	40(8)	-2(6)	22(7)	1(6)
C15	73(9)	45(7)	35(8)	-17(7)	12(7)	4(6)
C16	23(7)	47(7)	38(8)	10(6)	11(6)	-8(5)
C17	38(8)	47(7)	27(7)	13(5)	5(7)	-5(6)
C18	40(8)	44(7)	36(8)	1(6)	16(7)	-6(6)
C19	49(8)	34(7)	57(9)	8(6)	21(7)	7(6)
C20	78(10)	39(7)	42(8)	4(6)	25(8)	16(6)
C21	59(9)	49(7)	25(8)	-3(7)	17(7)	-3(6)
C22	32(7)	38(7)	66(10)	-14(6)	21(7)	-8(6)
C23	26(7)	37(6)	27(7)	0(5)	12(6)	0(5)
C24	22(6)	55(7)	41(7)	-2(6)	8(6)	-6(6)
C25	43(8)	49(7)	31(8)	13(5)	11(7)	-3(5)
C26	59(9)	51(7)	27(7)	11(5)	21(7)	-1(6)
C27	45(8)	44(6)	45(8)	10(5)	22(7)	-13(5)
C28	33(7)	34(6)	32(7)	3(6)	13(6)	6(6)
C29	31(7)	52(7)	20(7)	6(5)	7(6)	15(6)
C30	37(8)	40(6)	21(6)	6(5)	14(6)	7(6)
C31	30(7)	33(6)	29(7)	-4(5)	6(6)	5(5)
C32	39(7)	37(6)	18(7)	-4(5)	5(6)	-7(5)
C33	39(8)	41(7)	39(8)	12(6)	26(7)	11(6)
C34	29(7)	44(7)	29(7)	3(5)	15(6)	5(5)
C35	45(8)	29(5)	19(6)	2(4)	6(6)	-2(5)
C36	39(7)	46(6)	33(7)	-4(5)	20(6)	-19(5)
C37	38(8)	76(7)	51(8)	-12(6)	27(7)	-7(6)
C38	40(7)	24(6)	56(8)	-10(5)	32(7)	-4(5)
C39	48(8)	30(6)	47(8)	8(5)	23(6)	-2(5)
C40	45(8)	54(7)	71(9)	-22(6)	8(7)	1(6)
C41	64(9)	48(7)	47(9)	11(6)	15(8)	-1(6)
C42	71(10)	57(7)	73(10)	0(7)	31(9)	6(7)
C43	64(9)	82(8)	111(11)	26(7)	67(9)	1(7)
C44	57(9)	49(6)	35(8)	-9(5)	14(7)	5(6)
C45	25(7)	68(7)	59(8)	-6(7)	-1(6)	12(7)
C46	46(8)	105(9)	75(9)	-5(8)	6(7)	21(8)
C1A	101(11)	115(10)	82(11)	-16(9)	54(9)	-5(9)
C2A	140(14)	171(15)	187(17)	-142(14)	119(13)	-100(13)
C3A	320(30)	77(11)	420(30)	-141(16)	320(20)	-129(14)
C4A	79(11)	70(9)	111(12)	17(8)	58(10)	4(8)
C5A	96(14)	182(16)	104(15)	27(11)	54(12)	71(12)

C6A	119(14)	156(13)	133(16)	-82(11)	54(12)	-54(11)

Table SC5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H2	5898	4165	6181	50
H3	5468	1584	6311	48
H5	4286	882	6420	38
H7	3955	1223	7331	41
H8	3253	-49	7659	57
H9	2213	-212	6993	52
H10	1877	913	6024	53
H12	2367	465	5085	45
H14	1760	599	3702	50
H15	1322	2889	3017	65
H19	857	8590	3788	56
H20	1030	9286	4874	63
H22	1734	7662	6023	54
H24	1438	4914	6456	50
H25	1667	3963	7426	51
H26	2686	3590	8117	54
H27	3487	4467	7849	52
H29	3670	7234	7496	43
H31	4797	9053	7649	39
H32	5438	8972	7013	40
H35A	5924	6900	6423	40
H35B	5623	8399	6103	40
H36A	5571	7573	5163	45
H36B	5714	5916	5398	45
H37A	6599	7030	5351	78
H37B	6569	8307	5794	78
H37C	6712	6641	6031	78
H38A	4102	6583	5304	43
H38B	4585	6743	5020	43
H39A	4312	9143	4847	48
H39B	4646	9339	5555	48
H40A	3642	10278	5221	92
H40B	3383	8694	4942	92
H40C	3720	8892	5656	92
H41A	1768	7502	3259	66
H41B	1949	5922	3107	66
H42A	2719	5783	4055	80
H42B	2530	7345	4222	80
H43A	3384	7613	3966	113
H43B	3012	6908	3316	113
H43C	2822	8483	3485	113
H44A	858	5257	2769	58
H44B	718	6824	2974	58
H45A	256	5654	3548	68

H45B	407	4075	3356	68
H46A	-630	4695	2750	122
H46B	-406	6162	2534	122
H46C	-255	4572	2341	122
H1AA	-821	-2093	3670	140
H1AB	-1115	-920	3137	140
H1AC	-428	-1405	3340	140
H2AA	-226	-203	4230	178
H2AB	-904	275	4030	178
H3AA	-751	1757	3457	259
H3AB	-83	1241	3618	259
H4AA	-422	2696	4467	96
H4AB	-254	3679	4016	96
H5AA	709	2568	4405	147
H5AB	540	1658	4874	147
H6AA	1130	3574	5339	203
H6AB	645	4652	4868	203
H6AC	474	3734	5340	203

Table SC6. Torsion angles [°] for **8**.

N8-Fe1-O1-Fe2	-133.6(4)	O1-Fe2-N4-C16	-87.6(10)
N1-Fe1-O1-Fe2	135.4(4)	N5-Fe2-N4-C16	21.7(9)
N2-Fe1-O1-Fe2	51.8(4)	N6-Fe2-N4-C16	76.4(11)
N7-Fe1-O1-Fe2	-50.6(4)	N3-Fe2-N4-C16	174.4(10)
N5-Fe2-O1-Fe1	139.4(4)	O1-Fe2-N4-C13	90.5(6)
N4-Fe2-O1-Fe1	-131.9(4)	N5-Fe2-N4-C13	-160.2(7)
N6-Fe2-O1-Fe1	57.7(4)	N6-Fe2-N4-C13	-105.5(7)
N3-Fe2-O1-Fe1	-49.0(4)	N3-Fe2-N4-C13	-7.5(6)
O1-Fe1-N1-C1	98.5(8)	O1-Fe2-N5-C18	93.7(9)
N8-Fe1-N1-C1	-16.2(8)	N4-Fe2-N5-C18	-18.1(9)
N2-Fe1-N1-C1	-158.3(8)	N6-Fe2-N5-C18	-168.6(9)
N7-Fe1-N1-C1	-71.6(10)	N3-Fe2-N5-C18	-71.5(11)
O1-Fe1-N1-C4	-110.1(6)	O1-Fe2-N5-C21	-89.5(7)
N8-Fe1-N1-C4	135.2(7)	N4-Fe2-N5-C21	158.8(7)
N2-Fe1-N1-C4	-6.9(6)	N6-Fe2-N5-C21	8.2(6)
N7-Fe1-N1-C4	79.8(8)	N3-Fe2-N5-C21	105.3(8)
O1-Fe1-N2-C5	115.3(6)	O1-Fe2-N6-C22	102.4(6)
N8-Fe1-N2-C5	-57.5(8)	N5-Fe2-N6-C22	-7.4(6)
N1-Fe1-N2-C5	6.5(6)	N4-Fe2-N6-C22	-62.6(8)
N7-Fe1-N2-C5	-137.2(6)	N3-Fe2-N6-C22	-152.4(6)
O1-Fe1-N2-C6	-72.8(8)	O1-Fe2-N6-C23	-82.6(7)
N8-Fe1-N2-C6	114.3(8)	N5-Fe2-N6-C23	167.6(7)
N1-Fe1-N2-C6	178.3(8)	N4-Fe2-N6-C23	112.4(8)
N7-Fe1-N2-C6	34.7(8)	N3-Fe2-N6-C23	22.6(7)
O1-Fe2-N3-C12	-105.1(6)	O1-Fe1-N7-C29	-118.3(6)
N5-Fe2-N3-C12	60.9(9)	N8-Fe1-N7-C29	-4.4(6)
N4-Fe2-N3-C12	7.1(6)	N1-Fe1-N7-C29	52.2(8)
N6-Fe2-N3-C12	150.1(6)	N2-Fe1-N7-C29	132.7(6)
O1-Fe2-N3-C11	74.0(8)	O1-Fe1-N7-C28	65.6(8)
N5-Fe2-N3-C11	-120.0(9)	N8-Fe1-N7-C28	179.4(8)
N4-Fe2-N3-C11	-173.9(9)	N1-Fe1-N7-C28	-123.9(8)
N6-Fe2-N3-C11	-30.9(9)	N2-Fe1-N7-C28	-43.5(8)

O1-Fe1-N8-C33	-88.3(9)	Fe2-N4-C16-C15	176.3(7)
N1-Fe1-N8-C33	21.2(8)	C13-N4-C16-C17	176.4(9)
N2-Fe1-N8-C33	84.0(9)	Fe2-N4-C16-C17	-5.5(15)
N7-Fe1-N8-C33	171.5(9)	C14-C15-C16-N4	1.3(12)
O1-Fe1-N8-C30	105.5(6)	C14-C15-C16-C17	-176.8(10)
N1-Fe1-N8-C30	-144.9(7)	N4-C16-C17-C18	-22.6(13)
N2-Fe1-N8-C30	-82.1(8)	C15-C16-C17-C18	155.3(10)
N7-Fe1-N8-C30	5.3(6)	N4-C16-C17-C44	-144.9(9)
C4-N1-C1-C2	3.5(10)	C15-C16-C17-C44	33.0(15)
Fe1-N1-C1-C2	157.0(6)	N4-C16-C17-C41	99.7(11)
C4-N1-C1-C34	-173.1(7)	C15-C16-C17-C41	-82.3(12)
Fe1-N1-C1-C34	-19.5(12)	C21-N5-C18-C19	5.4(10)
N1-C1-C2-C3	-1.7(10)	Fe2-N5-C18-C19	-177.6(6)
C34-C1-C2-C3	174.5(8)	C21-N5-C18-C17	-178.6(8)
C1-C2-C3-C4	-0.9(10)	Fe2-N5-C18-C17	-1.5(14)
C2-C3-C4-N1	3.1(11)	C16-C17-C18-N5	25.7(13)
C2-C3-C4-C5	-161.6(11)	C44-C17-C18-N5	147.6(8)
C1-N1-C4-C3	-4.0(10)	C41-C17-C18-N5	-96.2(10)
Fe1-N1-C4-C3	-162.6(6)	C16-C17-C18-C19	-159.0(9)
C1-N1-C4-C5	164.7(8)	C44-C17-C18-C19	-37.2(13)
Fe1-N1-C4-C5	6.1(10)	C41-C17-C18-C19	79.0(12)
C6-N2-C5-C4	-178.1(8)	N5-C18-C19-C20	-5.5(11)
Fe1-N2-C5-C4	-5.4(11)	C17-C18-C19-C20	178.8(9)
C3-C4-C5-N2	164.2(10)	C18-C19-C20-C21	3.3(12)
N1-C4-C5-N2	-0.2(13)	C18-N5-C21-C20	-3.3(11)
C5-N2-C6-C11	-124.7(9)	Fe2-N5-C21-C20	178.9(7)
Fe1-N2-C6-C11	63.9(11)	C18-N5-C21-C22	170.3(8)
C5-N2-C6-C7	58.0(11)	Fe2-N5-C21-C22	-7.5(11)
Fe1-N2-C6-C7	-113.4(8)	C19-C20-C21-N5	-0.1(12)
C11-C6-C7-C8	0.0(13)	C19-C20-C21-C22	-171.8(11)
N2-C6-C7-C8	177.3(7)	C23-N6-C22-C21	-169.4(8)
C6-C7-C8-C9	0.0(13)	Fe2-N6-C22-C21	6.0(10)
C7-C8-C9-C10	0.2(13)	N5-C21-C22-N6	0.6(13)
C8-C9-C10-C11	-0.5(14)	C20-C21-C22-N6	172.1(11)
C7-C6-C11-C10	-0.2(14)	C22-N6-C23-C24	62.9(11)
N2-C6-C11-C10	-177.5(8)	Fe2-N6-C23-C24	-111.6(8)
C7-C6-C11-N3	179.4(7)	C22-N6-C23-C28	-118.1(9)
N2-C6-C11-N3	2.2(13)	Fe2-N6-C23-C28	67.4(10)
C9-C10-C11-C6	0.5(14)	C28-C23-C24-C25	-2.5(13)
C9-C10-C11-N3	-179.1(8)	N6-C23-C24-C25	176.5(7)
C12-N3-C11-C6	108.4(10)	C23-C24-C25-C26	-0.8(14)
Fe2-N3-C11-C6	-70.6(11)	C24-C25-C26-C27	2.8(13)
C12-N3-C11-C10	-72.0(12)	C25-C26-C27-C28	-1.4(13)
Fe2-N3-C11-C10	109.0(9)	C26-C27-C28-C23	-1.8(13)
C11-N3-C12-C13	175.3(9)	C26-C27-C28-N7	179.2(7)
Fe2-N3-C12-C13	-5.5(11)	C24-C23-C28-C27	3.8(13)
C16-N4-C13-C12	-174.2(8)	N6-C23-C28-C27	-175.2(7)
Fe2-N4-C13-C12	7.1(10)	C24-C23-C28-N7	-177.2(7)
C16-N4-C13-C14	1.7(11)	N6-C23-C28-N7	3.8(12)
Fe2-N4-C13-C14	-176.9(6)	C29-N7-C28-C27	-61.8(11)
N3-C12-C13-N4	-0.7(13)	Fe1-N7-C28-C27	114.3(8)
N3-C12-C13-C14	-175.0(11)	C29-N7-C28-C23	119.2(9)
N4-C13-C14-C15	-0.9(11)	Fe1-N7-C28-C23	-64.7(11)
C12-C13-C14-C15	173.7(11)	C28-N7-C29-C30	179.9(7)
C13-C14-C15-C16	-0.2(12)	Fe1-N7-C29-C30	3.0(10)
C13-N4-C16-C15	-1.9(11)	C33-N8-C30-C31	0.2(10)

Fe1-N8-C30-C31	170.1(5)
C33-N8-C30-C29	-175.2(7)
Fe1-N8-C30-C29	-5.3(10)
N7-C29-C30-N8	1.2(12)
N7-C29-C30-C31	-172.6(9)
N8-C30-C31-C32	0.6(10)
C29-C30-C31-C32	174.5(10)
C30-C31-C32-C33	-1.1(10)
C30-N8-C33-C32	-0.9(10)
Fe1-N8-C33-C32	-168.3(6)
C30-N8-C33-C34	178.1(7)
Fe1-N8-C33-C34	10.8(13)
C31-C32-C33-N8	1.3(10)
C31-C32-C33-C34	-177.5(9)
N8-C33-C34-C35	-172.4(7)
C32-C33-C34-C35	6.3(14)
N8-C33-C34-C1	-51.6(10)
C32-C33-C34-C1	127.2(10)
N8-C33-C34-C38	64.3(10)
C32-C33-C34-C38	-116.9(11)
N1-C1-C34-C33	56.5(10)
C2-C1-C34-C33	-119.4(10)
N1-C1-C34-C35	176.3(7)
C2-C1-C34-C35	0.3(12)
N1-C1-C34-C38	-60.3(10)
C2-C1-C34-C38	123.8(9)
C33-C34-C35-C36	-171.8(7)
C1-C34-C35-C36	70.8(9)
C38-C34-C35-C36	-50.2(9)
C34-C35-C36-C37	-165.9(7)
C33-C34-C38-C39	56.2(10)
C35-C34-C38-C39	-65.8(10)
C1-C34-C38-C39	170.9(7)
C34-C38-C39-C40	-106.4(9)
C16-C17-C41-C42	-67.5(11)
C18-C17-C41-C42	56.7(11)
C44-C17-C41-C42	175.3(8)
C17-C41-C42-C43	-179.5(8)
C16-C17-C44-C45	62.0(11)
C18-C17-C44-C45	-62.2(10)
C41-C17-C44-C45	179.2(7)
C17-C44-C45-C46	-179.5(8)
C1A-C2A-C3A-C4A	-176.5(13)
C2A-C3A-C4A-C5A	87(2)
C3A-C4A-C5A-C6A	-177.9(13)

Figure SD1. View of **9** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. The hydrogen atoms have been removed for clarity.

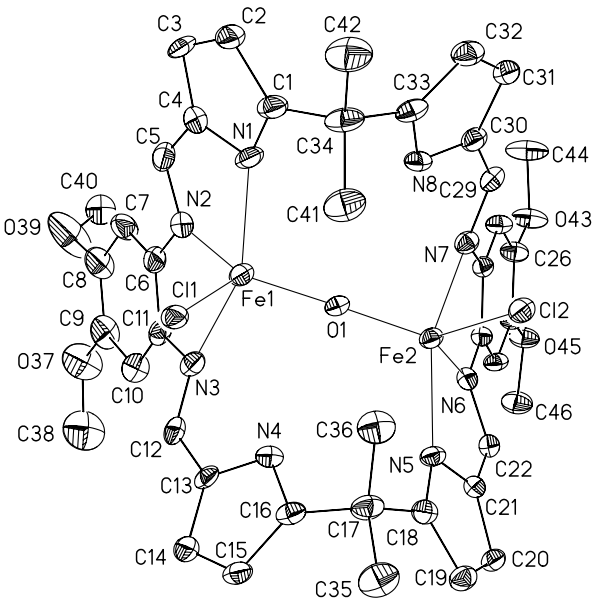

Figure SD2. Unit cell packing diagram for **9**. The view is approximately down the **a** axis.

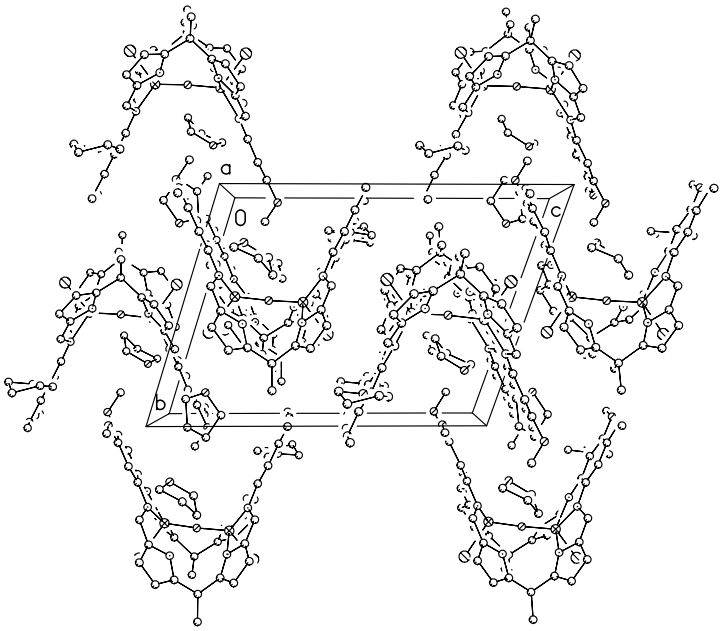

Table SD1. Crystal data and structure refinement for **9**.

Empirical formula	C54 H66 Cl2 Fe2 N8 O8	
Formula weight	1137.75	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.9485(3) Å	α= 106.450(2)°.
	b = 13.4105(3) Å	β= 92.570(2)°.
	c = 17.2908(5) Å	γ = 109.053(2)°.
Volume	2690.43(12) $Å^3$	
Z	2	
Density (calculated)	1.404 Mg/m^3	
Absorption coefficient	0.700 mm^{-1}	
F(000)	1192	
Crystal size	0.20 x 0.19 x 0.15 mm	
Theta range for data collection	3.13 to 25.00°.	
Index ranges	-15<=h<=15, -15<=k<=15, -20<=l<=20	
Reflections collected	17341	
Independent reflections	9442 [R(int) = 0.0680]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9442 / 443 / 665	
Goodness-of-fit on F^2	1.495	
Final R indices [I>2sigma(I)]	R1 = 0.0689, wR2 = 0.1114	
R indices (all data)	R1 = 0.1441, wR2 = 0.1240	
Largest diff. peak and hole	0.654 and -0.548 $e.Å^{-3}$	

Table SD2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe1	2558(1)	5472(1)	8700(1)	36(1)
Fe2	1588(1)	5229(1)	6616(1)	30(1)
Fe1A	1649(6)	5285(5)	8635(4)	28(2)
Fe2A	2570(8)	5329(8)	6692(6)	25(2)
Cl1	1787(1)	3955(1)	9101(1)	37(1)
Cl2	1822(1)	3867(1)	5597(1)	37(1)
O1	2078(2)	5303(2)	7649(2)	30(1)
N1	4163(3)	5254(3)	8658(2)	41(1)
N2	3486(3)	6847(3)	9589(2)	44(1)
N3	1358(3)	6340(3)	9306(2)	37(1)
N4	-158(3)	4332(3)	8121(2)	35(1)
N5	-194(3)	4386(3)	6422(2)	31(1)
N6	1076(3)	6317(3)	6268(2)	33(1)
N7	3153(3)	6525(3)	6421(2)	33(1)
N8	4072(3)	5032(3)	6889(2)	37(1)
C1	4707(4)	4547(5)	8349(3)	46(1)
C2	5703(4)	4852(5)	8859(3)	53(2)
C3	5786(4)	5774(5)	9499(3)	58(2)
C4	4837(4)	6018(5)	9361(3)	48(1)

C5	4475(4)	6838(5)	9821(3)	56(2)
C6	3089(4)	7665(4)	10014(3)	47(1)
C7	3749(4)	8696(5)	10569(3)	64(2)
C8	3292(5)	9420(5)	10982(3)	73(2)
C9	2147(5)	9159(5)	10829(3)	60(2)
C10	1473(4)	8157(4)	10263(3)	51(2)
C11	1953(4)	7407(4)	9867(3)	40(1)
C12	327(4)	5886(4)	9381(3)	38(1)
C13	-417(4)	4865(4)	8842(3)	33(1)
C14	-1473(4)	4207(4)	8900(3)	43(1)
C15	-1830(4)	3279(4)	8217(3)	38(1)
C16	-1002(4)	3362(4)	7732(3)	34(1)
C17	-954(4)	2706(4)	6894(3)	43(1)
C18	-1022(4)	3440(4)	6380(3)	34(1)
C19	-1992(4)	3350(4)	5917(3)	38(1)
C20	-1748(4)	4278(4)	5670(3)	37(1)
C21	-638(4)	4918(4)	5985(3)	31(1)
C22	16(4)	5906(4)	5927(3)	34(1)
C23	1821(3)	7333(4)	6215(3)	32(1)
C24	1494(4)	8166(4)	6077(3)	35(1)
C25	2274(4)	9085(4)	5985(3)	34(1)
C26	3394(4)	9190(4)	6037(3)	40(1)
C27	3711(4)	8376(4)	6200(3)	37(1)
C28	2913(4)	7419(4)	6278(3)	30(1)
C29	4063(4)	6388(4)	6191(3)	36(1)
C30	4484(4)	5598(4)	6369(3)	37(1)
C31	5345(4)	5266(4)	6067(3)	42(1)
C32	5412(4)	4469(4)	6423(3)	45(1)
C33	4622(4)	4346(4)	6928(3)	41(1)
C34	4358(4)	3684(4)	7514(4)	50(2)
C35	-1948(4)	1611(4)	6616(3)	59(2)
C36	126(4)	2445(4)	6841(3)	53(2)
O37	1748(4)	9946(3)	11243(3)	94(1)
C38	579(6)	9668(5)	11132(4)	103(2)
O39	3890(4)	10414(5)	11550(3)	151(2)
C40	4442(10)	11263(8)	11371(7)	68(4)
C40A	4856(9)	10999(9)	11558(7)	73(4)
C41	3121(4)	2986(4)	7369(3)	61(2)
C42	5018(4)	2910(4)	7422(4)	69(2)
O43	4087(2)	10145(3)	5942(2)	55(1)
C44	5243(4)	10341(5)	6064(4)	75(2)
O45	2064(2)	9965(3)	5860(2)	47(1)
C46	950(4)	9929(4)	5871(3)	55(2)
O1A	-516(3)	7640(3)	8782(2)	63(1)
C2A	-559(4)	7039(5)	7954(3)	55(2)
C3A	-1730(4)	6318(5)	7640(3)	63(2)
C4A	-2360(4)	6963(5)	8160(3)	57(2)
C5A	-1622(5)	7421(5)	8964(3)	67(2)
O1B	6261(3)	8329(3)	5954(3)	74(1)
C2B	6940(4)	8415(5)	6646(3)	65(2)
C3B	7998(5)	8327(5)	6372(4)	74(2)
C4B	8028(4)	8637(4)	5606(3)	56(2)
C5B	6828(4)	8212(5)	5272(3)	57(2)
O1C	6409(5)	8709(5)	11261(4)	73(2)
C2C	6649(9)	9702(9)	11962(6)	119(2)
C3C	7410(9)	10652(7)	11745(7)	119(2)

C4C	7972(8)	10163(8)	11116(7)	119(2)
C5C	7259(9)	8957(8)	10770(6)	119(2)
O1D	6309(8)	9341(10)	11202(6)	73(2)
C2D	6976(12)	9435(19)	11943(9)	119(2)
C3D	8135(11)	9707(17)	11813(10)	119(2)
C4D	8170(10)	9782(18)	10979(11)	119(2)
C5D	7109(12)	9944(17)	10771(10)	119(2)

Table SD3. Bond lengths [Å] and angles [°] for **9**.

Fe1-O1	1.820(3)	C3-H3	0.96
Fe1-N2	1.998(4)	C4-C5	1.391(7)
Fe1-N1	2.193(4)	C5-H5	0.96
Fe1-Cl1	2.2698(14)	C6-C11	1.390(6)
Fe1-N3	2.346(4)	C6-C7	1.401(7)
Fe2-O1	1.834(3)	C7-C8	1.351(7)
Fe2-N6	2.006(4)	C7-H7	0.96
Fe2-N5	2.175(3)	C8-O39	1.363(6)
Fe2-Cl2	2.2622(12)	C8-C9	1.401(7)
Fe2-N7	2.309(4)	C9-O37	1.362(6)
Fe1A-N3	1.717(7)	C9-C10	1.392(7)
Fe1A-O1	1.820(7)	C10-C11	1.387(6)
Fe1A-Cl1	2.207(6)	C10-H10	0.96
Fe1A-N4	2.262(8)	C12-C13	1.417(6)
Fe1A-C12	2.399(8)	C12-H12	0.96
Fe2A-N7	1.740(11)	C13-C14	1.390(6)
Fe2A-O1	1.806(11)	C14-C15	1.379(6)
Fe2A-N8	2.140(10)	C14-H14	0.96
Fe2A-Cl2	2.205(10)	C15-C16	1.386(6)
N1-C1	1.365(6)	C15-H15	0.96
N1-C4	1.380(6)	C16-C17	1.484(6)
N2-C5	1.330(6)	C17-C18	1.520(6)
N2-C6	1.397(6)	C17-C35	1.535(6)
N3-C12	1.304(5)	C17-C36	1.549(6)
N3-C11	1.417(5)	C18-C19	1.411(5)
N4-C16	1.360(5)	C19-C20	1.372(6)
N4-C13	1.366(5)	C19-H19	0.96
N4-H4N	0.90	C20-C21	1.399(6)
N5-C18	1.348(5)	C20-H20	0.96
N5-C21	1.395(5)	C21-C22	1.354(6)
N6-C22	1.336(5)	C22-H22	0.96
N6-C23	1.419(6)	C23-C28	1.377(5)
N7-C29	1.313(5)	C23-C24	1.392(6)
N7-C28	1.413(5)	C24-C25	1.370(6)
N8-C33	1.348(5)	C24-H24	0.96
N8-C30	1.354(6)	C25-O45	1.365(5)
N8-H8N	0.90	C25-C26	1.407(6)
C1-C2	1.400(6)	C26-O43	1.362(5)
C1-C34	1.510(7)	C26-C27	1.377(6)
C2-C3	1.376(7)	C27-C28	1.406(6)
C2-H2	0.96	C27-H27	0.96
C3-C4	1.398(6)	C29-C30	1.435(6)

C29-H29	0.96	C4A-H4AB	0.96
C30-C31	1.400(6)	C5A-H5AA	0.96
C31-C32	1.400(6)	C5A-H5AB	0.96
C31-H31	0.96	O1B-C2B	1.408(5)
C32-C33	1.375(7)	O1B-C5B	1.414(6)
C32-H32	0.96	C2B-C3B	1.500(7)
C33-C34	1.509(7)	C2B-H2BA	0.96
C34-C42	1.525(6)	C2B-H2BB	0.96
C34-C41	1.535(6)	C3B-C4B	1.495(7)
C35-H35A	0.96	C3B-H3BA	0.96
C35-H35B	0.96	C3B-H3BB	0.96
C35-H35C	0.96	C4B-C5B	1.493(6)
C36-H36A	0.96	C4B-H4BA	0.96
C36-H36B	0.96	C4B-H4BB	0.96
C36-H36C	0.96	C5B-H5BA	0.96
O37-C38	1.426(7)	C5B-H5BB	0.96
C38-H38A	0.96	O1C-C5C	1.431(9)
C38-H38B	0.96	O1C-C2C	1.456(8)
C38-H38C	0.96	O1C-H2DA	1.4349
O39-C40A	1.236(10)	C2C-C3C	1.490(8)
O39-C40	1.260(10)	C2C-H2CA	0.96
C40-C40A	0.832(14)	C2C-H2CB	0.96
C40-H40A	0.96	C2C-H2DA	1.3585
C40-H40B	0.96	C2C-H2DB	0.7332
C40-H40C	0.96	C3C-C4C	1.457(8)
C40-H40D	1.3762	C3C-H3CA	0.96
C40-H40F	0.5426	C3C-H3CB	0.96
C40A-H40A	1.1559	C3C-H5DA	1.4196
C40A-H40B	0.9793	C4C-C5C	1.502(8)
C40A-H40D	0.96	C4C-H4CA	0.96
C40A-H40E	0.96	C4C-H4CB	0.96
C40A-H40F	0.96	C4C-H4DA	1.5641
C41-H41A	0.96	C4C-H4DB	1.0407
C41-H41B	0.96	C4C-H5DA	1.5066
C41-H41C	0.96	C5C-H5CA	0.96
C42-H42A	0.96	C5C-H5CB	0.96
C42-H42B	0.96	C5C-H4DA	1.2978
C42-H42C	0.96	O1D-C2D	1.463(9)
O43-C44	1.428(5)	O1D-C5D	1.465(10)
C44-H44A	0.96	C2D-C3D	1.468(8)
C44-H44B	0.96	C2D-H2CA	0.7869
C44-H44C	0.96	C2D-H2CB	1.5471
O45-C46	1.427(5)	C2D-H2DA	0.96
C46-H46A	0.96	C2D-H2DB	0.96
C46-H46B	0.96	C3D-C4D	1.475(9)
C46-H46C	0.96	C3D-H4CA	1.3351
O1A-C2A	1.418(5)	C3D-H3DA	0.96
O1A-C5A	1.434(6)	C3D-H3DB	0.96
C2A-C3A	1.483(6)	C4D-C5D	1.503(9)
C2A-H2AA	0.96	C4D-H4CA	0.8452
C2A-H2AB	0.96	C4D-H4CB	1.2668
C3A-C4A	1.520(7)	C4D-H5CB	1.5403
C3A-H3AA	0.96	C4D-H4DA	0.96
C3A-H3AB	0.96	C4D-H4DB	0.96
C4A-C5A	1.496(6)	C5D-H4CB	1.2266
C4A-H4AA	0.96	C5D-H5CA	1.5007

C5D-H5DA	0.96	C5D-H5DB	0.96
O1-Fe1-N2	129.39(15)	C23-N6-Fe2	122.5(3)
O1-Fe1-N1	104.34(14)	C29-N7-C28	116.9(4)
N2-Fe1-N1	80.32(16)	C29-N7-Fe2A	100.1(4)
O1-Fe1-Cl1	114.77(10)	C28-N7-Fe2A	142.3(5)
N2-Fe1-Cl1	115.18(12)	C29-N7-Fe2	128.5(3)
N1-Fe1-Cl1	93.42(11)	C28-N7-Fe2	111.1(3)
O1-Fe1-N3	96.89(12)	C33-N8-C30	109.8(4)
N2-Fe1-N3	73.02(15)	C33-N8-Fe2A	151.3(4)
N1-Fe1-N3	152.77(14)	C30-N8-Fe2A	88.3(4)
Cl1-Fe1-N3	92.95(11)	C33-N8-H8N	125.0
O1-Fe2-N6	128.35(13)	C30-N8-H8N	125.2
O1-Fe2-N5	105.82(14)	N1-C1-C2	110.1(5)
N6-Fe2-N5	79.29(15)	N1-C1-C34	123.9(4)
O1-Fe2-Cl2	115.25(9)	C2-C1-C34	125.4(5)
N6-Fe2-Cl2	115.79(11)	C3-C2-C1	107.5(5)
N5-Fe2-Cl2	92.59(9)	C3-C2-H2	127.2
O1-Fe2-N7	98.07(12)	C1-C2-H2	125.3
N6-Fe2-N7	73.88(14)	C2-C3-C4	106.2(5)
N5-Fe2-N7	151.62(13)	C2-C3-H3	126.7
Cl2-Fe2-N7	90.85(10)	C4-C3-H3	127.0
N3-Fe1A-O1	124.9(4)	N1-C4-C5	118.4(5)
N3-Fe1A-N4	92.2(3)	N1-C4-C3	110.5(5)
O1-Fe1A-N4	94.6(3)	C5-C4-C3	131.0(5)
Cl1-Fe1A-N4	92.4(3)	N2-C5-C4	119.7(5)
N7-Fe2A-O1	124.8(6)	N2-C5-H5	120.0
N7-Fe2A-N8	96.6(5)	C4-C5-H5	120.3
O1-Fe2A-N8	99.9(4)	C11-C6-N2	116.0(4)
N7-Fe2A-Cl2	110.7(5)	C11-C6-C7	119.3(5)
O1-Fe2A-Cl2	119.3(5)	N2-C6-C7	124.7(5)
N8-Fe2A-Cl2	95.8(4)	C8-C7-C6	120.9(5)
Fe2A-O1-Fe1A	177.2(4)	C8-C7-H7	119.3
Fe1-O1-Fe2	176.03(17)	C6-C7-H7	119.8
C1-N1-C4	105.6(4)	C7-C8-O39	123.3(6)
C1-N1-Fe1	145.9(3)	C7-C8-C9	119.6(5)
C4-N1-Fe1	105.9(3)	O39-C8-C9	117.1(6)
C5-N2-C6	122.3(4)	O37-C9-C10	122.7(5)
C5-N2-Fe1	113.3(4)	O37-C9-C8	116.4(5)
C6-N2-Fe1	123.7(3)	C10-C9-C8	120.8(5)
C12-N3-C11	116.6(4)	C11-C10-C9	118.7(5)
C12-N3-Fe1A	104.3(4)	C11-C10-H10	120.9
C11-N3-Fe1A	137.6(4)	C9-C10-H10	120.4
C12-N3-Fe1	128.6(3)	C10-C11-C6	120.6(5)
C11-N3-Fe1	111.3(3)	C10-C11-N3	124.5(4)
C16-N4-C13	110.2(4)	C6-C11-N3	114.9(5)
C16-N4-Fe1A	150.7(3)	N3-C12-C13	124.7(5)
C13-N4-Fe1A	88.5(3)	N3-C12-H12	117.7
C16-N4-H4N	124.8	C13-C12-H12	117.6
C13-N4-H4N	125.0	N4-C13-C14	106.7(4)
Fe1A-N4-H4N	42.4	N4-C13-C12	122.1(5)
C18-N5-C21	105.9(3)	C14-C13-C12	131.2(5)
C18-N5-Fe2	145.5(3)	C15-C14-C13	108.0(5)
C21-N5-Fe2	106.0(3)	C15-C14-H14	126.4
C22-N6-C23	122.0(4)	C13-C14-H14	125.6
C22-N6-Fe2	114.0(3)	C14-C15-C16	107.9(4)

C14-C15-H15	126.5	N8-C33-C32	108.3(5)
C16-C15-H15	125.5	N8-C33-C34	119.3(5)
N4-C16-C15	107.1(4)	C32-C33-C34	132.2(4)
N4-C16-C17	119.5(4)	C33-C34-C1	104.5(4)
C15-C16-C17	132.9(4)	C33-C34-C42	110.8(4)
C16-C17-C18	104.1(4)	C1-C34-C42	110.1(4)
C16-C17-C35	109.6(4)	C33-C34-C41	111.0(4)
C18-C17-C35	110.7(4)	C1-C34-C41	111.6(4)
C16-C17-C36	112.0(4)	C42-C34-C41	108.9(4)
C18-C17-C36	111.3(4)	C17-C35-H35A	109.9
C35-C17-C36	109.1(4)	C17-C35-H35B	109.0
N5-C18-C19	110.4(4)	H35A-C35-H35B	109.5
N5-C18-C17	123.2(4)	C17-C35-H35C	109.5
C19-C18-C17	125.5(4)	H35A-C35-H35C	109.5
C20-C19-C18	107.2(4)	H35B-C35-H35C	109.5
C20-C19-H19	126.7	C17-C36-H36A	109.4
C18-C19-H19	126.1	C17-C36-H36B	109.6
C19-C20-C21	106.6(4)	H36A-C36-H36B	109.5
C19-C20-H20	127.4	C17-C36-H36C	109.4
C21-C20-H20	126.0	H36A-C36-H36C	109.4
C22-C21-N5	119.0(4)	H36B-C36-H36C	109.5
C22-C21-C20	131.2(4)	C9-O37-C38	117.2(5)
N5-C21-C20	109.9(4)	O37-C38-H38A	109.8
N6-C22-C21	118.6(4)	O37-C38-H38B	108.7
N6-C22-H22	120.9	H38A-C38-H38B	109.5
C21-C22-H22	120.5	O37-C38-H38C	109.9
C28-C23-C24	121.6(4)	H38A-C38-H38C	109.5
C28-C23-N6	114.4(4)	H38B-C38-H38C	109.5
C24-C23-N6	123.9(4)	C40A-O39-C40	38.9(7)
C25-C24-C23	119.2(4)	C40A-O39-C8	126.7(7)
C25-C24-H24	120.4	C40-O39-C8	123.5(8)
C23-C24-H24	120.4	O39-C40-H40A	110.7
O45-C25-C24	124.9(4)	O39-C40-H40B	110.9
O45-C25-C26	114.7(4)	H40A-C40-H40B	109.5
C24-C25-C26	120.4(4)	C40A-C40-H40C	170.5
O43-C26-C27	125.5(4)	O39-C40-H40C	106.7
O43-C26-C25	114.7(4)	H40A-C40-H40C	109.5
C27-C26-C25	119.8(5)	H40B-C40-H40C	109.5
C26-C27-C28	120.1(4)	O39-C40A-H40B	111.5
C26-C27-H27	120.0	O39-C40A-H40D	113.1
C28-C27-H27	119.8	O39-C40A-H40E	116.0
C23-C28-C27	118.8(4)	H40D-C40A-H40E	109.5
C23-C28-N7	116.9(4)	H40D-C40A-H40F	109.5
C27-C28-N7	124.3(4)	H40E-C40A-H40F	109.5
N7-C29-C30	123.7(5)	C34-C41-H41A	110.3
N7-C29-H29	118.3	C34-C41-H41B	108.7
C30-C29-H29	117.9	H41A-C41-H41B	109.5
N8-C30-C31	108.0(4)	C34-C41-H41C	109.4
N8-C30-C29	123.1(4)	H41A-C41-H41C	109.5
C31-C30-C29	128.9(5)	H41B-C41-H41C	109.5
C30-C31-C32	106.1(5)	C34-C42-H42A	109.8
C30-C31-H31	126.3	C34-C42-H42B	109.4
C32-C31-H31	127.6	H42A-C42-H42B	109.5
C33-C32-C31	107.9(4)	C34-C42-H42C	109.3
C33-C32-H32	125.5	H42A-C42-H42C	109.5
C31-C32-H32	126.6	H42B-C42-H42C	109.5

C26-O43-C44	116.9(4)	C3B-C4B-H4BB	110.8
O43-C44-H44A	109.3	H4BA-C4B-H4BB	109.2
O43-C44-H44B	109.2	O1B-C5B-C4B	106.4(4)
H44A-C44-H44B	109.5	O1B-C5B-H5BA	110.4
O43-C44-H44C	109.9	C4B-C5B-H5BA	110.8
H44A-C44-H44C	109.5	O1B-C5B-H5BB	110.2
H44B-C44-H44C	109.5	C4B-C5B-H5BB	110.1
C25-O45-C46	116.1(4)	H5BA-C5B-H5BB	109.0
O45-C46-H46A	109.7	C5C-O1C-C2C	106.7(7)
O45-C46-H46B	109.1	C5C-O1C-H2DA	119.2
H46A-C46-H46B	109.5	O1C-C2C-C3C	107.4(6)
O45-C46-H46C	109.6	O1C-C2C-H2CA	109.6
H46A-C46-H46C	109.5	C3C-C2C-H2CA	108.4
H46B-C46-H46C	109.5	O1C-C2C-H2CB	111.0
C2A-O1A-C5A	108.8(4)	C3C-C2C-H2CB	111.5
O1A-C2A-C3A	106.9(4)	H2CA-C2C-H2CB	108.8
O1A-C2A-H2AA	110.0	H2CB-C2C-H2DA	112.1
C3A-C2A-H2AA	111.1	C4C-C3C-C2C	105.5(5)
O1A-C2A-H2AB	110.4	C4C-C3C-H3CA	110.0
C3A-C2A-H2AB	109.8	C2C-C3C-H3CA	112.8
H2AA-C2A-H2AB	108.8	C4C-C3C-H3CB	111.0
C2A-C3A-C4A	102.9(4)	C2C-C3C-H3CB	108.8
C2A-C3A-H3AA	110.4	H3CA-C3C-H3CB	108.7
C4A-C3A-H3AA	109.6	C2C-C3C-H5DA	117.4
C2A-C3A-H3AB	112.0	C3C-C4C-C5C	105.7(5)
C4A-C3A-H3AB	112.8	C3C-C4C-H4CA	111.0
H3AA-C3A-H3AB	109.1	C5C-C4C-H4CA	111.3
C5A-C4A-C3A	100.4(4)	C3C-C4C-H4CB	110.1
C5A-C4A-H4AA	113.3	C5C-C4C-H4CB	110.2
C3A-C4A-H4AA	112.5	H4CA-C4C-H4CB	108.6
C5A-C4A-H4AB	110.5	C5C-C4C-H5DA	101.1
C3A-C4A-H4AB	110.2	H4CA-C4C-H5DA	147.7
H4AA-C4A-H4AB	109.6	H4DA-C4C-H5DA	133.0
O1A-C5A-C4A	106.1(4)	H4DB-C4C-H5DA	121.9
O1A-C5A-H5AA	110.3	O1C-C5C-C4C	109.1(6)
C4A-C5A-H5AA	111.8	O1C-C5C-H5CA	108.8
O1A-C5A-H5AB	110.1	C4C-C5C-H5CA	110.7
C4A-C5A-H5AB	109.5	O1C-C5C-H5CB	110.1
H5AA-C5A-H5AB	109.0	C4C-C5C-H5CB	109.4
C2B-O1B-C5B	109.6(4)	H5CA-C5C-H5CB	108.6
O1B-C2B-C3B	106.7(5)	C2D-O1D-C5D	104.2(8)
O1B-C2B-H2BA	109.2	O1D-C2D-C3D	108.7(7)
C3B-C2B-H2BA	109.9	C3D-C2D-H2CA	103.1
O1B-C2B-H2BB	111.1	O1D-C2D-H2DA	110.8
C3B-C2B-H2BB	111.1	C3D-C2D-H2DA	111.9
H2BA-C2B-H2BB	108.9	O1D-C2D-H2DB	108.2
C4B-C3B-C2B	104.0(4)	C3D-C2D-H2DB	108.4
C4B-C3B-H3BA	110.2	H2DA-C2D-H2DB	108.7
C2B-C3B-H3BA	111.7	C2D-C3D-C4D	106.8(5)
C4B-C3B-H3BB	110.9	C2D-C3D-H3DA	108.6
C2B-C3B-H3BB	111.0	C4D-C3D-H3DA	106.4
H3BA-C3B-H3BB	109.0	H4CA-C3D-H3DA	110.8
C5B-C4B-C3B	101.6(4)	C2D-C3D-H3DB	112.2
C5B-C4B-H4BA	112.4	C4D-C3D-H3DB	114.2
C3B-C4B-H4BA	112.0	H3DA-C3D-H3DB	108.4
C5B-C4B-H4BB	110.7	C3D-C4D-C5D	103.9(6)

C3D-C4D-H4DA	114.7	H4CB-C5D-H5CA	105.4
C5D-C4D-H4DA	112.5	O1D-C5D-H5DA	108.6
C3D-C4D-H4DB	107.0	C4D-C5D-H5DA	112.6
C5D-C4D-H4DB	109.8	O1D-C5D-H5DB	111.8
H4DA-C4D-H4DB	108.7	C4D-C5D-H5DB	109.2
O1D-C5D-C4D	105.6(7)	H5DA-C5D-H5DB	109.1

Table SD4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe1	27(1)	44(1)	35(1)	16(1)	-1(1)	8(1)
Fe2	25(1)	33(1)	31(1)	6(1)	0(1)	13(1)
Cl1	29(1)	47(1)	44(1)	26(1)	5(1)	13(1)
Cl2	34(1)	38(1)	35(1)	0(1)	0(1)	19(1)
O1	23(2)	33(2)	34(2)	9(1)	-1(1)	10(1)
N1	24(2)	54(3)	47(3)	26(2)	-4(2)	8(2)
N2	40(3)	60(3)	32(2)	15(2)	7(2)	16(2)
N3	35(2)	36(3)	38(2)	14(2)	-3(2)	8(2)
N4	25(2)	34(2)	42(3)	11(2)	5(2)	8(2)
N5	22(2)	29(2)	35(2)	0(2)	0(2)	7(2)
N6	32(2)	37(2)	28(2)	9(2)	8(2)	11(2)
N7	33(2)	32(2)	34(2)	6(2)	0(2)	15(2)
N8	25(2)	48(3)	43(3)	16(2)	7(2)	19(2)
C1	28(3)	64(4)	58(4)	41(3)	7(3)	14(3)
C2	36(3)	89(5)	55(4)	42(4)	11(3)	31(3)
C3	25(3)	106(5)	50(4)	41(4)	-6(3)	18(3)
C4	40(3)	71(4)	37(3)	24(3)	12(3)	16(3)
C5	43(3)	80(4)	34(3)	26(3)	-1(3)	3(3)
C6	41(3)	56(4)	28(3)	7(3)	1(3)	4(3)
C7	40(3)	83(5)	39(3)	-2(3)	9(3)	0(3)
C8	61(4)	67(4)	43(4)	-14(3)	11(3)	-12(4)
C9	80(4)	39(4)	47(4)	-8(3)	17(3)	21(3)
C10	56(3)	46(4)	50(3)	13(3)	5(3)	18(3)
C11	42(3)	33(3)	30(3)	6(3)	-6(2)	-1(3)
C12	46(3)	44(3)	28(3)	14(3)	-1(3)	20(3)
C13	29(3)	37(3)	34(3)	16(3)	-8(2)	10(2)
C14	35(3)	57(4)	41(3)	26(3)	3(3)	14(3)
C15	26(3)	38(3)	48(3)	21(3)	-3(3)	4(2)
C16	26(3)	30(3)	47(3)	17(3)	-2(3)	7(2)
C17	30(3)	33(3)	52(3)	4(3)	-1(2)	3(2)
C18	31(3)	29(3)	34(3)	0(2)	5(2)	9(2)
C19	33(3)	34(3)	38(3)	2(3)	0(2)	9(2)
C20	28(3)	47(3)	32(3)	7(3)	-1(2)	14(3)
C21	27(3)	37(3)	28(3)	8(2)	6(2)	12(3)
C22	32(3)	43(3)	27(3)	9(2)	5(2)	14(3)
C23	24(3)	36(3)	29(3)	7(2)	4(2)	6(2)
C24	23(3)	38(3)	42(3)	9(3)	2(2)	14(3)
C25	29(3)	35(3)	42(3)	12(3)	4(2)	18(3)
C26	30(3)	30(3)	59(3)	12(3)	9(2)	10(3)
C27	25(3)	36(3)	50(3)	10(3)	4(2)	13(2)

C28	29(3)	34(3)	29(3)	10(2)	3(2)	14(2)
C29	36(3)	36(3)	33(3)	7(2)	-6(2)	13(2)
C30	35(3)	41(3)	35(3)	4(3)	-3(2)	19(3)
C31	34(3)	52(3)	37(3)	9(3)	2(2)	19(3)
C32	37(3)	47(3)	55(4)	11(3)	1(3)	23(3)
C33	31(3)	42(3)	52(3)	15(3)	-6(3)	18(3)
C34	31(3)	49(3)	78(4)	30(3)	2(3)	19(3)
C35	56(3)	31(3)	74(4)	11(3)	-3(3)	4(3)
C36	53(3)	43(3)	68(4)	13(3)	8(3)	25(3)
O37	95(3)	57(3)	99(3)	-10(3)	25(3)	16(3)
C38	118(6)	77(5)	112(6)	1(4)	30(5)	54(5)
O39	126(4)	105(4)	94(4)	-58(3)	57(3)	-55(3)
C41	49(3)	47(3)	81(4)	20(3)	-2(3)	12(3)
C42	62(4)	61(4)	104(5)	39(4)	12(3)	36(3)
O43	29(2)	38(2)	102(3)	27(2)	16(2)	12(2)
C44	29(3)	58(4)	142(5)	42(4)	14(3)	13(3)
O45	34(2)	45(2)	72(2)	26(2)	12(2)	21(2)
C46	42(3)	59(4)	79(4)	29(3)	14(3)	30(3)
O1A	48(2)	72(3)	53(3)	8(2)	2(2)	13(2)
C2A	54(4)	72(4)	44(4)	21(3)	13(3)	28(3)
C3A	76(4)	54(4)	50(4)	10(3)	1(3)	20(3)
C4A	49(3)	69(4)	58(4)	27(3)	9(3)	21(3)
C5A	67(4)	71(4)	59(4)	17(3)	7(3)	21(3)
O1B	49(2)	119(4)	85(3)	55(3)	30(2)	50(2)
C2B	49(4)	70(4)	70(4)	23(3)	6(3)	13(3)
C3B	56(4)	85(5)	88(5)	30(4)	8(3)	34(3)
C4B	49(4)	40(3)	82(4)	17(3)	26(3)	19(3)
C5B	52(4)	63(4)	72(4)	29(3)	21(3)	31(3)

Table SD5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **9**.

	x	y	z	U(eq)
H4N	479	4586	7930	42
H8N	3516	5103	7168	44
H2	6221	4472	8773	64
H3	6376	6167	9950	70
H5	4929	7386	10309	67
H7	4535	8886	10666	77
H10	691	7988	10156	61
H12	51	6272	9832	45
H14	-1879	4377	9339	51
H15	-2524	2673	8097	46
H19	-2689	2748	5795	46
H20	-2237	4465	5350	44
H22	-280	6302	5649	41
H24	728	8089	6032	41
H27	4478	8458	6257	45
H29	4466	6833	5880	44
H31	5787	5531	5686	50

H32	5920	4077	6336	55
H35A	-2623	1761	6647	88
H35B	-1932	1210	6063	88
H35C	-1906	1172	6961	88
H36A	750	3129	7016	80
H36B	162	2005	7186	80
H36C	136	2043	6287	80
H38A	395	10279	11456	155
H38B	324	9515	10566	155
H38C	232	9023	11292	155
H40A	4818	11872	11856	102
H40B	4970	11110	11028	102
H40C	3923	11455	11082	102
H40D	5176	11573	12071	110
H40E	5352	10608	11392	110
H40F	4726	11326	11154	110
H41A	2689	3457	7424	91
H41B	2933	2465	6827	91
H41C	2971	2590	7759	91
H42A	5794	3336	7515	103
H42B	4854	2515	7811	103
H42C	4816	2390	6880	103
H44A	5646	11035	5983	112
H44B	5461	10372	6611	112
H44C	5401	9751	5684	112
H46A	888	10580	5777	83
H46B	473	9278	5450	83
H46C	740	9898	6392	83
H2AA	-92	6605	7916	65
H2AB	-313	7540	7643	65
H3AA	-1880	5616	7737	75
H3AB	-1913	6188	7068	75
H4AA	-3095	6499	8178	69
H4AB	-2390	7554	7961	69
H5AA	-1698	8090	9301	81
H5AB	-1799	6877	9245	81
H2BA	6583	7812	6849	78
H2BB	7073	9105	7069	78
H3BA	8003	7586	6261	88
H3BB	8623	8831	6774	88
H4BA	8441	8296	5240	67
H4BB	8340	9428	5726	67
H5BA	6681	8632	4942	69
H5BB	6596	7444	4947	69
H2CA	7020	9621	12421	143
H2CB	5982	9823	12104	143
H3CA	7942	11191	12201	143
H3CB	6981	11012	11540	143
H4CA	8701	10252	11340	143
H4CB	8034	10513	10698	143
H5CA	6920	8791	10221	143
H5CB	7704	8507	10765	143
H2DA	6708	8764	12086	143
H2DB	6923	10037	12379	143
H3DA	8358	9092	11819	143
H3DB	8619	10359	12229	143

H4DA	8251	9154	10586	143
H4DB	8788	10435	11011	143
H5DA	7175	10711	10953	143
H5DB	6885	9650	10190	143

Table SD6. Torsion angles [°] for **9**.

N7-Fe2A-O1-Fe1A	-89(8)	N1-Fe1-N2-C5	-12.8(3)
N8-Fe2A-O1-Fe1A	16(9)	Cl1-Fe1-N2-C5	76.4(4)
N7-Fe2A-O1-Fe1	-83.8(8)	N3-Fe1-N2-C5	161.6(4)
N8-Fe2A-O1-Fe1	21.6(7)	O1-Fe1-N2-C6	75.6(4)
Cl2-Fe2A-O1-Fe1	124.0(5)	N1-Fe1-N2-C6	176.3(4)
N7-Fe2A-O1-Fe2	90.1(7)	Cl1-Fe1-N2-C6	-94.5(4)
N8-Fe2A-O1-Fe2	-164.5(7)	N3-Fe1-N2-C6	-9.3(4)
Cl2-Fe2A-O1-Fe2	-62.0(4)	O1-Fe1A-N3-C12	119.3(5)
Fe1-Fe1A-O1-Fe2A	6(9)	Cl1-Fe1A-N3-C12	-71.8(4)
N3-Fe1A-O1-Fe2A	108(8)	N4-Fe1A-N3-C12	22.0(4)
Cl1-Fe1A-O1-Fe2A	-61(9)	Fe1-Fe1A-N3-C11	6.1(8)
N4-Fe1A-O1-Fe2A	-156(8)	O1-Fe1A-N3-C11	-75.7(7)
C12-Fe1A-O1-Fe2A	148(8)	Cl1-Fe1A-N3-C11	93.3(6)
Cl1-Fe1A-O1-Fe2	120.1(4)	N4-Fe1A-N3-C11	-172.9(4)
N4-Fe1A-O1-Fe2	24.9(5)	C12-Fe1A-N3-C11	165.1(7)
C12-Fe1A-O1-Fe2	-31.2(7)	O1-Fe1-N3-C12	81.4(4)
Fe1A-Fe1-O1-Fe2A	-179.5(7)	N2-Fe1-N3-C12	-149.5(4)
N2-Fe1-O1-Fe2A	70.6(6)	N1-Fe1-N3-C12	-137.4(4)
N1-Fe1-O1-Fe2A	-18.6(6)	Cl1-Fe1-N3-C12	-34.0(4)
Cl1-Fe1-O1-Fe2A	-119.3(5)	O1-Fe1-N3-C11	-120.7(3)
N3-Fe1-O1-Fe2A	144.2(6)	N2-Fe1-N3-C11	8.5(3)
Cl1-Fe1-O1-Fe1A	60.3(3)	N1-Fe1-N3-C11	20.6(5)
N3-Fe1-O1-Fe1A	-36.2(3)	Cl1-Fe1-N3-C11	123.9(3)
N2-Fe1-O1-Fe2	-33(3)	N3-Fe1A-N4-C16	-156.0(7)
N1-Fe1-O1-Fe2	-123(3)	O1-Fe1A-N4-C16	78.7(8)
Cl1-Fe1-O1-Fe2	137(3)	Cl1-Fe1A-N4-C16	-39.4(8)
N3-Fe1-O1-Fe2	40(3)	C12-Fe1A-N4-C16	-143.2(7)
N6-Fe2-O1-Fe1A	65.5(5)	N3-Fe1A-N4-C13	-24.8(3)
N5-Fe2-O1-Fe1A	-23.3(4)	O1-Fe1A-N4-C13	-150.0(3)
Cl2-Fe2-O1-Fe1A	-123.9(4)	Cl1-Fe1A-N4-C13	91.9(3)
N7-Fe2-O1-Fe1A	141.3(4)	C12-Fe1A-N4-C13	-11.9(3)
Fe2A-Fe2-O1-Fe1	109(3)	O1-Fe2-N5-C18	-61.2(6)
N6-Fe2-O1-Fe1	-6(3)	N6-Fe2-N5-C18	171.7(6)
N5-Fe2-O1-Fe1	-94(3)	Cl2-Fe2-N5-C18	55.9(5)
Cl2-Fe2-O1-Fe1	165(3)	N7-Fe2-N5-C18	152.5(5)
N7-Fe2-O1-Fe1	70(3)	O1-Fe2-N5-C21	141.6(3)
Fe1A-Fe1-N1-C1	15.1(13)	N6-Fe2-N5-C21	14.5(3)
O1-Fe1-N1-C1	-61.7(6)	Cl2-Fe2-N5-C21	-101.2(2)
N2-Fe1-N1-C1	169.9(6)	N7-Fe2-N5-C21	-4.6(4)
Cl1-Fe1-N1-C1	54.9(6)	O1-Fe2-N6-C22	-116.3(3)
N3-Fe1-N1-C1	158.1(5)	N5-Fe2-N6-C22	-14.6(3)
O1-Fe1-N1-C4	141.4(3)	Cl2-Fe2-N6-C22	73.1(3)
N2-Fe1-N1-C4	13.0(3)	N7-Fe2-N6-C22	156.1(3)
Cl1-Fe1-N1-C4	-102.0(3)	O1-Fe2-N6-C23	77.3(4)
N3-Fe1-N1-C4	1.3(5)	N5-Fe2-N6-C23	179.1(3)
O1-Fe1-N2-C5	-113.5(3)	Cl2-Fe2-N6-C23	-93.2(3)

N7-Fe2-N6-C23	-10.2(3)	O37-C9-C10-C11	179.6(5)
O1-Fe2A-N7-C29	129.0(6)	C8-C9-C10-C11	1.7(8)
N8-Fe2A-N7-C29	22.0(5)	C9-C10-C11-C6	-1.9(8)
Cl2-Fe2A-N7-C29	-76.8(5)	C9-C10-C11-N3	177.0(4)
C30-Fe2A-N7-C29	7.5(3)	N2-C6-C11-C10	179.4(5)
Fe2-Fe2A-N7-C28	12.4(10)	C7-C6-C11-C10	-0.1(7)
O1-Fe2A-N7-C28	-62.3(10)	N2-C6-C11-N3	0.4(6)
N8-Fe2A-N7-C28	-169.3(5)	C7-C6-C11-N3	-179.1(4)
Cl2-Fe2A-N7-C28	91.9(7)	C12-N3-C11-C10	-25.2(7)
C29-Fe2A-N7-C28	168.7(8)	Fe1A-N3-C11-C10	171.0(5)
C30-Fe2A-N7-C28	176.2(6)	Fe1-N3-C11-C10	173.9(4)
O1-Fe2-N7-C29	82.3(4)	C12-N3-C11-C6	153.8(4)
N6-Fe2-N7-C29	-150.0(4)	Fe1A-N3-C11-C6	-10.0(7)
N5-Fe2-N7-C29	-130.4(4)	Fe1-N3-C11-C6	-7.1(5)
Cl2-Fe2-N7-C29	-33.4(4)	C11-N3-C12-C13	175.2(4)
O1-Fe2-N7-C28	-119.9(3)	Fe1A-N3-C12-C13	-16.0(5)
N6-Fe2-N7-C28	7.7(3)	Fe1-N3-C12-C13	-27.8(6)
N5-Fe2-N7-C28	27.4(4)	Fe1-Fe1A-C12-N3	30.9(7)
Cl2-Fe2-N7-C28	124.4(3)	O1-Fe1A-C12-N3	-86.8(6)
Fe2-Fe2A-N8-C33	19(3)	Cl1-Fe1A-C12-N3	119.1(4)
N7-Fe2A-N8-C33	-155.7(7)	N4-Fe1A-C12-N3	-155.1(4)
O1-Fe2A-N8-C33	77.1(10)	N3-Fe1A-C12-C13	166.8(5)
Cl2-Fe2A-N8-C33	-44.0(10)	O1-Fe1A-C12-C13	79.9(5)
C29-Fe2A-N8-C33	-142.7(8)	Cl1-Fe1A-C12-C13	-74.2(3)
C30-Fe2A-N8-C33	-130.5(9)	N4-Fe1A-C12-C13	11.6(2)
N7-Fe2A-N8-C30	-25.2(4)	C16-N4-C13-C14	-0.8(5)
O1-Fe2A-N8-C30	-152.4(5)	Fe1A-N4-C13-C14	-157.7(3)
C4-N1-C1-C2	1.1(6)	C16-N4-C13-C12	178.6(4)
Fe1-N1-C1-C2	-155.8(4)	Fe1A-N4-C13-C12	21.6(4)
C4-N1-C1-C34	-170.2(5)	N3-C12-C13-N4	-9.4(6)
Fe1-N1-C1-C34	32.9(9)	Fe1A-C12-C13-N4	-20.5(4)
N1-C1-C2-C3	-0.4(6)	N3-C12-C13-C14	169.8(4)
C34-C1-C2-C3	170.7(5)	Fe1A-C12-C13-C14	158.7(5)
C1-C2-C3-C4	-0.4(6)	N4-C13-C14-C15	0.7(5)
C1-N1-C4-C5	-178.6(5)	C12-C13-C14-C15	-178.6(4)
Fe1-N1-C4-C5	-11.9(6)	C13-C14-C15-C16	-0.4(5)
C1-N1-C4-C3	-1.4(6)	C13-N4-C16-C15	0.6(5)
Fe1-N1-C4-C3	165.4(4)	Fe1A-N4-C16-C15	127.4(7)
C2-C3-C4-N1	1.1(6)	C13-N4-C16-C17	173.2(4)
C2-C3-C4-C5	177.9(6)	Fe1A-N4-C16-C17	-59.9(9)
C6-N2-C5-C4	-178.4(5)	C14-C15-C16-N4	-0.1(5)
Fe1-N2-C5-C4	10.6(6)	C14-C15-C16-C17	-171.4(5)
N1-C4-C5-N2	2.0(8)	N4-C16-C17-C18	-66.1(5)
C3-C4-C5-N2	-174.6(5)	C15-C16-C17-C18	104.3(6)
C5-N2-C6-C11	-161.4(5)	N4-C16-C17-C35	175.5(4)
Fe1-N2-C6-C11	8.7(6)	C15-C16-C17-C35	-14.1(7)
C5-N2-C6-C7	18.1(8)	N4-C16-C17-C36	54.2(6)
Fe1-N2-C6-C7	-171.8(4)	C15-C16-C17-C36	-135.4(5)
C11-C6-C7-C8	2.5(8)	C21-N5-C18-C19	0.5(5)
N2-C6-C7-C8	-177.0(5)	Fe2-N5-C18-C19	-156.7(4)
C6-C7-C8-O39	177.5(5)	C21-N5-C18-C17	-169.2(4)
C6-C7-C8-C9	-2.8(9)	Fe2-N5-C18-C17	33.6(8)
C7-C8-C9-O37	-177.4(6)	C16-C17-C18-N5	70.9(5)
O39-C8-C9-O37	2.4(8)	C35-C17-C18-N5	-171.5(4)
C7-C8-C9-C10	0.7(9)	C36-C17-C18-N5	-49.9(6)
O39-C8-C9-C10	-179.6(6)	C16-C17-C18-C19	-97.2(5)

C35-C17-C18-C19	20.5(6)
C36-C17-C18-C19	142.0(4)
N5-C18-C19-C20	-0.3(5)
C17-C18-C19-C20	169.0(4)
C18-C19-C20-C21	0.0(5)
C18-N5-C21-C22	179.7(4)
Fe2-N5-C21-C22	-13.5(5)
C18-N5-C21-C20	-0.4(5)
Fe2-N5-C21-C20	166.3(3)
C19-C20-C21-C22	-179.9(5)
C19-C20-C21-N5	0.2(5)
C23-N6-C22-C21	178.3(4)
Fe2-N6-C22-C21	11.9(5)
N5-C21-C22-N6	2.3(6)
C20-C21-C22-N6	-177.5(4)
C22-N6-C23-C28	-154.1(4)
Fe2-N6-C23-C28	11.1(5)
C22-N6-C23-C24	23.2(7)
Fe2-N6-C23-C24	-171.6(3)
C28-C23-C24-C25	1.4(7)
N6-C23-C24-C25	-175.8(4)
C23-C24-C25-O45	-178.9(4)
C23-C24-C25-C26	-0.7(7)
O45-C25-C26-O43	-1.1(6)
C24-C25-C26-O43	-179.4(4)
O45-C25-C26-C27	177.0(4)
C24-C25-C26-C27	-1.3(7)
O43-C26-C27-C28	-179.4(5)
C25-C26-C27-C28	2.8(7)
C24-C23-C28-C27	0.1(7)
N6-C23-C28-C27	177.5(4)
C24-C23-C28-N7	179.8(4)
N6-C23-C28-N7	-2.8(6)
C26-C27-C28-C23	-2.1(7)
C26-C27-C28-N7	178.1(4)
C29-N7-C28-C23	155.8(4)
Fe2A-N7-C28-C23	-11.8(9)
Fe2-N7-C28-C23	-4.8(5)
C29-N7-C28-C27	-24.5(6)
Fe2A-N7-C28-C27	168.0(6)
Fe2-N7-C28-C27	174.9(4)
C28-N7-C29-C30	173.2(4)
Fe2A-N7-C29-C30	-14.5(6)
Fe2-N7-C29-C30	-30.1(6)
C28-N7-C29-Fe2A	-172.3(5)
Fe2-Fe2A-C29-N7	31.2(7)
O1-Fe2A-C29-N7	-79.4(8)
N8-Fe2A-C29-N7	-155.9(5)
N7-Fe2A-C29-C30	167.7(5)
O1-Fe2A-C29-C30	88.3(8)
N8-Fe2A-C29-C30	11.8(3)
C33-N8-C30-C31	-0.6(5)
Fe2A-N8-C30-C31	-157.7(4)
C33-N8-C30-C29	179.4(4)
Fe2A-N8-C30-C29	22.2(5)
N7-C29-C30-N8	-9.8(7)
N7-C29-C30-C31	170.1(4)
C30-C31-C32-C33	-0.7(5)
C30-N8-C33-C32	0.1(5)
Fe2A-N8-C33-C32	126.2(8)
C30-N8-C33-C34	175.9(4)
Fe2A-N8-C33-C34	-58.0(10)
C31-C32-C33-N8	0.4(5)
C31-C32-C33-C34	-174.7(5)
N8-C33-C34-C1	-65.1(5)
C32-C33-C34-C1	109.5(6)
N8-C33-C34-C42	176.4(4)
C32-C33-C34-C42	-9.0(8)
N8-C33-C34-C41	55.3(6)
C32-C33-C34-C41	-130.1(5)
N1-C1-C34-C33	70.8(6)
C2-C1-C34-C33	-99.1(5)
N1-C1-C34-C42	-170.1(5)
C2-C1-C34-C42	19.9(7)
N1-C1-C34-C41	-49.2(7)
C2-C1-C34-C41	140.9(5)
C10-C9-O37-C38	5.7(8)
C8-C9-O37-C38	-176.3(6)
C7-C8-O39-C40A	30.6(14)
C9-C8-O39-C40A	-149.1(11)
C7-C8-O39-C40	78.5(12)
C9-C8-O39-C40	-101.3(10)
C27-C26-O43-C44	-3.5(7)
C25-C26-O43-C44	174.4(4)
C24-C25-O45-C46	3.3(6)
C26-C25-O45-C46	-174.9(4)
C5A-O1A-C2A-C3A	-6.8(6)
O1A-C2A-C3A-C4A	28.3(5)
C2A-C3A-C4A-C5A	-37.5(5)
C2A-O1A-C5A-C4A	-18.1(6)
C3A-C4A-C5A-O1A	34.4(6)
C5B-O1B-C2B-C3B	-1.0(6)
O1B-C2B-C3B-C4B	21.6(6)
C2B-C3B-C4B-C5B	-32.4(5)
C2B-O1B-C5B-C4B	-20.3(6)
C3B-C4B-C5B-O1B	32.7(5)
C5C-O1C-C2C-C3C	19.0(12)
O1C-C2C-C3C-C4C	-24.6(12)
C2C-C3C-C4C-C5C	20.0(13)
C2C-O1C-C5C-C4C	-6.3(12)
C3C-C4C-C5C-O1C	-8.9(13)
C5D-O1D-C2D-C3D	-20(2)
O1D-C2D-C3D-C4D	0(2)
C2D-C3D-C4D-C5D	19(2)
C2D-O1D-C5D-C4D	31.9(18)
C3D-C4D-C5D-O1D	-31.9(19)

Figure SE1. View of **10** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. The hydrogen atoms have been removed for clarity.

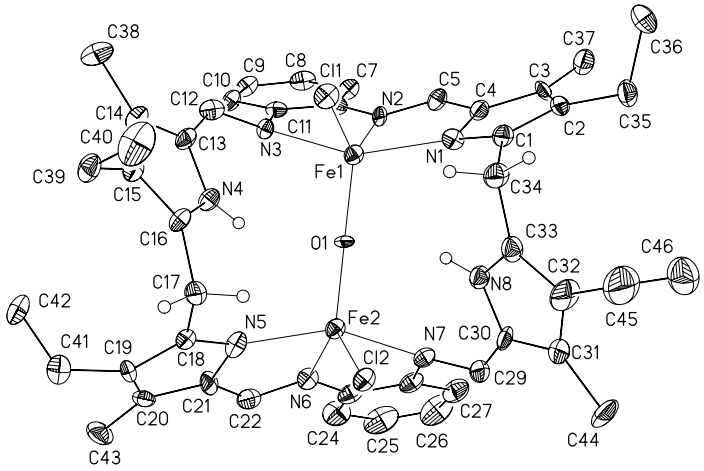

Figure SE2. Unit cell packing diagram for **10**. The view is approximately down the **b** axis. There are columnar shaped voids that lie near 0, y, ¼ in which the disordered n-hexane solvate molecules reside.

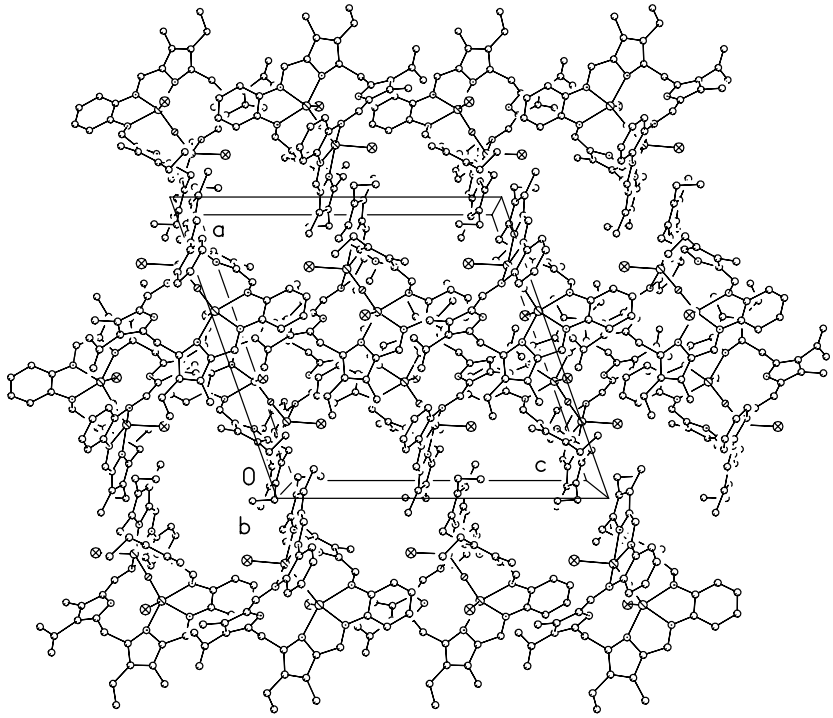

Table SE1. Crystal data and structure refinement for **10**.

Empirical formula	C49 H57 Cl2 Fe2 N8 O	
Formula weight	956.63	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 17.8779(6) Å	α= 90°.
	b = 15.3460(7) Å	β= 109.606(3)°.
	c = 18.5817(8) Å	γ = 90°.
Volume	4802.4(3) $Å^3$	
Z	4	
Density (calculated)	1.323 Mg/m^3	
Absorption coefficient	0.760 mm^{-1}	
F(000)	2004	
Crystal size	0.30 x 0.25 x 0.11 mm	
Theta range for data collection	2.92 to 25.00°.	
Index ranges	-21<=h<=21, -18<=k<=18, -22<=l<=21	
Reflections collected	15560	
Independent reflections	8382 [R(int) = 0.0860]	
Completeness to theta = 25.00°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8382 / 20 / 542	
Goodness-of-fit on F^2	1.994	
Final R indices [I>2sigma(I)]	R1 = 0.1066, wR2 = 0.1500	
R indices (all data)	R1 = 0.1731, wR2 = 0.1568	
Extinction coefficient	$2.9(3)x10^{-6}$	
Largest diff. peak and hole	0.946 and -0.706 $e.Å^{-3}$	

Table SE2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe1	1241(1)	1881(1)	4983(1)	28(1)
Fe2	2761(1)	698(1)	4482(1)	29(1)
Cl1	1108(1)	3288(1)	4592(1)	34(1)
Cl2	2831(1)	1059(1)	3322(1)	30(1)
O1	2004(3)	1272(2)	4750(2)	26(1)
N1	182(3)	1521(3)	4136(3)	30(1)
N2	629(3)	1300(3)	5611(2)	25(1)
N3	1891(3)	2241(3)	6188(3)	24(1)
N4	2959(3)	2858(3)	5510(3)	31(2)
N5	3819(4)	1359(3)	5045(3)	39(2)
N6	3466(4)	-252(3)	5155(3)	32(2)
N7	2127(3)	-542(3)	4054(3)	32(2)
N8	1010(3)	660(3)	3172(3)	34(2)
C1	-258(4)	1666(4)	3396(3)	31(2)
C2	-1044(4)	1380(4)	3204(3)	30(2)
C3	-1115(4)	1032(4)	3858(4)	29(2)
C4	-360(4)	1139(4)	4423(3)	32(2)
C5	-92(4)	1020(4)	5236(3)	32(2)

C6	944(4)	1275(4)	6412(4)	32(2)
C7	642(4)	802(4)	6899(3)	35(2)
C8	1038(5)	857(4)	7695(4)	39(2)
C9	1702(5)	1362(4)	7986(4)	36(2)
C10	1996(4)	1829(4)	7529(3)	32(2)
C11	1611(4)	1801(4)	6728(3)	29(2)
C12	2265(4)	2978(4)	6412(3)	35(2)
C13	2725(4)	3356(4)	6012(3)	32(2)
C14	3004(4)	4210(4)	5976(3)	33(2)
C15	3379(4)	4203(4)	5422(3)	34(2)
C16	3341(4)	3356(4)	5151(3)	33(2)
C17	3708(4)	2914(4)	4612(4)	37(2)
C18	4195(4)	2136(4)	5030(4)	33(2)
C19	4985(4)	2121(5)	5477(4)	37(2)
C20	5146(5)	1290(5)	5791(4)	42(2)
C21	4424(4)	821(5)	5506(4)	36(2)
C22	4216(5)	-20(5)	5551(4)	40(2)
C23	3186(5)	-1116(4)	5136(4)	40(2)
C24	3533(5)	-1780(5)	5666(4)	56(2)
C25	3143(7)	-2580(5)	5598(6)	77(3)
C26	2451(7)	-2725(5)	5031(6)	77(3)
C27	2080(5)	-2083(4)	4485(4)	53(2)
C28	2466(5)	-1261(4)	4539(4)	41(2)
C29	1699(4)	-705(5)	3342(4)	40(2)
C30	1222(4)	-91(5)	2878(4)	37(2)
C31	848(5)	-32(6)	2082(4)	56(2)
C32	423(5)	763(6)	1928(4)	66(3)
C33	543(4)	1176(5)	2628(4)	38(2)
C34	172(5)	1972(4)	2845(3)	42(2)
C35	-1687(4)	1432(4)	2443(4)	44(2)
C36	-2336(4)	2061(4)	2419(4)	48(2)
C37	-1821(5)	619(5)	3957(4)	49(2)
C38	2894(5)	4974(4)	6421(4)	50(2)
C39	3694(5)	4981(4)	5120(4)	41(2)
C40	3090(6)	5297(5)	4375(4)	76(3)
C41	5541(5)	2890(5)	5646(4)	63(3)
C42	5521(5)	3396(5)	6347(5)	85(3)
C43	5916(4)	951(5)	6358(4)	59(2)
C44	888(6)	-697(6)	1502(4)	90(3)
C45	-70(6)	1120(7)	1129(6)	117(4)
C46	-670(8)	834(8)	730(6)	74(4)
C46A	63(15)	1675(14)	808(11)	67(9)

Table SE3. Bond lengths [Å] and angles [°] for **10**.

Fe1-O1	1.821(4)	Fe2-N7	2.221(5)
Fe1-N2	2.053(5)	Fe2-Cl2	2.2685(17)
Fe1-N1	2.090(5)	N1-C1	1.353(7)
Fe1-N3	2.218(5)	N1-C4	1.384(8)
Fe1-Cl1	2.2656(18)	N2-C5	1.314(8)
Fe2-O1	1.819(4)	N2-C6	1.404(7)
Fe2-N6	2.055(5)	N3-C12	1.308(7)
Fe2-N5	2.092(6)	N3-C11	1.431(7)

N4-C16	1.343(8)	C26-C27	1.411(10)
N4-C13	1.374(7)	C26-H26	0.96
N4-H4N	0.8999	C27-C28	1.425(9)
N5-C18	1.374(8)	C27-H27	0.96
N5-C21	1.401(8)	C29-C30	1.365(9)
N6-C22	1.343(8)	C29-H29	0.96
N6-C23	1.414(8)	C30-C31	1.407(9)
N7-C29	1.311(7)	C31-C32	1.414(10)
N7-C28	1.424(8)	C31-C44	1.504(9)
N8-C33	1.335(8)	C32-C33	1.396(9)
N8-C30	1.382(8)	C32-C45	1.550(12)
N8-H8N	0.8999	C33-C34	1.509(9)
C1-C2	1.399(9)	C34-H34A	0.96
C1-C34	1.546(9)	C34-H34B	0.96
C2-C3	1.372(8)	C35-C36	1.498(9)
C2-C35	1.495(8)	C35-H35A	0.96
C3-C4	1.414(9)	C35-H35B	0.96
C3-C37	1.478(9)	C36-H36A	0.96
C4-C5	1.435(8)	C36-H36B	0.96
C5-H5	0.96	C36-H36C	0.96
C6-C11	1.396(9)	C37-H37A	0.96
C6-C7	1.402(8)	C37-H37B	0.9603
C7-C8	1.411(8)	C37-H37C	0.96
C7-H7	0.96	C38-H37A	0.96
C8-C9	1.369(9)	C38-H37B	0.9603
C8-H8	0.96	C38-H37C	0.96
C9-C10	1.345(8)	C39-C40	1.522(9)
C9-H9	0.96	C39-H39A	0.96
C10-C11	1.416(8)	C39-H39B	0.96
C10-H10	0.96	C40-H40A	0.96
C12-C13	1.406(9)	C40-H40B	0.96
C12-H12	0.96	C40-H40C	0.96
C13-C14	1.411(8)	C41-C42	1.527(9)
C14-C15	1.405(9)	C41-H41A	0.96
C14-C38	1.484(8)	C41-H41B	0.96
C15-C16	1.387(8)	C42-H42A	0.96
C15-C39	1.508(8)	C42-H42B	0.96
C16-C17	1.528(8)	C42-H42C	0.96
C17-C18	1.527(8)	C43-H43A	0.96
C17-H17A	0.96	C43-H43B	0.96
C17-H17B	0.96	C43-H43C	0.96
C18-C19	1.378(9)	C44-H44A	0.96
C19-C20	1.392(9)	C44-H44B	0.96
C19-C41	1.506(9)	C44-H44C	0.96
C20-C21	1.417(9)	C45-C46A	1.110(12)
C20-C43	1.517(9)	C45-C46	1.166(11)
C21-C22	1.353(9)	C45-H46E	1.5280
C22-H22	0.96	C46-C46A	1.81(3)
C23-C28	1.407(9)	C46-H46A	0.96
C23-C24	1.408(9)	C46-H46B	0.96
C24-C25	1.397(11)	C46-H46C	0.96
C24-H24	0.96	C46A-H46D	0.96
C25-C26	1.347(12)	C46A-H46E	0.96
C25-H25	0.96	C46A-H46F	0.96

O1-Fe1-N2	119.80(19)	O1-Fe1-N1	104.29(19)

N2-Fe1-N1	78.0(2)	N2-C5-H5	122.3
O1-Fe1-N3	100.78(19)	C4-C5-H5	121.7
N2-Fe1-N3	74.52(19)	C11-C6-C7	119.2(6)
N1-Fe1-N3	149.5(2)	C11-C6-N2	114.3(6)
O1-Fe1-Cl1	114.79(14)	C7-C6-N2	126.4(6)
N2-Fe1-Cl1	125.31(15)	C6-C7-C8	118.6(7)
N1-Fe1-Cl1	92.26(14)	C6-C7-H7	120.7
N3-Fe1-Cl1	92.85(13)	C8-C7-H7	120.7
O1-Fe2-N6	122.5(2)	C9-C8-C7	120.8(6)
O1-Fe2-N5	105.0(2)	C9-C8-H8	119.4
N6-Fe2-N5	76.8(2)	C7-C8-H8	119.9
O1-Fe2-N7	100.18(19)	C10-C9-C8	121.5(6)
N6-Fe2-N7	75.2(2)	C10-C9-H9	119.7
N5-Fe2-N7	149.5(2)	C8-C9-H9	118.8
O1-Fe2-Cl2	115.19(13)	C9-C10-C11	119.5(7)
N6-Fe2-Cl2	122.25(16)	C9-C10-H10	120.9
N5-Fe2-Cl2	91.59(15)	C11-C10-H10	119.5
N7-Fe2-Cl2	93.06(13)	C6-C11-C10	120.3(6)
Fe2-O1-Fe1	177.4(2)	C6-C11-N3	115.4(5)
C1-N1-C4	102.5(6)	C10-C11-N3	124.2(6)
C1-N1-Fe1	142.4(5)	N3-C12-C13	121.1(6)
C4-N1-Fe1	113.4(4)	N3-C12-H12	120.3
C5-N2-C6	121.8(6)	C13-C12-H12	118.6
C5-N2-Fe1	117.1(4)	N4-C13-C12	119.6(6)
C6-N2-Fe1	120.9(4)	N4-C13-C14	107.0(6)
C12-N3-C11	116.5(5)	C12-C13-C14	133.4(6)
C12-N3-Fe1	125.1(4)	C15-C14-C13	106.9(6)
C11-N3-Fe1	113.7(4)	C15-C14-C38	126.8(6)
C16-N4-C13	110.0(5)	C13-C14-C38	126.3(6)
C16-N4-H4N	124.9	C16-C15-C14	107.2(6)
C13-N4-H4N	125.0	C16-C15-C39	125.9(6)
C18-N5-C21	104.0(6)	C14-C15-C39	126.6(6)
C18-N5-Fe2	141.0(5)	N4-C16-C15	108.9(6)
C21-N5-Fe2	113.8(4)	N4-C16-C17	118.4(5)
C22-N6-C23	122.8(6)	C15-C16-C17	132.4(7)
C22-N6-Fe2	116.2(4)	C18-C17-C16	108.1(5)
C23-N6-Fe2	120.7(5)	C18-C17-H17A	110.8
C29-N7-C28	118.2(6)	C16-C17-H17A	110.5
C29-N7-Fe2	125.4(4)	C18-C17-H17B	109.5
C28-N7-Fe2	112.3(4)	C16-C17-H17B	109.2
C33-N8-C30	112.4(6)	H17A-C17-H17B	108.7
C33-N8-H8N	123.8	N5-C18-C19	112.5(6)
C30-N8-H8N	123.8	N5-C18-C17	119.3(6)
N1-C1-C2	113.6(6)	C19-C18-C17	127.9(6)
N1-C1-C34	118.3(6)	C18-C19-C20	107.1(6)
C2-C1-C34	127.3(6)	C18-C19-C41	125.7(7)
C3-C2-C1	106.3(6)	C20-C19-C41	127.0(7)
C3-C2-C35	126.0(7)	C19-C20-C21	106.0(6)
C1-C2-C35	127.8(6)	C19-C20-C43	128.0(7)
C2-C3-C4	105.2(6)	C21-C20-C43	125.9(7)
C2-C3-C37	127.9(6)	C22-C21-N5	115.4(7)
C4-C3-C37	126.8(6)	C22-C21-C20	134.1(7)
N1-C4-C3	112.4(6)	N5-C21-C20	110.4(6)
N1-C4-C5	115.4(6)	N6-C22-C21	117.6(6)
C3-C4-C5	131.7(7)	N6-C22-H22	120.9
N2-C5-C4	116.0(6)	C21-C22-H22	121.5

C28-C23-C24	120.6(7)	H37B-C37-H37C	109.4
C28-C23-N6	113.0(6)	C14-C38-H37A	109.6
C24-C23-N6	126.3(7)	C14-C38-H37B	109.2
C25-C24-C23	118.9(8)	H37A-C38-H37B	109.5
C25-C24-H24	121.9	C14-C38-H37C	109.6
C23-C24-H24	119.2	H37A-C38-H37C	109.5
C26-C25-C24	121.0(8)	H37B-C38-H37C	109.4
C26-C25-H25	118.9	C15-C39-C40	110.6(6)
C24-C25-H25	120.1	C15-C39-H39A	111.1
C25-C26-C27	122.3(8)	C40-C39-H39A	109.6
C25-C26-H26	118.7	C15-C39-H39B	108.7
C27-C26-H26	119.1	C40-C39-H39B	108.3
C26-C27-C28	117.9(8)	H39A-C39-H39B	108.5
C26-C27-H27	122.0	C39-C40-H40A	111.8
C28-C27-H27	120.1	C39-C40-H40B	107.6
C23-C28-C27	119.3(7)	H40A-C40-H40B	109.5
C23-C28-N7	117.3(6)	C39-C40-H40C	109.0
C27-C28-N7	123.2(7)	H40A-C40-H40C	109.5
N7-C29-C30	122.4(6)	H40B-C40-H40C	109.5
N7-C29-H29	118.3	C19-C41-C42	111.9(7)
C30-C29-H29	119.3	C19-C41-H41A	109.9
C29-C30-N8	121.4(6)	C42-C41-H41A	109.0
C29-C30-C31	133.3(7)	C19-C41-H41B	108.4
N8-C30-C31	105.3(7)	C42-C41-H41B	109.2
C30-C31-C32	107.6(6)	H41A-C41-H41B	108.4
C30-C31-C44	126.1(8)	C41-C42-H42A	111.3
C32-C31-C44	126.3(7)	C41-C42-H42B	108.6
C33-C32-C31	107.4(6)	H42A-C42-H42B	109.5
C33-C32-C45	126.2(8)	C41-C42-H42C	108.5
C31-C32-C45	126.3(7)	H42A-C42-H42C	109.5
N8-C33-C32	107.3(7)	H42B-C42-H42C	109.5
N8-C33-C34	119.8(6)	C20-C43-H43A	108.7
C32-C33-C34	132.3(7)	C20-C43-H43B	109.0
C33-C34-C1	107.0(5)	H43A-C43-H43B	109.5
C33-C34-H34A	110.8	C20-C43-H43C	110.7
C1-C34-H34A	110.1	H43A-C43-H43C	109.5
C33-C34-H34B	110.1	H43B-C43-H43C	109.5
C1-C34-H34B	110.0	C31-C44-H44A	111.1
H34A-C34-H34B	108.9	C31-C44-H44B	108.8
C2-C35-C36	113.8(6)	H44A-C44-H44B	109.5
C2-C35-H35A	109.0	C31-C44-H44C	108.4
C36-C35-H35A	108.6	H44A-C44-H44C	109.5
C2-C35-H35B	108.8	H44B-C44-H44C	109.5
C36-C35-H35B	108.6	C46A-C45-C46	105.4(18)
H35A-C35-H35B	107.8	C46A-C45-C32	129.1(12)
C35-C36-H36A	110.4	C46-C45-C32	125.5(10)
C35-C36-H36B	109.0	C45-C46-H46A	118.0
H36A-C36-H36B	109.5	C45-C46-H46B	104.7
C35-C36-H36C	109.0	C46A-C46-H46B	121.1
H36A-C36-H36C	109.5	H46A-C46-H46B	109.5
H36B-C36-H36C	109.5	C45-C46-H46C	105.4
C3-C37-H37A	109.4	C46A-C46-H46C	120.8
C3-C37-H37B	109.7	H46A-C46-H46C	109.5
H37A-C37-H37B	109.5	H46B-C46-H46C	109.5
C3-C37-H37C	109.3	C45-C46A-H46D	123.1
H37A-C37-H37C	109.5	C46-C46A-H46E	108.5

H46D-C46A-H46E	109.5	H46D-C46A-H46F	109.5
C45-C46A-H46F	109.2	H46E-C46A-H46F	109.5

Table SE4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe1	32(1)	30(1)	21(1)	1(1)	8(1)	1(1)
Fe2	33(1)	27(1)	25(1)	0(1)	8(1)	1(1)
Cl1	47(1)	31(1)	24(1)	10(1)	9(1)	4(1)
Cl2	40(1)	30(1)	20(1)	3(1)	10(1)	0(1)
O1	23(3)	31(2)	28(2)	-8(2)	13(2)	8(2)
N1	32(4)	34(3)	25(3)	8(3)	11(3)	3(3)
N2	27(4)	32(3)	10(3)	-2(2)	0(3)	-2(3)
N3	30(4)	22(3)	24(3)	1(3)	11(3)	-7(3)
N4	42(4)	20(3)	30(3)	0(3)	13(3)	-3(3)
N5	52(5)	33(3)	30(3)	-4(3)	10(3)	-8(3)
N6	39(5)	27(3)	25(3)	7(3)	4(3)	7(3)
N7	40(4)	32(3)	26(3)	-2(3)	15(3)	1(3)
N8	34(4)	39(3)	26(3)	-3(3)	7(3)	-2(3)
C1	35(5)	36(4)	22(4)	0(3)	8(4)	2(4)
C2	25(5)	36(4)	24(4)	-1(3)	3(3)	6(4)
C3	12(4)	30(4)	42(4)	-1(3)	4(4)	-2(3)
C4	36(5)	31(4)	27(4)	-5(3)	7(4)	2(4)
C5	43(5)	26(4)	27(4)	-2(3)	12(4)	-6(4)
C6	31(5)	34(4)	35(4)	8(4)	17(4)	2(4)
C7	45(5)	31(4)	31(4)	0(3)	16(4)	-2(4)
C8	58(6)	36(4)	33(4)	12(4)	27(4)	9(4)
C9	56(6)	27(4)	25(4)	3(3)	14(4)	4(4)
C10	43(5)	31(4)	20(4)	-2(3)	9(3)	-3(4)
C11	32(5)	24(4)	38(4)	2(3)	21(4)	4(4)
C12	43(5)	37(4)	26(4)	6(4)	12(4)	12(4)
C13	42(5)	32(4)	18(4)	-5(3)	5(4)	3(4)
C14	47(5)	25(4)	28(4)	-3(3)	13(4)	-3(4)
C15	39(5)	28(4)	34(4)	-3(3)	8(4)	-3(4)
C16	45(5)	30(4)	24(4)	-7(3)	11(4)	-3(4)
C17	32(5)	35(4)	44(4)	-4(4)	14(4)	-5(4)
C18	33(5)	30(4)	37(4)	-10(3)	13(4)	-3(4)
C19	18(5)	42(5)	49(5)	-14(4)	7(4)	-7(4)
C20	25(5)	61(5)	40(4)	-16(4)	11(4)	10(4)
C21	24(5)	42(5)	27(4)	1(4)	-8(3)	5(4)
C22	42(6)	47(5)	26(4)	0(4)	5(4)	17(4)
C23	60(6)	27(4)	38(4)	0(4)	21(4)	8(4)
C24	67(7)	35(5)	61(5)	13(4)	16(5)	18(5)
C25	125(11)	31(5)	79(7)	13(5)	42(7)	20(6)
C26	132(11)	22(5)	81(7)	7(5)	42(7)	0(6)
C27	71(7)	29(4)	62(5)	-7(4)	28(5)	-3(4)
C28	56(6)	22(4)	48(5)	-6(4)	20(4)	5(4)
C29	33(5)	43(5)	46(5)	-14(4)	15(4)	-10(4)
C30	37(5)	47(5)	25(4)	-19(4)	6(4)	-12(4)
C31	38(6)	86(7)	39(5)	-26(5)	5(4)	3(5)

C32	80(8)	90(7)	18(4)	-2(5)	4(4)	21(6)
C33	34(5)	53(5)	27(4)	-2(4)	9(4)	-6(4)
C34	48(6)	47(5)	28(4)	1(4)	9(4)	8(4)
C35	36(6)	46(5)	38(4)	-3(4)	-4(4)	1(4)
C36	35(5)	54(5)	48(5)	15(4)	5(4)	6(4)
C37	51(6)	51(5)	40(4)	-10(4)	7(4)	-4(5)
C38	75(7)	37(4)	50(5)	-2(4)	37(5)	7(4)
C39	51(6)	30(4)	45(4)	-6(4)	20(4)	-14(4)
C40	117(10)	44(5)	59(6)	15(5)	20(6)	-10(5)
C41	48(6)	60(5)	77(6)	-23(5)	15(5)	-11(5)
C42	70(8)	84(7)	103(7)	-68(6)	30(6)	-28(6)
C43	28(5)	91(6)	51(5)	-8(5)	4(4)	15(5)
C44	84(8)	123(8)	44(5)	-53(5)	-1(5)	29(6)
C45	109(8)	149(8)	63(6)	-23(6)	-12(5)	52(7)
C46	61(8)	82(7)	75(7)	-2(6)	20(6)	-15(7)
C46A	58(12)	66(11)	71(12)	14(8)	12(9)	-20(9)

Table SE5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10**.

	x	y	z	U(eq)
H4N	2867	2284	5432	37
H8N	1168	786	3673	40
H5	-423	756	5489	38
H7	180	441	6696	41
H8	840	539	8038	47
H9	1961	1382	8530	43
H10	2460	2184	7738	38
H12	2227	3273	6854	42
H17A	3301	2730	4153	44
H17B	4050	3319	4480	44
H22	4590	-439	5852	48
H24	4031	-1671	6062	67
H25	3369	-3039	5956	92
H26	2199	-3282	5005	92
H27	1584	-2187	4084	63
H29	1725	-1277	3144	48
H34A	-200	2239	2401	50
H34B	576	2389	3096	50
H35A	-1458	1601	2065	53
H35B	-1916	863	2310	53
H36A	-2732	2067	1920	72
H36B	-2112	2633	2542	72
H36C	-2575	1887	2789	72
H37A	-2254	634	3482	74
H37B	-1968	927	4340	74
H37C	-1701	24	4115	74
H37A	3145	5475	6293	75
H37B	3131	4852	6956	75
H37C	2338	5086	6303	75
H39A	3825	5448	5485	49

H39B	4168	4812	5021	49
H40A	3286	5784	4166	113
H40B	2620	5467	4480	113
H40C	2965	4827	4013	113
H41A	6074	2695	5731	76
H41B	5386	3269	5210	76
H42A	5870	3890	6445	128
H42B	5679	3014	6780	128
H42C	4987	3591	6257	128
H43A	6309	1403	6457	88
H43B	6090	455	6142	88
H43C	5842	785	6828	88
H44A	584	-515	993	134
H44B	684	-1240	1613	134
H44C	1434	-769	1540	134
H46A	-921	1111	246	110
H46B	-1016	858	1028	110
H46C	-559	236	650	110
H46D	-290	1861	318	101
H46E	525	1410	749	101
H46F	220	2170	1141	101

Table SE6. Torsion angles [°] for **10**.

N6-Fe2-O1-Fe1	171(6)	N2-Fe1-N3-C11	7.7(4)
N5-Fe2-O1-Fe1	87(6)	N1-Fe1-N3-C11	34.3(6)
N7-Fe2-O1-Fe1	-110(6)	Cl1-Fe1-N3-C11	133.6(4)
Cl2-Fe2-O1-Fe1	-12(6)	O1-Fe2-N5-C18	-70.6(7)
N2-Fe1-O1-Fe2	158(6)	N6-Fe2-N5-C18	168.9(7)
N1-Fe1-O1-Fe2	74(6)	N7-Fe2-N5-C18	144.8(6)
N3-Fe1-O1-Fe2	-124(6)	Cl2-Fe2-N5-C18	46.0(7)
Cl1-Fe1-O1-Fe2	-26(6)	O1-Fe2-N5-C21	124.8(5)
O1-Fe1-N1-C1	-77.8(7)	N6-Fe2-N5-C21	4.3(4)
N2-Fe1-N1-C1	164.2(7)	N7-Fe2-N5-C21	-19.8(7)
N3-Fe1-N1-C1	138.0(7)	Cl2-Fe2-N5-C21	-118.5(4)
Cl1-Fe1-N1-C1	38.5(7)	O1-Fe2-N6-C22	-103.9(5)
O1-Fe1-N1-C4	120.7(4)	N5-Fe2-N6-C22	-4.3(5)
N2-Fe1-N1-C4	2.6(4)	N7-Fe2-N6-C22	163.3(5)
N3-Fe1-N1-C4	-23.5(6)	Cl2-Fe2-N6-C22	79.1(5)
Cl1-Fe1-N1-C4	-123.0(4)	O1-Fe2-N6-C23	82.0(5)
O1-Fe1-N2-C5	-101.9(5)	N5-Fe2-N6-C23	-178.5(5)
N1-Fe1-N2-C5	-2.2(5)	N7-Fe2-N6-C23	-10.8(5)
N3-Fe1-N2-C5	164.4(5)	Cl2-Fe2-N6-C23	-95.0(5)
Cl1-Fe1-N2-C5	82.0(5)	O1-Fe2-N7-C29	92.1(6)
O1-Fe1-N2-C6	83.5(5)	N6-Fe2-N7-C29	-146.7(6)
N1-Fe1-N2-C6	-176.8(5)	N5-Fe2-N7-C29	-122.5(6)
N3-Fe1-N2-C6	-10.2(4)	Cl2-Fe2-N7-C29	-24.1(6)
Cl1-Fe1-N2-C6	-92.6(5)	O1-Fe2-N7-C28	-111.3(4)
O1-Fe1-N3-C12	94.8(6)	N6-Fe2-N7-C28	9.8(4)
N2-Fe1-N3-C12	-147.0(6)	N5-Fe2-N7-C28	34.0(6)
N1-Fe1-N3-C12	-120.4(6)	Cl2-Fe2-N7-C28	132.4(4)
Cl1-Fe1-N3-C12	-21.1(5)	C4-N1-C1-C2	-1.1(7)
O1-Fe1-N3-C11	-110.5(4)	Fe1-N1-C1-C2	-163.8(5)

C4-N1-C1-C34	-171.3(5)	C13-N4-C16-C17	175.3(6)
Fe1-N1-C1-C34	26.0(10)	C14-C15-C16-N4	0.4(8)
N1-C1-C2-C3	0.2(8)	C39-C15-C16-N4	-174.2(6)
C34-C1-C2-C3	169.3(6)	C14-C15-C16-C17	-172.9(7)
N1-C1-C2-C35	-179.6(6)	C39-C15-C16-C17	12.5(12)
C34-C1-C2-C35	-10.4(11)	N4-C16-C17-C18	-49.2(8)
C1-C2-C3-C4	0.9(7)	C15-C16-C17-C18	123.6(8)
C35-C2-C3-C4	-179.4(6)	C21-N5-C18-C19	-2.4(8)
C1-C2-C3-C37	-178.3(6)	Fe2-N5-C18-C19	-167.9(5)
C35-C2-C3-C37	1.4(11)	C21-N5-C18-C17	-176.5(6)
C1-N1-C4-C3	1.7(7)	Fe2-N5-C18-C17	18.1(10)
Fe1-N1-C4-C3	170.3(4)	C16-C17-C18-N5	83.0(7)
C1-N1-C4-C5	-171.4(5)	C16-C17-C18-C19	-90.0(8)
Fe1-N1-C4-C5	-2.8(7)	N5-C18-C19-C20	1.3(8)
C2-C3-C4-N1	-1.6(7)	C17-C18-C19-C20	174.7(6)
C37-C3-C4-N1	177.6(6)	N5-C18-C19-C41	-173.5(6)
C2-C3-C4-C5	170.0(6)	C17-C18-C19-C41	-0.1(12)
C37-C3-C4-C5	-10.8(12)	C18-C19-C20-C21	0.3(8)
C6-N2-C5-C4	175.8(5)	C41-C19-C20-C21	175.1(7)
Fe1-N2-C5-C4	1.3(7)	C18-C19-C20-C43	-176.3(7)
N1-C4-C5-N2	1.1(8)	C41-C19-C20-C43	-1.5(12)
C3-C4-C5-N2	-170.4(6)	C18-N5-C21-C22	-173.9(6)
C5-N2-C6-C11	-163.3(6)	Fe2-N5-C21-C22	-3.8(8)
Fe1-N2-C6-C11	11.1(7)	C18-N5-C21-C20	2.6(7)
C5-N2-C6-C7	14.9(10)	Fe2-N5-C21-C20	172.7(4)
Fe1-N2-C6-C7	-170.8(5)	C19-C20-C21-C22	173.7(8)
C11-C6-C7-C8	-1.8(9)	C43-C20-C21-C22	-9.6(13)
N2-C6-C7-C8	-179.8(6)	C19-C20-C21-N5	-1.9(8)
C6-C7-C8-C9	0.2(10)	C43-C20-C21-N5	174.9(6)
C7-C8-C9-C10	0.7(11)	C23-N6-C22-C21	177.8(6)
C8-C9-C10-C11	0.1(10)	Fe2-N6-C22-C21	3.7(8)
C7-C6-C11-C10	2.6(10)	N5-C21-C22-N6	0.1(10)
N2-C6-C11-C10	-179.1(6)	C20-C21-C22-N6	-175.3(7)
C7-C6-C11-N3	178.4(5)	C22-N6-C23-C28	-164.0(6)
N2-C6-C11-N3	-3.4(8)	Fe2-N6-C23-C28	9.8(8)
C9-C10-C11-C6	-1.7(10)	C22-N6-C23-C24	19.9(11)
C9-C10-C11-N3	-177.1(6)	Fe2-N6-C23-C24	-166.3(6)
C12-N3-C11-C6	152.3(6)	C28-C23-C24-C25	-1.1(11)
Fe1-N3-C11-C6	-4.6(7)	N6-C23-C24-C25	174.7(7)
C12-N3-C11-C10	-32.1(9)	C23-C24-C25-C26	0.9(13)
Fe1-N3-C11-C10	171.0(5)	C24-C25-C26-C27	-0.7(15)
C11-N3-C12-C13	164.6(6)	C25-C26-C27-C28	0.8(14)
Fe1-N3-C12-C13	-41.3(9)	C24-C23-C28-C27	1.2(11)
C16-N4-C13-C12	175.6(6)	N6-C23-C28-C27	-175.1(6)
C16-N4-C13-C14	-1.9(8)	C24-C23-C28-N7	176.3(6)
N3-C12-C13-N4	-17.1(10)	N6-C23-C28-N7	0.0(9)
N3-C12-C13-C14	159.6(7)	C26-C27-C28-C23	-1.0(11)
N4-C13-C14-C15	2.1(8)	C26-C27-C28-N7	-175.8(7)
C12-C13-C14-C15	-174.9(7)	C29-N7-C28-C23	150.1(7)
N4-C13-C14-C38	-179.9(6)	Fe2-N7-C28-C23	-8.3(8)
C12-C13-C14-C38	3.1(13)	C29-N7-C28-C27	-35.0(10)
C13-C14-C15-C16	-1.5(8)	Fe2-N7-C28-C27	166.6(5)
C38-C14-C15-C16	-179.6(7)	C28-N7-C29-C30	166.5(7)
C13-C14-C15-C39	173.0(6)	Fe2-N7-C29-C30	-38.2(10)
C38-C14-C15-C39	-5.0(12)	N7-C29-C30-N8	-16.2(11)
C13-N4-C16-C15	0.9(8)	N7-C29-C30-C31	164.2(8)

C33-N8-C30-C29	-180.0(7)
C33-N8-C30-C31	-0.3(8)
C29-C30-C31-C32	179.7(8)
N8-C30-C31-C32	0.1(9)
C29-C30-C31-C44	0.2(15)
N8-C30-C31-C44	-179.4(8)
C30-C31-C32-C33	0.1(10)
C44-C31-C32-C33	179.6(8)
C30-C31-C32-C45	178.7(7)
C44-C31-C32-C45	-1.8(14)
C30-N8-C33-C32	0.4(9)
C30-N8-C33-C34	172.7(6)
C31-C32-C33-N8	-0.3(9)
C45-C32-C33-N8	-178.9(7)
C31-C32-C33-C34	-171.3(8)
C45-C32-C33-C34	10.1(14)
N8-C33-C34-C1	-52.6(9)
C32-C33-C34-C1	117.5(9)
N1-C1-C34-C33	79.2(7)
C2-C1-C34-C33	-89.5(8)
C3-C2-C35-C36	69.3(9)
C1-C2-C35-C36	-111.0(8)
C16-C15-C39-C40	77.0(9)
C14-C15-C39-C40	-96.6(8)
C18-C19-C41-C42	88.1(10)
C20-C19-C41-C42	-85.8(9)
C33-C32-C45-C46A	70(3)
C31-C32-C45-C46A	-109(2)
C33-C32-C45-C46	-111.5(15)
C31-C32-C45-C46	70.1(18)