Supporting Information

Six-coordinate Ferric Porphyrins Containing Bidentate *N*-*t*-Butyl-*N*-nitrosohydroxylaminato Ligands: Structure, Magnetism, IR spectroelectrochemistry, and Reactivity

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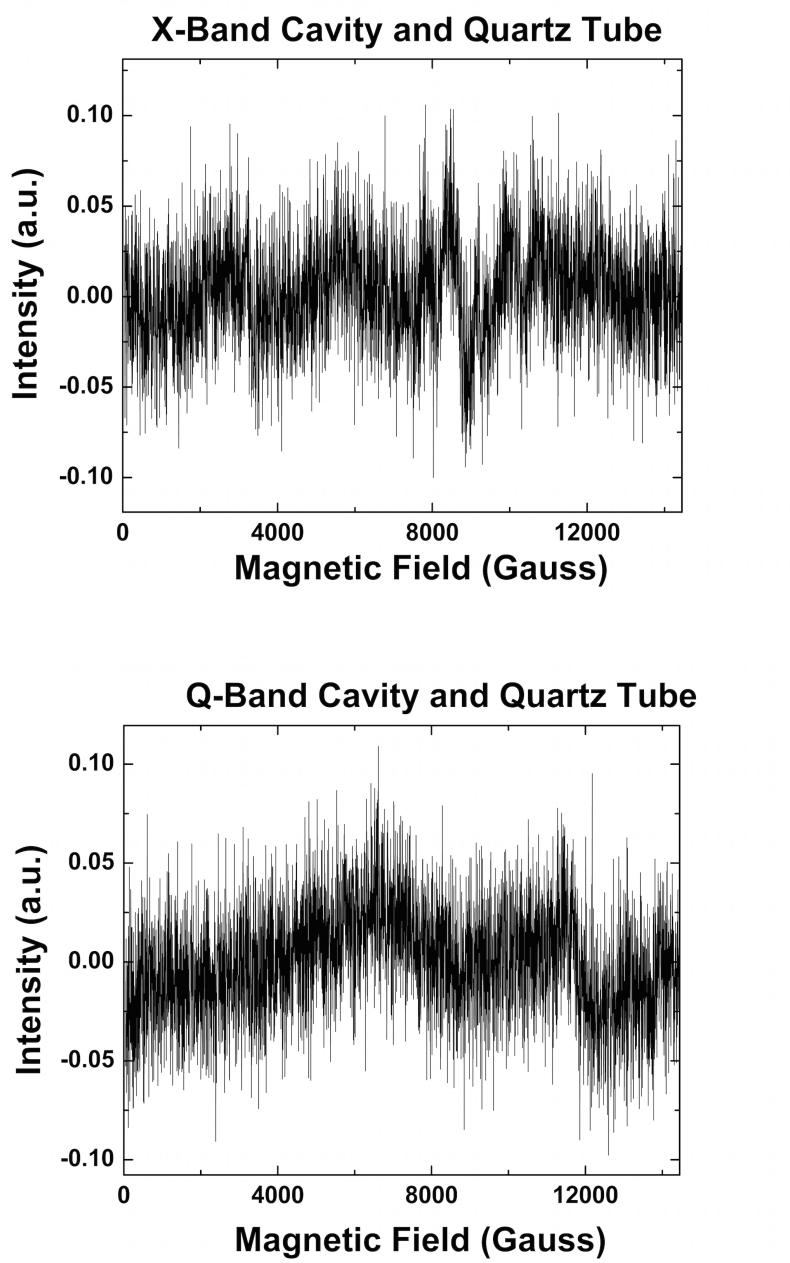

Figure S1. X-bnad (top) and Q-band (bottom) cavity and quartz tube profiles.

X-ray crystallography experimental

The data were corrected for absorption by the semi-empirical method.[1] The structures were solved by direct methods and refined by full-matrix least-squares methods on F^2.[2] Hydrogen atom positions of hydrogens bonded to carbons were initially determined by geometry and refined by a riding model. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atom displacement parameters were set to 1.2x (1.5x for methyl) the isotropic equivalent displacement parameters of the bonded atoms.

(OEP)Fe(η^2-ON(*t*-Bu)NO) (1). A black plate-shaped crystal of dimensions 0.26 x 0.23 x 0.02 mm was selected for structural analysis. The ligand was found to be disordered and was modeled in two orientations. The occupancies of the disordered atoms refined to 0.671(6) and 0.329(6) for the unprimed and primed atoms, respectively. Restraints (SADI, RIGU, and SIMU) on the positional and displacement parameters of the disordered atoms were required. Cell parameters were determined from a non-linear least squares fit of 4620 peaks in the range $2.26 < \theta < 25.89°$. A total of 20526 data were measured in the range $1.976 < \theta < 26.153°$ using ϕ and ω oscillation frames. The data were merged to form a set of 7394 independent data with R(int) = 0.0680 and a coverage of 99.7%.

The monoclinic space group $P2_1/c$ was determined by systematic absences and statistical tests and verified by subsequent refinement. A total of 515 parameters were refined against 381 restraints and 7394 data to give $wR(F^2) = 0.2382$ and S = 1.014 for weights of $w = 1/[\sigma^2(F^2) + (0.1200\ P)^2 + 6.4000\ P]$, where $P = [F_o^2 + 2F_c^2]/3$. The final R(F) was 0.0808 for the 4649 observed, [$F > 4\sigma(F)$], data. The largest shift/s.u. was 0.004 in the final refinement cycle. The final difference map had maxima and minima of 1.231 and -0.877 e/Å^3, respectively.

(TPP)Fe(η^2-ON(*t*-Bu)NO) (2). A black prism-shaped crystal of dimensions 0.48 x 0.30 x 0.30 mm was selected for structural analysis. Cell parameters were determined from a non-linear least squares fit of 9070 peaks in the range $2.21 < \theta < 28.40°$. A total of 20598 data were measured in the range $1.22 < \theta < 26.00°$ using ϕ and ω oscillation frames. The data were merged to form a set of 8306 independent data with R(int) = 0.0410 and a coverage of 99.9%.

The triclinic space group $P\bar{1}$ was determined by statistical tests and verified by subsequent refinement. Restraints (SADI, RIGU, and SIMU) on the positional and displacement parameters of the disordered CH_2Cl_2 were required. A total of 626 parameters were refined against 401 restraints and 8306 data to give wR(F^2) = 0.1613 and S = 1.005 for weights of w = 1/[$\sigma^2(F^2)$ + (0.0800 P)^2 + 4.0000 P], where P = [F_o^2 + 2F_c^2]/3. The final R(F) was 0.0584 for the 6817 observed, [$F > 4\sigma(F)$], data. The largest shift/s.u. was 0.003 in the final refinement cycle. The final difference map had maxima and minima of 0.627 and -0.863 e/Å^3, respectively.

(T(*p*-OMe)PP)Fe(PhNO)(1-MeIm) (6). A purple block-shaped crystal of dimensions 0.320 x 0.240 x 0.070 mm was selected for structural analysis. Cell parameters were determined from a non-linear least squares fit of 7775 peaks in the range 2.22 < θ < 24.74°. A total of 45452 data were measured in the range 1.769 < θ < 26.105° using ϕ and ω oscillation frames. The data were corrected for absorption by the empirical method giving minimum and maximum transmission factors of 0.897 and 0.976. The data were merged to form a set of 10179 independent data with R(int) = 0.0494 and a coverage of 100.0%. The triclinic space group $P\bar{1}$ was determined by statistical tests and verified by subsequent refinement. A severely disordered solvent was removed from the model using *Squeeze*.[34] A total of 640 parameters were refined against 10179 data to give wR(F^2) = 0.1165 and S = 0.986 for weights of w = 1/[$\sigma^2(F^2)$ + (0.0550 P)^2 + 1.7000 P], where P = F_o^2 + 2F_c^2]/3. The final R(F) was 0.0436 for the 7656 observed, [$F > 4\sigma(F)$], data. The largest shift/s.u. was 0.001 in the final refinement cycle. The final difference map had maxima and minima of 0.351 and -0.254 e/Å^3, respectively.

(1) L. Krause, R. Herbst-Irmer, G. M. Sheldrick, and D. Stalke (2015) *J. Appl. Cryst., 48*, 3-10.

(2) (a) G. M. Sheldrick (2015). *Acta Cryst., A71*, 3-8. (b) G. M. Sheldrick (2015) *Acta Cryst., C71*, 3-8.

Table 1. Crystallographic statistics.

Complex	**1**	**2**•(CH_2Cl_2)	**6**
Empirical formula (fw)	$C_{40}H_{53}FeN_6O_2$ (705.73)	$C_{48}H_{37}FeN_6O_2$•CH_2Cl_2 (870.61)	$C_{58}H_{47}FeN_7O_5$ (977.87)
Crystal system, space group	monoclinic, $P2_1/c$	triclinic, $P\bar{1}$	triclinic, $P\bar{1}$
Unit cell dimensions			
a (Å)	18.019(5)	9.7262(15)	9.8358(13)
b (Å)	13.583(4)	13.217(2)	11.9775(16)
c (Å)	17.340(4)	17.511(3)	23.149(3)
α (°)	90	95.746(3)	81.837(2)
β (°)	118.552(7)	105.162(3)	79.205(2)
γ (°)	90	100.150(4)	74.975(2)
Volume (Å^3)	3727.9(17)	2113.2(6)	2574.7(6)
Z, Z'	4, 1	2, 1	2, 1
F(000)	1508	902	1020
Absorption coefficient (mm^{-1})	0.447	0.532	0.348
Max. and min. transmission	0.991 and 0.893	0.857 and 0.784	0.976 and 0.897
Theta range for data collection (°)	1.976–26.153	1.219–25.999	1.769–26.105
Reflections collected	20526	20598	45452
Independent reflections	7394 [R(int) =0.0680]	8306 [R(int) = 0.0410]	10179[R(int) = 0.0494]
Data/restraints/parameters	7394/381/515	8306/401/626	10179/0/640
wR(F^2 all data) [a]	*wR*2 = 0.2382	*wR*2 = 0.1613	*wR2* = 0.1165
R(*F* obsd data) [b]	*R*1 = 0.0808	*R*1 = 0.0584	*R1* = 0.0436
Goodness-of-fit on F^2	1.014	1.005	0.986
Observed data [$I > 2\sigma(I)$]	4649	6817	7656
Largest and mean shift / s.u.	0.014 and 0.000	0.003 and 0.000	0.000 and 0.000
Largest diff. peak and hole (e/Å^3)	1.231 and –0.877	0.627 and –0.863	0.351 and –0.254

[a] $wR2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$ [b] $R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$

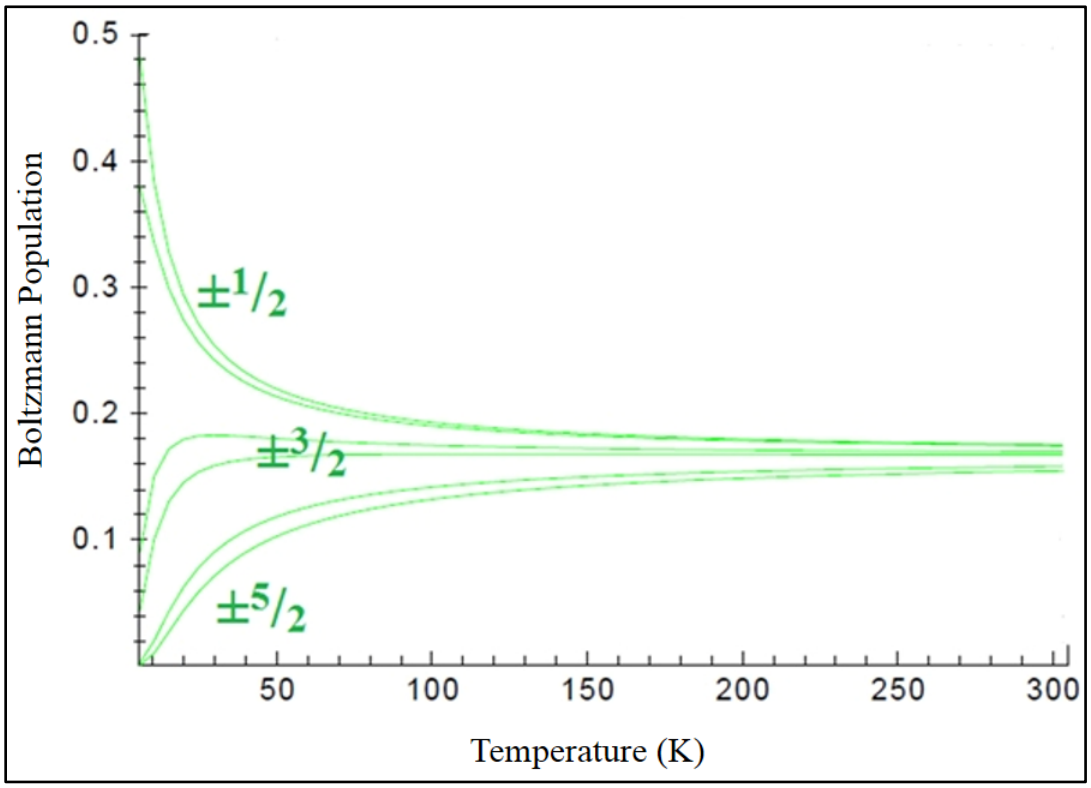

Figure S2. The Boltzmann populations for compounds **1** and **2** are calculated using S = $^{5}/_{2}$, D = 3.89 cm^{-1}, and $g_{average}$ = 2.00. The green numbers represent the M_s quantum numbers in the high-field limit. At low temperatures (< 50 K) it is seen that the ± 1/2 states are the most populated, thus the effective magnetic moment of 1 and 2 shows a decrease at low temperatures.

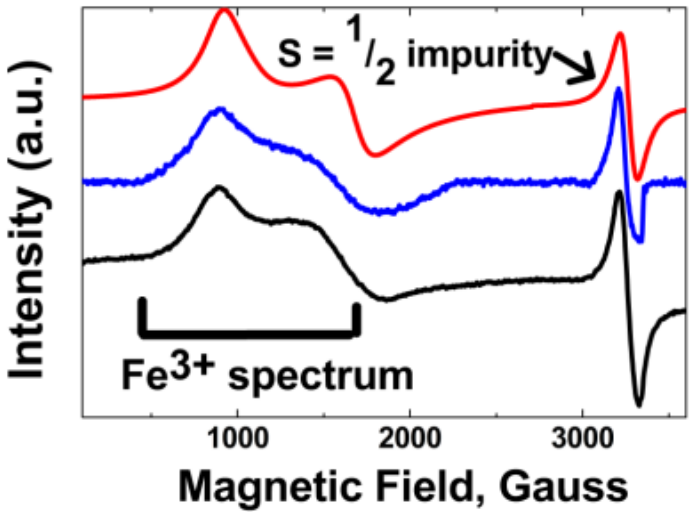

Figure S3. X-band EPR spectra of **1** (blue trace) and **2** (black trace). The red trace is the best fit simulation to the spectra. At high field (g ~2.02), a sharp peak is observed that cannot be simulated simultaneously with the low field peaks. This peak was separately simulated using $g_z = 2.02 \pm 0.03$, $g_{x,y} = 2.06 \pm 0.03$ and $S = ½$, and was later combined with the Fe^{3+} simulation to produce the red trace above. The high field peak is tentatively attributed to a small amount of a low-spin $S = {}^1/_2$ impurity. The relative amount of this impurity was determined by performing a double integration of the EPR spectra as shown in Figure S3.

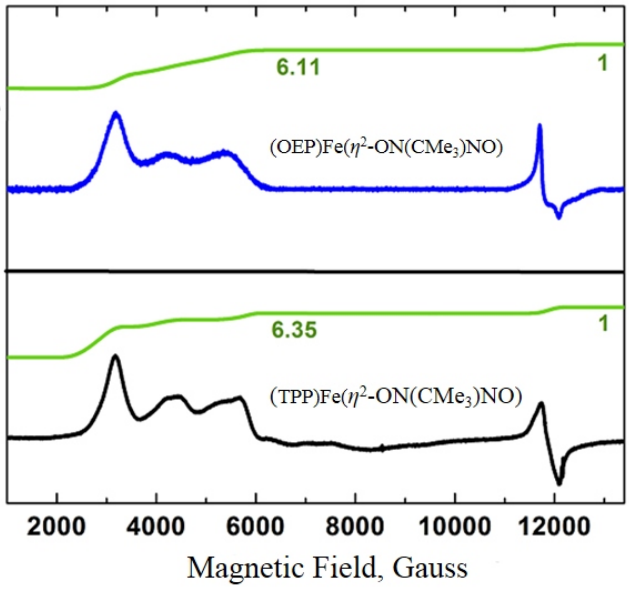

Figure S4. Q-band EPR spectra of **1** and **2**. The blue and black traces are the original EPR spectra while the green traces are the second integral of the experimental data. The measured relative intensities are listed in green. It is seen that the high field peak, which is attributed to $S={}^1/_2$ impurity, is approximately 16% of the OEP and TPP spectra.

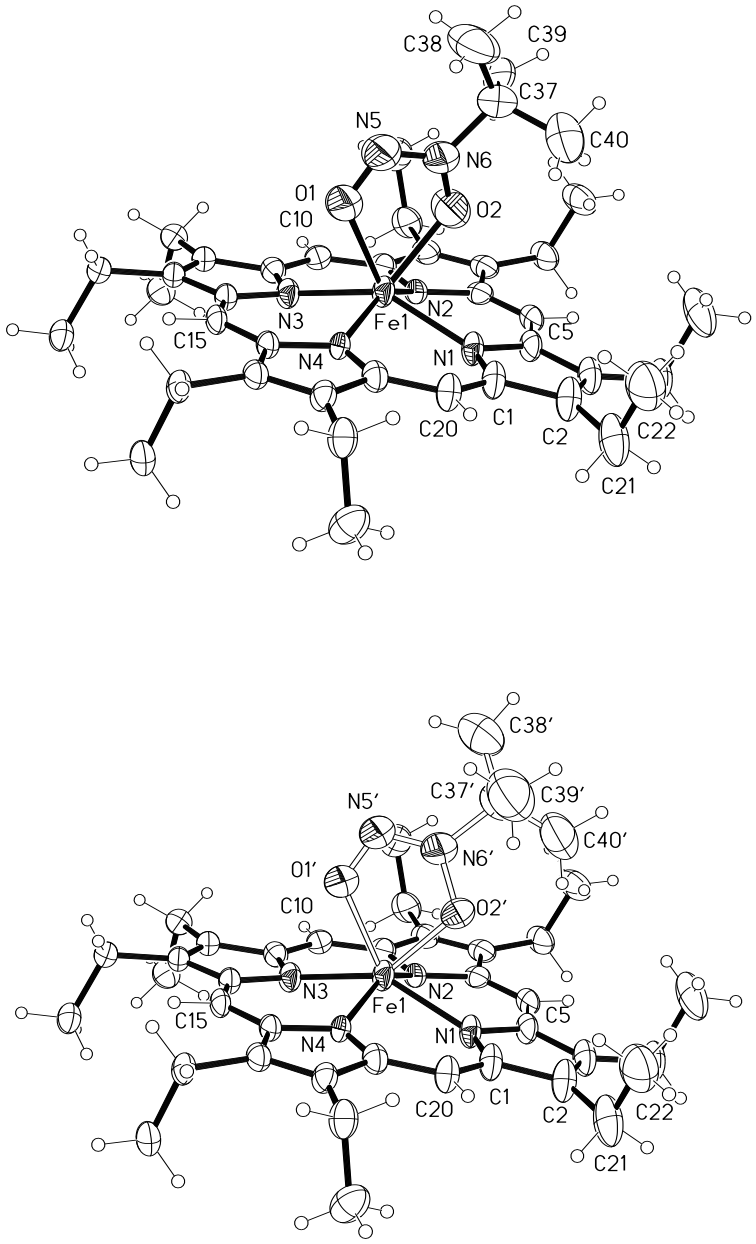

Figure S5. Molecular structures of **1** showing the disordered axial NONOate positions.

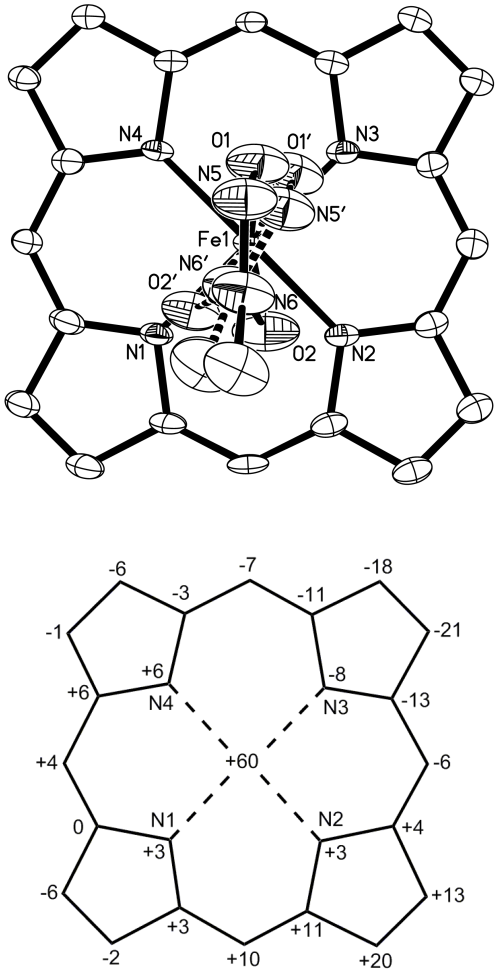

Figure S6. (*Top*) View of the disordered bidentate ligand orientations in (OEP)Fe(η^2-ON(*t*-Bu)NO) (**1**). relative to the porphyrin core, with the ligand facing the viewer and the minor disordered component represented by dashed lines. The peripheral por and C*Me*$_3$ substituents have been omitted for clarity. (*Bottom*) Perpendicular atom displacements (in units of 0.01 Å) of the porphyrin core from the 24-atom mean porphyrin plane.

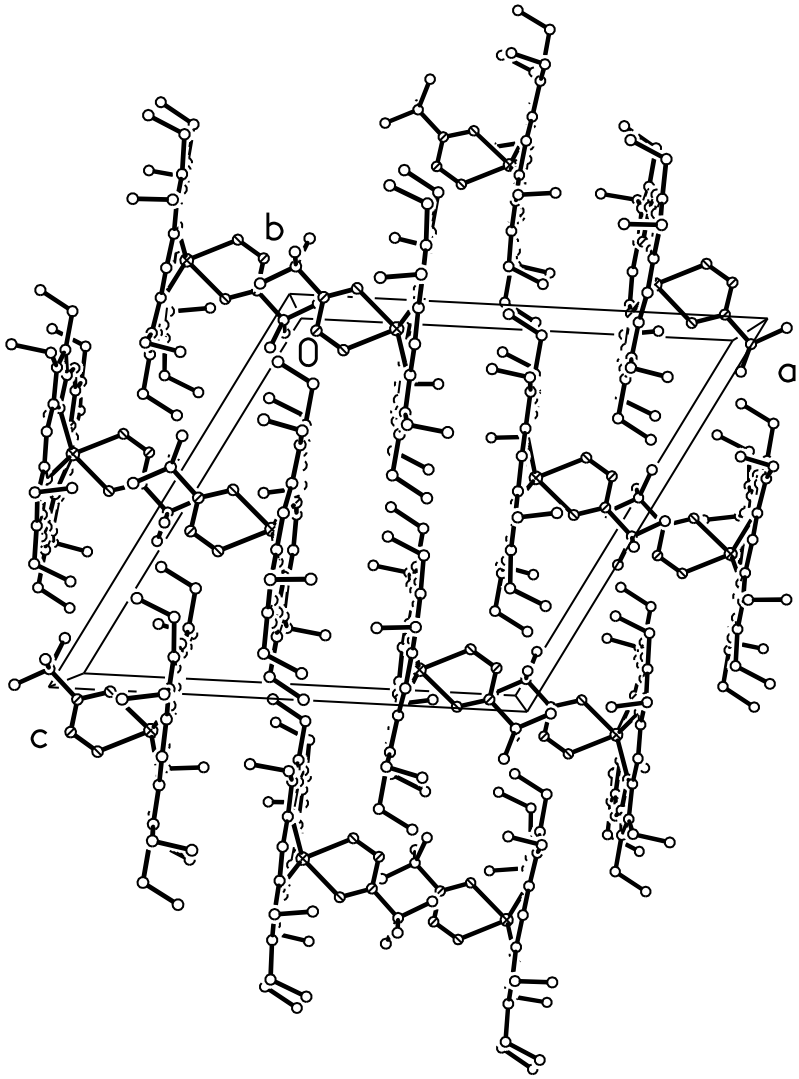

Figure S7. Crystal packing for **1**.

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0.26656(4)	0.30722(5)	0.58359(4)	0.0319(2)
O(1)	0.1868(6)	0.3107(7)	0.6421(6)	0.0731(18)
O(2)	0.1409(4)	0.2681(7)	0.4937(4)	0.0747(15)
O(1')	0.1886(10)	0.2736(15)	0.6405(12)	0.072(2)
O(2')	0.1404(4)	0.3485(11)	0.4976(7)	0.0657(17)
N(1)	0.2601(3)	0.3932(3)	0.4797(2)	0.0327(9)
N(2)	0.2785(2)	0.1873(3)	0.5153(2)	0.0300(9)
N(3)	0.3455(2)	0.2266(3)	0.6963(2)	0.0310(9)
N(4)	0.3190(2)	0.4318(3)	0.6594(2)	0.0269(8)
N(5)	0.1093(6)	0.3124(9)	0.5983(5)	0.0718(16)
N(6)	0.0844(4)	0.2971(8)	0.5185(5)	0.0702(13)
N(5')	0.1111(12)	0.2776(17)	0.5961(9)	0.0718(18)
N(6')	0.0863(7)	0.3024(16)	0.5180(8)	0.0711(15)
C(1)	0.2569(3)	0.4949(4)	0.4743(3)	0.0390(12)
C(2)	0.2286(4)	0.5275(4)	0.3844(3)	0.0448(14)
C(3)	0.2123(3)	0.4438(4)	0.3352(3)	0.0399(13)
C(4)	0.2321(3)	0.3610(4)	0.3945(3)	0.0340(11)
C(5)	0.2228(3)	0.2630(4)	0.3698(3)	0.0338(11)
C(6)	0.2433(3)	0.1821(4)	0.4250(3)	0.0315(11)
C(7)	0.2314(3)	0.0806(4)	0.3965(3)	0.0361(12)
C(8)	0.2620(3)	0.0253(4)	0.4697(3)	0.0364(12)
C(9)	0.2904(3)	0.0912(4)	0.5437(3)	0.0322(11)
C(10)	0.3272(3)	0.0633(4)	0.6312(3)	0.0315(10)
C(11)	0.3535(3)	0.1251(3)	0.7021(3)	0.0296(10)
C(12)	0.3897(3)	0.0936(4)	0.7936(3)	0.0318(11)
C(13)	0.4024(3)	0.1761(3)	0.8417(3)	0.0291(10)
C(14)	0.3754(3)	0.2585(3)	0.7816(3)	0.0289(10)
C(15)	0.3782(3)	0.3564(3)	0.8051(3)	0.0271(10)
C(16)	0.3547(3)	0.4369(3)	0.7503(3)	0.0278(10)
C(17)	0.3628(3)	0.5378(3)	0.7780(3)	0.0286(10)
C(18)	0.3335(3)	0.5953(4)	0.7045(3)	0.0296(10)
C(19)	0.3063(3)	0.5279(4)	0.6311(3)	0.0313(11)
C(20)	0.2769(3)	0.5566(4)	0.5445(3)	0.0353(11)
C(21)	0.2201(4)	0.6365(5)	0.3547(4)	0.0589(17)
C(22)	0.1362(4)	0.6725(5)	0.3346(4)	0.070(2)
C(23)	0.1780(4)	0.4354(4)	0.2371(3)	0.0461(14)
C(24)	0.0831(4)	0.4178(6)	0.1887(4)	0.071(2)
C(25)	0.1862(3)	0.0491(4)	0.3016(3)	0.0413(13)

C(26)	0.0913(3)	0.0637(5)	0.2620(4)	0.0580(17)
C(27)	0.2620(4)	-0.0859(4)	0.4772(4)	0.0471(14)
C(28)	0.1897(4)	-0.1232(4)	0.4925(4)	0.0556(16)
C(29)	0.4094(3)	-0.0110(4)	0.8240(3)	0.0342(11)
C(30)	0.4962(3)	-0.0432(4)	0.8384(3)	0.0386(12)
C(31)	0.4374(3)	0.1824(4)	0.9399(3)	0.0318(11)
C(32)	0.5326(3)	0.1999(4)	0.9900(3)	0.0337(11)
C(33)	0.4035(3)	0.5712(4)	0.8723(3)	0.0311(11)
C(34)	0.4990(3)	0.5753(4)	0.9139(3)	0.0378(12)
C(35)	0.3334(3)	0.7055(3)	0.6988(3)	0.0363(12)
C(36)	0.4099(4)	0.7440(4)	0.6928(4)	0.0491(14)
C(37)	-0.0079(6)	0.2853(5)	0.4482(5)	0.0774(16)
C(38)	-0.0607(5)	0.3156(8)	0.4912(7)	0.083(2)
C(39)	-0.0201(6)	0.1779(7)	0.4208(6)	0.069(2)
C(40)	-0.0202(7)	0.3536(7)	0.3738(6)	0.091(3)
C(37')	-0.0043(8)	0.3118(10)	0.4431(7)	0.0791(17)
C(38')	-0.0527(10)	0.2238(13)	0.4498(13)	0.091(3)
C(39')	-0.0377(12)	0.4088(12)	0.4574(12)	0.091(3)
C(40')	0.0016(12)	0.3112(15)	0.3585(8)	0.084(3)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Fe(1)-N(4)	2.073(4)	C(12)-C(13)	1.351(7)
Fe(1)-N(2)	2.084(4)	C(12)-C(29)	1.497(7)
Fe(1)-N(3)	2.094(4)	C(13)-C(14)	1.446(6)
Fe(1)-N(1)	2.104(4)	C(13)-C(31)	1.509(6)
Fe(1)-O(2)	2.113(6)	C(14)-C(15)	1.384(6)
Fe(1)-O(2')	2.114(6)	C(15)-C(16)	1.376(6)
Fe(1)-O(1')	2.116(5)	C(15)-H(15)	0.9500
Fe(1)-O(1)	2.118(5)	C(16)-C(17)	1.437(6)
O(1)-N(5)	1.231(7)	C(17)-C(18)	1.366(6)
O(2)-N(6)	1.340(9)	C(17)-C(33)	1.507(6)
O(1')-N(5')	1.232(8)	C(18)-C(19)	1.450(6)
O(2')-N(6')	1.342(9)	C(18)-C(35)	1.501(7)
N(1)-C(1)	1.383(7)	C(19)-C(20)	1.389(6)
N(1)-C(4)	1.385(5)	C(20)-H(20)	0.9500
N(2)-C(9)	1.375(6)	C(21)-C(22)	1.465(9)
N(2)-C(6)	1.382(6)	C(21)-H(21A)	0.9900
N(3)-C(14)	1.381(5)	C(21)-H(21B)	0.9900
N(3)-C(11)	1.384(6)	C(22)-H(22A)	0.9798
N(4)-C(19)	1.375(6)	C(22)-H(22B)	0.9799
N(4)-C(16)	1.391(5)	C(22)-H(22C)	0.9799
N(5)-N(6)	1.250(8)	C(23)-C(24)	1.521(8)
N(6)-C(37)	1.529(9)	C(23)-H(23A)	0.9900
N(5')-N(6')	1.252(9)	C(23)-H(23B)	0.9900
N(6')-C(37')	1.529(9)	C(24)-H(24A)	0.9798
C(1)-C(20)	1.377(7)	C(24)-H(24B)	0.9798
C(1)-C(2)	1.457(6)	C(24)-H(24C)	0.9798
C(2)-C(3)	1.366(7)	C(25)-C(26)	1.521(7)
C(2)-C(21)	1.552(8)	C(25)-H(25A)	0.9900
C(3)-C(4)	1.448(7)	C(25)-H(25B)	0.9900
C(3)-C(23)	1.511(6)	C(26)-H(26A)	0.9798
C(4)-C(5)	1.384(7)	C(26)-H(26B)	0.9799
C(5)-C(6)	1.386(7)	C(26)-H(26C)	0.9799
C(5)-H(5)	0.9500	C(27)-C(28)	1.534(8)
C(6)-C(7)	1.446(7)	C(27)-H(27A)	0.9900
C(7)-C(8)	1.345(7)	C(27)-H(27B)	0.9900
C(7)-C(25)	1.508(6)	C(28)-H(28A)	0.9797
C(8)-C(9)	1.444(6)	C(28)-H(28B)	0.9799
C(8)-C(27)	1.515(7)	C(28)-H(28C)	0.9796
C(9)-C(10)	1.387(6)	C(29)-C(30)	1.525(7)
C(10)-C(11)	1.373(6)	C(29)-H(29A)	0.9900
C(10)-H(10)	0.9500	C(29)-H(29B)	0.9900
C(11)-C(12)	1.461(6)	C(30)-H(30A)	0.9798

C(30)-H(30B)	0.9799	C(37)-C(38)	1.518(6)
C(30)-H(30C)	0.9796	C(38)-H(38A)	0.9800
C(31)-C(32)	1.526(7)	C(38)-H(38B)	0.9800
C(31)-H(31A)	0.9900	C(38)-H(38C)	0.9800
C(31)-H(31B)	0.9900	C(39)-H(39A)	0.9800
C(32)-H(32A)	0.9798	C(39)-H(39B)	0.9800
C(32)-H(32B)	0.9799	C(39)-H(39C)	0.9800
C(32)-H(32C)	0.9798	C(40)-H(40A)	0.9800
C(33)-C(34)	1.516(7)	C(40)-H(40B)	0.9800
C(33)-H(33A)	0.9900	C(40)-H(40C)	0.9800
C(33)-H(33B)	0.9900	C(37')-C(38')	1.518(6)
C(34)-H(34A)	0.9798	C(37')-C(39')	1.519(6)
C(34)-H(34B)	0.9799	C(37')-C(40')	1.519(6)
C(34)-H(34C)	0.9798	C(38')-H(38D)	0.9800
C(35)-C(36)	1.523(7)	C(38')-H(38E)	0.9800
C(35)-H(35A)	0.9900	C(38')-H(38F)	0.9800
C(35)-H(35B)	0.9900	C(39')-H(39D)	0.9800
C(36)-H(36A)	0.9799	C(39')-H(39E)	0.9800
C(36)-H(36B)	0.9797	C(39')-H(39F)	0.9800
C(36)-H(36C)	0.9799	C(40')-H(40D)	0.9800
C(37)-C(40)	1.517(6)	C(40')-H(40E)	0.9800
C(37)-C(39)	1.518(6)	C(40')-H(40F)	0.9800

N(4)-Fe(1)-N(2)	149.17(15)	N(1)-Fe(1)-O(1)	128.7(3)
N(4)-Fe(1)-N(3)	86.25(15)	O(2)-Fe(1)-O(1)	68.0(3)
N(2)-Fe(1)-N(3)	85.01(15)	N(5)-O(1)-Fe(1)	122.3(8)
N(4)-Fe(1)-N(1)	84.93(14)	N(6)-O(2)-Fe(1)	113.6(5)
N(2)-Fe(1)-N(1)	85.75(15)	N(5')-O(1')-Fe(1)	120.3(14)
N(3)-Fe(1)-N(1)	145.55(16)	N(6')-O(2')-Fe(1)	111.2(8)
N(4)-Fe(1)-O(2)	132.5(3)	C(1)-N(1)-C(4)	105.1(4)
N(2)-Fe(1)-O(2)	75.5(2)	C(1)-N(1)-Fe(1)	126.6(3)
N(3)-Fe(1)-O(2)	124.6(3)	C(4)-N(1)-Fe(1)	125.5(3)
N(1)-Fe(1)-O(2)	84.7(2)	C(9)-N(2)-C(6)	105.4(4)
N(4)-Fe(1)-O(2')	104.0(4)	C(9)-N(2)-Fe(1)	125.4(3)
N(2)-Fe(1)-O(2')	100.1(4)	C(6)-N(2)-Fe(1)	124.6(3)
N(3)-Fe(1)-O(2')	145.0(3)	C(14)-N(3)-C(11)	105.1(4)
N(1)-Fe(1)-O(2')	69.4(3)	C(14)-N(3)-Fe(1)	125.4(3)
N(4)-Fe(1)-O(1')	94.8(6)	C(11)-N(3)-Fe(1)	126.1(3)
N(2)-Fe(1)-O(1')	111.6(6)	C(19)-N(4)-C(16)	105.4(4)
N(3)-Fe(1)-O(1')	76.0(6)	C(19)-N(4)-Fe(1)	126.9(3)
N(1)-Fe(1)-O(1')	137.9(6)	C(16)-N(4)-Fe(1)	125.7(3)
O(2')-Fe(1)-O(1')	69.9(6)	O(1)-N(5)-N(6)	112.3(10)
N(4)-Fe(1)-O(1)	83.5(3)	N(5)-N(6)-O(2)	118.6(8)
N(2)-Fe(1)-O(1)	124.5(3)	N(5)-N(6)-C(37)	125.3(7)
N(3)-Fe(1)-O(1)	83.0(3)	O(2)-N(6)-C(37)	114.6(6)

O(1')-N(5')-N(6')	113.6(19)	C(15)-C(14)-C(13)	125.4(4)
N(5')-N(6')-O(2')	118.8(13)	C(16)-C(15)-C(14)	127.2(4)
N(5')-N(6')-C(37')	128.8(12)	C(16)-C(15)-H(15)	116.4
O(2')-N(6')-C(37')	110.5(8)	C(14)-C(15)-H(15)	116.4
C(20)-C(1)-N(1)	124.3(4)	C(15)-C(16)-N(4)	124.5(4)
C(20)-C(1)-C(2)	124.7(5)	C(15)-C(16)-C(17)	125.4(4)
N(1)-C(1)-C(2)	111.0(4)	N(4)-C(16)-C(17)	110.1(4)
C(3)-C(2)-C(1)	106.0(5)	C(18)-C(17)-C(16)	107.5(4)
C(3)-C(2)-C(21)	128.9(5)	C(18)-C(17)-C(33)	127.6(4)
C(1)-C(2)-C(21)	125.0(5)	C(16)-C(17)-C(33)	124.7(4)
C(2)-C(3)-C(4)	107.2(4)	C(17)-C(18)-C(19)	106.0(4)
C(2)-C(3)-C(23)	128.0(5)	C(17)-C(18)-C(35)	128.2(4)
C(4)-C(3)-C(23)	124.7(5)	C(19)-C(18)-C(35)	125.6(4)
C(5)-C(4)-N(1)	124.3(4)	N(4)-C(19)-C(20)	124.5(4)
C(5)-C(4)-C(3)	125.1(4)	N(4)-C(19)-C(18)	110.9(4)
N(1)-C(4)-C(3)	110.6(4)	C(20)-C(19)-C(18)	124.5(4)
C(4)-C(5)-C(6)	126.5(4)	C(1)-C(20)-C(19)	126.0(5)
C(4)-C(5)-H(5)	116.7	C(1)-C(20)-H(20)	117.0
C(6)-C(5)-H(5)	116.7	C(19)-C(20)-H(20)	117.0
N(2)-C(6)-C(5)	124.7(4)	C(22)-C(21)-C(2)	108.9(6)
N(2)-C(6)-C(7)	110.4(4)	C(22)-C(21)-H(21A)	109.9
C(5)-C(6)-C(7)	124.9(4)	C(2)-C(21)-H(21A)	109.9
C(8)-C(7)-C(6)	106.5(4)	C(22)-C(21)-H(21B)	109.9
C(8)-C(7)-C(25)	129.4(5)	C(2)-C(21)-H(21B)	109.9
C(6)-C(7)-C(25)	123.9(5)	H(21A)-C(21)-H(21B)	108.3
C(7)-C(8)-C(9)	107.7(5)	C(21)-C(22)-H(22A)	109.6
C(7)-C(8)-C(27)	128.4(5)	C(21)-C(22)-H(22B)	109.2
C(9)-C(8)-C(27)	123.8(5)	H(22A)-C(22)-H(22B)	109.5
N(2)-C(9)-C(10)	124.2(4)	C(21)-C(22)-H(22C)	109.6
N(2)-C(9)-C(8)	110.0(4)	H(22A)-C(22)-H(22C)	109.5
C(10)-C(9)-C(8)	125.7(5)	H(22B)-C(22)-H(22C)	109.5
C(11)-C(10)-C(9)	126.3(5)	C(3)-C(23)-C(24)	112.4(4)
C(11)-C(10)-H(10)	116.8	C(3)-C(23)-H(23A)	109.1
C(9)-C(10)-H(10)	116.8	C(24)-C(23)-H(23A)	109.1
C(10)-C(11)-N(3)	124.3(4)	C(3)-C(23)-H(23B)	109.1
C(10)-C(11)-C(12)	125.2(4)	C(24)-C(23)-H(23B)	109.1
N(3)-C(11)-C(12)	110.4(4)	H(23A)-C(23)-H(23B)	107.9
C(13)-C(12)-C(11)	106.5(4)	C(23)-C(24)-H(24A)	109.5
C(13)-C(12)-C(29)	128.8(4)	C(23)-C(24)-H(24B)	109.6
C(11)-C(12)-C(29)	124.7(4)	H(24A)-C(24)-H(24B)	109.5
C(12)-C(13)-C(14)	107.3(4)	C(23)-C(24)-H(24C)	109.3
C(12)-C(13)-C(31)	127.0(4)	H(24A)-C(24)-H(24C)	109.5
C(14)-C(13)-C(31)	125.7(4)	H(24B)-C(24)-H(24C)	109.5
N(3)-C(14)-C(15)	123.9(4)	C(7)-C(25)-C(26)	111.0(4)
N(3)-C(14)-C(13)	110.7(4)	C(7)-C(25)-H(25A)	109.4

C(26)-C(25)-H(25A)	109.4	H(32B)-C(32)-H(32C)	109.5
C(7)-C(25)-H(25B)	109.4	C(17)-C(33)-C(34)	112.4(4)
C(26)-C(25)-H(25B)	109.4	C(17)-C(33)-H(33A)	109.1
H(25A)-C(25)-H(25B)	108.0	C(34)-C(33)-H(33A)	109.1
C(25)-C(26)-H(26A)	109.0	C(17)-C(33)-H(33B)	109.1
C(25)-C(26)-H(26B)	109.5	C(34)-C(33)-H(33B)	109.1
H(26A)-C(26)-H(26B)	109.5	H(33A)-C(33)-H(33B)	107.9
C(25)-C(26)-H(26C)	109.9	C(33)-C(34)-H(34A)	109.5
H(26A)-C(26)-H(26C)	109.5	C(33)-C(34)-H(34B)	109.4
H(26B)-C(26)-H(26C)	109.5	H(34A)-C(34)-H(34B)	109.5
C(8)-C(27)-C(28)	112.3(5)	C(33)-C(34)-H(34C)	109.5
C(8)-C(27)-H(27A)	109.1	H(34A)-C(34)-H(34C)	109.5
C(28)-C(27)-H(27A)	109.1	H(34B)-C(34)-H(34C)	109.5
C(8)-C(27)-H(27B)	109.1	C(18)-C(35)-C(36)	112.0(4)
C(28)-C(27)-H(27B)	109.1	C(18)-C(35)-H(35A)	109.2
H(27A)-C(27)-H(27B)	107.9	C(36)-C(35)-H(35A)	109.2
C(27)-C(28)-H(28A)	109.5	C(18)-C(35)-H(35B)	109.2
C(27)-C(28)-H(28B)	109.4	C(36)-C(35)-H(35B)	109.2
H(28A)-C(28)-H(28B)	109.5	H(35A)-C(35)-H(35B)	107.9
C(27)-C(28)-H(28C)	109.5	C(35)-C(36)-H(36A)	109.5
H(28A)-C(28)-H(28C)	109.5	C(35)-C(36)-H(36B)	109.3
H(28B)-C(28)-H(28C)	109.5	H(36A)-C(36)-H(36B)	109.5
C(12)-C(29)-C(30)	112.4(4)	C(35)-C(36)-H(36C)	109.6
C(12)-C(29)-H(29A)	109.1	H(36A)-C(36)-H(36C)	109.5
C(30)-C(29)-H(29A)	109.1	H(36B)-C(36)-H(36C)	109.5
C(12)-C(29)-H(29B)	109.1	C(40)-C(37)-C(39)	112.4(4)
C(30)-C(29)-H(29B)	109.1	C(40)-C(37)-C(38)	112.4(4)
H(29A)-C(29)-H(29B)	107.9	C(39)-C(37)-C(38)	112.5(4)
C(29)-C(30)-H(30A)	109.4	C(40)-C(37)-N(6)	106.0(5)
C(29)-C(30)-H(30B)	109.5	C(39)-C(37)-N(6)	106.9(5)
H(30A)-C(30)-H(30B)	109.5	C(38)-C(37)-N(6)	106.1(5)
C(29)-C(30)-H(30C)	109.5	C(37)-C(38)-H(38A)	108.3
H(30A)-C(30)-H(30C)	109.5	C(37)-C(38)-H(38B)	110.2
H(30B)-C(30)-H(30C)	109.5	H(38A)-C(38)-H(38B)	109.5
C(13)-C(31)-C(32)	113.6(4)	C(37)-C(38)-H(38C)	109.9
C(13)-C(31)-H(31A)	108.8	H(38A)-C(38)-H(38C)	109.5
C(32)-C(31)-H(31A)	108.8	H(38B)-C(38)-H(38C)	109.5
C(13)-C(31)-H(31B)	108.8	C(37)-C(39)-H(39A)	109.8
C(32)-C(31)-H(31B)	108.8	C(37)-C(39)-H(39B)	109.9
H(31A)-C(31)-H(31B)	107.7	H(39A)-C(39)-H(39B)	109.5
C(31)-C(32)-H(32A)	109.5	C(37)-C(39)-H(39C)	108.6
C(31)-C(32)-H(32B)	109.6	H(39A)-C(39)-H(39C)	109.5
H(32A)-C(32)-H(32B)	109.5	H(39B)-C(39)-H(39C)	109.5
C(31)-C(32)-H(32C)	109.3	C(37)-C(40)-H(40A)	108.7
H(32A)-C(32)-H(32C)	109.5	C(37)-C(40)-H(40B)	109.1

H(40A)-C(40)-H(40B)	109.5	H(38D)-C(38')-H(38F)	109.5
C(37)-C(40)-H(40C)	110.6	H(38E)-C(38')-H(38F)	109.5
H(40A)-C(40)-H(40C)	109.5	C(37')-C(39')-H(39D)	112.7
H(40B)-C(40)-H(40C)	109.5	C(37')-C(39')-H(39E)	110.4
C(38')-C(37')-C(39')	112.5(4)	H(39D)-C(39')-H(39E)	109.5
C(38')-C(37')-C(40')	112.3(4)	C(37')-C(39')-H(39F)	105.2
C(39')-C(37')-C(40')	112.3(4)	H(39D)-C(39')-H(39F)	109.5
C(38')-C(37')-N(6')	106.7(5)	H(39E)-C(39')-H(39F)	109.5
C(39')-C(37')-N(6')	106.2(5)	C(37')-C(40')-H(40D)	112.8
C(40')-C(37')-N(6')	106.4(5)	C(37')-C(40')-H(40E)	110.0
C(37')-C(38')-H(38D)	108.9	H(40D)-C(40')-H(40E)	109.5
C(37')-C(38')-H(38E)	105.6	C(37')-C(40')-H(40F)	105.5
H(38D)-C(38')-H(38E)	109.5	H(40D)-C(40')-H(40F)	109.5
C(37')-C(38')-H(38F)	113.8	H(40E)-C(40')-H(40F)	109.5

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. 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}
Fe(1)	38(1)	41(1)	17(1)	-4(1)	13(1)	0(1)
O(1)	53(2)	122(4)	46(2)	-6(3)	25(2)	-19(3)
O(2)	48(2)	129(4)	51(2)	-11(3)	27(2)	-8(3)
O(1')	52(3)	120(5)	47(3)	0(3)	26(2)	-18(3)
O(2')	43(3)	118(4)	47(3)	0(3)	30(2)	-11(3)
N(1)	37(2)	42(2)	17(2)	-1(2)	12(2)	8(2)
N(2)	29(2)	42(2)	20(2)	-6(2)	12(2)	-8(2)
N(3)	33(2)	38(2)	21(2)	-3(2)	12(2)	3(2)
N(4)	29(2)	37(2)	15(2)	-1(2)	10(2)	-3(2)
N(5)	52(2)	121(4)	49(2)	-7(2)	30(2)	-13(3)
N(6)	47(2)	120(3)	50(2)	-2(2)	28(2)	-11(2)
N(5')	51(2)	121(4)	49(2)	-2(3)	28(2)	-14(3)
N(6')	48(2)	121(3)	50(2)	-1(2)	28(2)	-11(2)
C(1)	44(3)	49(3)	19(2)	4(2)	11(2)	9(2)
C(2)	58(4)	51(3)	23(2)	4(2)	18(2)	15(3)
C(3)	39(3)	58(3)	19(2)	1(2)	11(2)	12(2)
C(4)	34(3)	52(3)	16(2)	-2(2)	12(2)	5(2)
C(5)	30(3)	57(3)	17(2)	-12(2)	13(2)	-4(2)
C(6)	29(3)	43(3)	28(2)	-11(2)	18(2)	-8(2)
C(7)	28(3)	52(3)	31(3)	-14(2)	15(2)	-8(2)
C(8)	34(3)	43(3)	34(3)	-10(2)	18(2)	-9(2)
C(9)	30(3)	38(3)	30(2)	-8(2)	16(2)	-6(2)
C(10)	30(3)	36(3)	31(2)	-1(2)	17(2)	-1(2)
C(11)	26(3)	36(3)	26(2)	-3(2)	12(2)	1(2)
C(12)	28(3)	43(3)	25(2)	3(2)	13(2)	-3(2)
C(13)	24(2)	41(3)	21(2)	2(2)	11(2)	0(2)
C(14)	27(3)	39(3)	19(2)	-2(2)	9(2)	-1(2)
C(15)	28(3)	37(3)	17(2)	-2(2)	10(2)	2(2)
C(16)	26(2)	40(3)	18(2)	-3(2)	10(2)	-1(2)
C(17)	25(2)	37(3)	22(2)	-3(2)	10(2)	0(2)
C(18)	31(3)	38(3)	22(2)	0(2)	14(2)	4(2)
C(19)	30(3)	41(3)	23(2)	1(2)	13(2)	5(2)
C(20)	44(3)	37(3)	23(2)	2(2)	15(2)	8(2)
C(21)	67(4)	74(4)	28(3)	-2(3)	16(3)	25(3)
C(22)	68(5)	83(5)	46(4)	-5(3)	16(3)	-2(4)
C(23)	53(3)	66(4)	18(2)	0(2)	15(2)	13(3)

C(24)	49(4)	128(6)	27(3)	-10(3)	11(3)	28(4)
C(25)	38(3)	55(3)	27(2)	-17(2)	13(2)	-9(2)
C(26)	38(3)	91(5)	39(3)	-24(3)	14(3)	-16(3)
C(27)	49(3)	45(3)	42(3)	-12(2)	17(3)	-9(3)
C(28)	66(4)	46(3)	52(4)	-7(3)	26(3)	-15(3)
C(29)	33(3)	35(3)	34(3)	-2(2)	15(2)	-2(2)
C(30)	35(3)	38(3)	41(3)	1(2)	17(2)	4(2)
C(31)	30(3)	44(3)	22(2)	2(2)	13(2)	-2(2)
C(32)	36(3)	41(3)	24(2)	-1(2)	14(2)	2(2)
C(33)	37(3)	38(3)	18(2)	-2(2)	13(2)	-2(2)
C(34)	36(3)	51(3)	20(2)	-3(2)	8(2)	-3(2)
C(35)	44(3)	36(3)	29(2)	-2(2)	17(2)	8(2)
C(36)	67(4)	40(3)	50(3)	-3(3)	35(3)	-6(3)
C(37)	51(2)	122(4)	58(2)	2(2)	24(2)	-13(3)
C(38)	49(4)	126(5)	71(4)	-6(4)	26(3)	-8(4)
C(39)	55(4)	117(5)	39(3)	-9(3)	25(3)	-21(4)
C(40)	64(4)	130(5)	63(4)	8(4)	17(3)	-6(4)
C(37')	52(2)	123(4)	58(2)	1(3)	23(2)	-11(3)
C(38')	59(4)	129(5)	69(4)	1(4)	18(4)	-17(4)
C(39')	63(4)	130(5)	66(4)	-1(4)	20(4)	-3(4)
C(40')	57(5)	126(6)	60(4)	0(4)	20(4)	-3(5)

Table S5. Hydrogen coordinates and isotropic displacement parameters for 1.

	x	y	z	U(eq)
H(5)	0.2000	0.2498	0.3088	0.041
H(10)	0.3349	-0.0053	0.6432	0.038
H(15)	0.3988	0.3694	0.8658	0.033
H(20)	0.2700	0.6253	0.5325	0.042
H(21A)	0.2642	0.6768	0.4019	0.071
H(21B)	0.2278	0.6417	0.3020	0.071
H(22A)	0.0928	0.6335	0.2868	0.105
H(22B)	0.1308	0.7417	0.3167	0.105
H(22C)	0.1287	0.6668	0.3868	0.105
H(23A)	0.2068	0.3804	0.2246	0.055
H(23B)	0.1909	0.4967	0.2150	0.055
H(24A)	0.0703	0.3554	0.2081	0.106
H(24B)	0.0634	0.4151	0.1253	0.106
H(24C)	0.0546	0.4718	0.2015	0.106
H(25A)	0.1983	-0.0212	0.2973	0.050
H(25B)	0.2075	0.0880	0.2679	0.050
H(26A)	0.0701	0.0219	0.2934	0.087
H(26B)	0.0636	0.0452	0.1998	0.087
H(26C)	0.0789	0.1328	0.2675	0.087
H(27A)	0.3166	-0.1074	0.5266	0.056
H(27B)	0.2567	-0.1156	0.4227	0.056
H(28A)	0.1947	-0.0941	0.5465	0.083
H(28B)	0.1929	-0.1951	0.4981	0.083
H(28C)	0.1354	-0.1044	0.4427	0.083
H(29A)	0.3658	-0.0546	0.7798	0.041
H(29B)	0.4071	-0.0184	0.8797	0.041
H(30A)	0.4988	-0.0354	0.7836	0.058
H(30B)	0.5056	-0.1124	0.8566	0.058
H(30C)	0.5398	-0.0024	0.8843	0.058
H(31A)	0.4244	0.1204	0.9610	0.038
H(31B)	0.4087	0.2367	0.9533	0.038
H(32A)	0.5618	0.1454	0.9788	0.051
H(32B)	0.5512	0.2038	1.0530	0.051
H(32C)	0.5459	0.2618	0.9702	0.051
H(33A)	0.3875	0.5254	0.9063	0.037
H(33B)	0.3819	0.6374	0.8751	0.037
H(34A)	0.5209	0.5099	0.9118	0.057
H(34B)	0.5226	0.5965	0.9752	0.057
H(34C)	0.5153	0.6223	0.8818	0.057

H(35A)	0.3333	0.7340	0.7513	0.044
H(35B)	0.2812	0.7273	0.6465	0.044
H(36A)	0.4616	0.7267	0.7464	0.074
H(36B)	0.4058	0.8158	0.6862	0.074
H(36C)	0.4112	0.7146	0.6419	0.074
H(38A)	-0.0363	0.3758	0.5250	0.124
H(38B)	-0.0601	0.2635	0.5306	0.124
H(38C)	-0.1190	0.3282	0.4461	0.124
H(39A)	0.0300	0.1535	0.4184	0.104
H(39B)	-0.0699	0.1707	0.3629	0.104
H(39C)	-0.0283	0.1398	0.4641	0.104
H(40A)	-0.0022	0.3193	0.3358	0.136
H(40B)	0.0145	0.4126	0.3983	0.136
H(40C)	-0.0796	0.3727	0.3394	0.136
H(38D)	-0.1134	0.2361	0.4139	0.136
H(38E)	-0.0386	0.2199	0.5118	0.136
H(38F)	-0.0380	0.1615	0.4319	0.136
H(39D)	-0.0425	0.4093	0.5114	0.136
H(39E)	-0.0929	0.4238	0.4072	0.136
H(39F)	0.0035	0.4584	0.4616	0.136
H(40D)	0.0453	0.3558	0.3605	0.126
H(40E)	-0.0531	0.3288	0.3089	0.126
H(40F)	0.0158	0.2433	0.3515	0.126

Table S6. Torsion angles [°] for **1**.

Fe(1)-O(1)-N(5)-N(6)	10.0(14)	C(6)-C(7)-C(8)-C(9)	1.9(5)
O(1)-N(5)-N(6)-O(2)	9.2(16)	C(25)-C(7)-C(8)-C(9)	-173.2(5)
O(1)-N(5)-N(6)-C(37)	174.2(8)	C(6)-C(7)-C(8)-C(27)	177.2(5)
Fe(1)-O(2)-N(6)-N(5)	-23.2(14)	C(25)-C(7)-C(8)-C(27)	2.1(9)
Fe(1)-O(2)-N(6)-C(37)	170.2(5)	C(6)-N(2)-C(9)-C(10)	177.9(5)
Fe(1)-O(1')-N(5')-N(6')	0(3)	Fe(1)-N(2)-C(9)-C(10)	-25.4(6)
O(1')-N(5')-N(6')-O(2')	-19(3)	C(6)-N(2)-C(9)-C(8)	-0.1(5)
O(1')-N(5')-N(6')-C(37')	177.7(16)	Fe(1)-N(2)-C(9)-C(8)	156.6(3)
Fe(1)-O(2')-N(6')-N(5')	29(3)	C(7)-C(8)-C(9)-N(2)	-1.2(6)
Fe(1)-O(2')-N(6')-C(37')	-165.6(8)	C(27)-C(8)-C(9)-N(2)	-176.8(5)
C(4)-N(1)-C(1)-C(20)	177.8(5)	C(7)-C(8)-C(9)-C(10)	-179.1(5)
Fe(1)-N(1)-C(1)-C(20)	15.9(7)	C(27)-C(8)-C(9)-C(10)	5.3(8)
C(4)-N(1)-C(1)-C(2)	-1.6(6)	N(2)-C(9)-C(10)-C(11)	3.2(8)
Fe(1)-N(1)-C(1)-C(2)	-163.5(4)	C(8)-C(9)-C(10)-C(11)	-179.2(5)
C(20)-C(1)-C(2)-C(3)	-177.6(5)	C(9)-C(10)-C(11)-N(3)	1.3(8)
N(1)-C(1)-C(2)-C(3)	1.8(6)	C(9)-C(10)-C(11)-C(12)	178.0(5)
C(20)-C(1)-C(2)-C(21)	2.6(9)	C(14)-N(3)-C(11)-C(10)	176.8(4)
N(1)-C(1)-C(2)-C(21)	-178.0(5)	Fe(1)-N(3)-C(11)-C(10)	16.8(7)
C(1)-C(2)-C(3)-C(4)	-1.2(6)	C(14)-N(3)-C(11)-C(12)	-0.3(5)
C(21)-C(2)-C(3)-C(4)	178.6(6)	Fe(1)-N(3)-C(11)-C(12)	-160.3(3)
C(1)-C(2)-C(3)-C(23)	177.4(5)	C(10)-C(11)-C(12)-C(13)	-176.5(5)
C(21)-C(2)-C(3)-C(23)	-2.8(10)	N(3)-C(11)-C(12)-C(13)	0.6(5)
C(1)-N(1)-C(4)-C(5)	-177.8(5)	C(10)-C(11)-C(12)-C(29)	4.8(8)
Fe(1)-N(1)-C(4)-C(5)	-15.6(7)	N(3)-C(11)-C(12)-C(29)	-178.2(4)
C(1)-N(1)-C(4)-C(3)	0.9(6)	C(11)-C(12)-C(13)-C(14)	-0.5(5)
Fe(1)-N(1)-C(4)-C(3)	163.0(3)	C(29)-C(12)-C(13)-C(14)	178.1(5)
C(2)-C(3)-C(4)-C(5)	178.8(5)	C(11)-C(12)-C(13)-C(31)	178.9(4)
C(23)-C(3)-C(4)-C(5)	0.2(8)	C(29)-C(12)-C(13)-C(31)	-2.4(8)
C(2)-C(3)-C(4)-N(1)	0.2(6)	C(11)-N(3)-C(14)-C(15)	-179.8(4)
C(23)-C(3)-C(4)-N(1)	-178.4(5)	Fe(1)-N(3)-C(14)-C(15)	-19.7(7)
N(1)-C(4)-C(5)-C(6)	-3.4(8)	C(11)-N(3)-C(14)-C(13)	0.0(5)
C(3)-C(4)-C(5)-C(6)	178.1(5)	Fe(1)-N(3)-C(14)-C(13)	160.1(3)
C(9)-N(2)-C(6)-C(5)	-178.4(4)	C(12)-C(13)-C(14)-N(3)	0.3(5)
Fe(1)-N(2)-C(6)-C(5)	24.7(6)	C(31)-C(13)-C(14)-N(3)	-179.1(4)
C(9)-N(2)-C(6)-C(7)	1.3(5)	C(12)-C(13)-C(14)-C(15)	-179.8(5)
Fe(1)-N(2)-C(6)-C(7)	-155.7(3)	C(31)-C(13)-C(14)-C(15)	0.7(7)
C(4)-C(5)-C(6)-N(2)	-1.4(8)	N(3)-C(14)-C(15)-C(16)	-1.5(8)
C(4)-C(5)-C(6)-C(7)	179.1(5)	C(13)-C(14)-C(15)-C(16)	178.7(5)
N(2)-C(6)-C(7)-C(8)	-2.0(5)	C(14)-C(15)-C(16)-N(4)	3.6(8)
C(5)-C(6)-C(7)-C(8)	177.6(5)	C(14)-C(15)-C(16)-C(17)	-176.5(5)
N(2)-C(6)-C(7)-C(25)	173.4(4)	C(19)-N(4)-C(16)-C(15)	-179.3(4)
C(5)-C(6)-C(7)-C(25)	-6.9(8)	Fe(1)-N(4)-C(16)-C(15)	15.9(6)

C(19)-N(4)-C(16)-C(17)	0.8(5)	C(4)-C(3)-C(23)-C(24)	81.2(7)
Fe(1)-N(4)-C(16)-C(17)	-163.9(3)	C(8)-C(7)-C(25)-C(26)	100.9(7)
C(15)-C(16)-C(17)-C(18)	179.3(4)	C(6)-C(7)-C(25)-C(26)	-73.5(6)
N(4)-C(16)-C(17)-C(18)	-0.9(5)	C(7)-C(8)-C(27)-C(28)	-98.9(6)
C(15)-C(16)-C(17)-C(33)	3.9(7)	C(9)-C(8)-C(27)-C(28)	75.7(6)
N(4)-C(16)-C(17)-C(33)	-176.2(4)	C(13)-C(12)-C(29)-C(30)	-93.2(6)
C(16)-C(17)-C(18)-C(19)	0.6(5)	C(11)-C(12)-C(29)-C(30)	85.2(6)
C(33)-C(17)-C(18)-C(19)	175.7(4)	C(12)-C(13)-C(31)-C(32)	94.1(6)
C(16)-C(17)-C(18)-C(35)	-175.9(5)	C(14)-C(13)-C(31)-C(32)	-86.6(6)
C(33)-C(17)-C(18)-C(35)	-0.7(8)	C(18)-C(17)-C(33)-C(34)	-92.8(6)
C(16)-N(4)-C(19)-C(20)	175.4(5)	C(16)-C(17)-C(33)-C(34)	81.6(6)
Fe(1)-N(4)-C(19)-C(20)	-20.1(7)	C(17)-C(18)-C(35)-C(36)	95.4(6)
C(16)-N(4)-C(19)-C(18)	-0.5(5)	C(19)-C(18)-C(35)-C(36)	-80.4(6)
Fe(1)-N(4)-C(19)-C(18)	164.0(3)	N(5)-N(6)-C(37)-C(40)	130.5(11)
C(17)-C(18)-C(19)-N(4)	-0.1(5)	O(2)-N(6)-C(37)-C(40)	-64.0(9)
C(35)-C(18)-C(19)-N(4)	176.5(4)	N(5)-N(6)-C(37)-C(39)	-109.5(11)
C(17)-C(18)-C(19)-C(20)	-175.9(5)	O(2)-N(6)-C(37)-C(39)	56.1(9)
C(35)-C(18)-C(19)-C(20)	0.6(8)	N(5)-N(6)-C(37)-C(38)	10.8(12)
N(1)-C(1)-C(20)-C(19)	2.7(9)	O(2)-N(6)-C(37)-C(38)	176.4(9)
C(2)-C(1)-C(20)-C(19)	-178.0(5)	N(5')-N(6')-C(37')-C(38')	-42(2)
N(4)-C(19)-C(20)-C(1)	-0.7(8)	O(2')-N(6')-C(37')-C(38')	153.9(15)
C(18)-C(19)-C(20)-C(1)	174.7(5)	N(5')-N(6')-C(37')-C(39')	78(2)
C(3)-C(2)-C(21)-C(22)	92.9(7)	O(2')-N(6')-C(37')-C(39')	-85.9(15)
C(1)-C(2)-C(21)-C(22)	-87.3(7)	N(5')-N(6')-C(37')-C(40')	-162(2)
C(2)-C(3)-C(23)-C(24)	-97.1(7)	O(2')-N(6')-C(37')-C(40')	33.9(15)

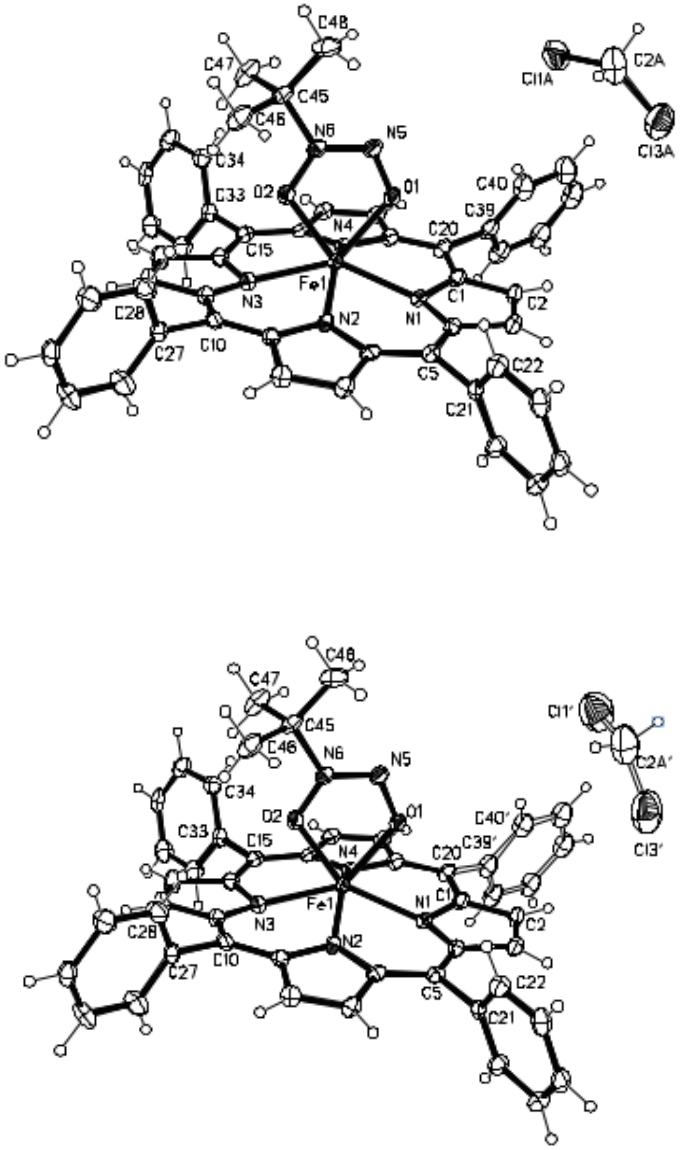

Figure S8. Molecular structure of **2**.CH_2Cl_2, showing the disordered CH_2Cl_2 and porphyrin phenyl (C39-C44) groups. The structure with the major disordered (85% occupancy) components is shown at the top.

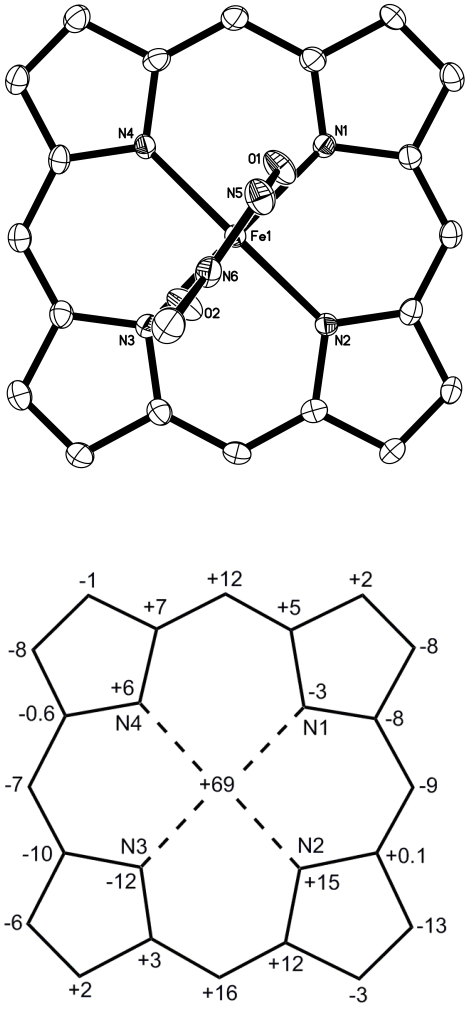

Figure S9. (*Top*) View of the bidentate ligand orientation relative to the porphyrin core, with the ligand facing the viewer. The peripheral por and C*Me*$_3$ substituents have been omitted for clarity. (*Bottom*) Perpendicular atom displacements (in units of 0.01 Å) of the porphyrin core from the 24-atom mean porphyrin plane..

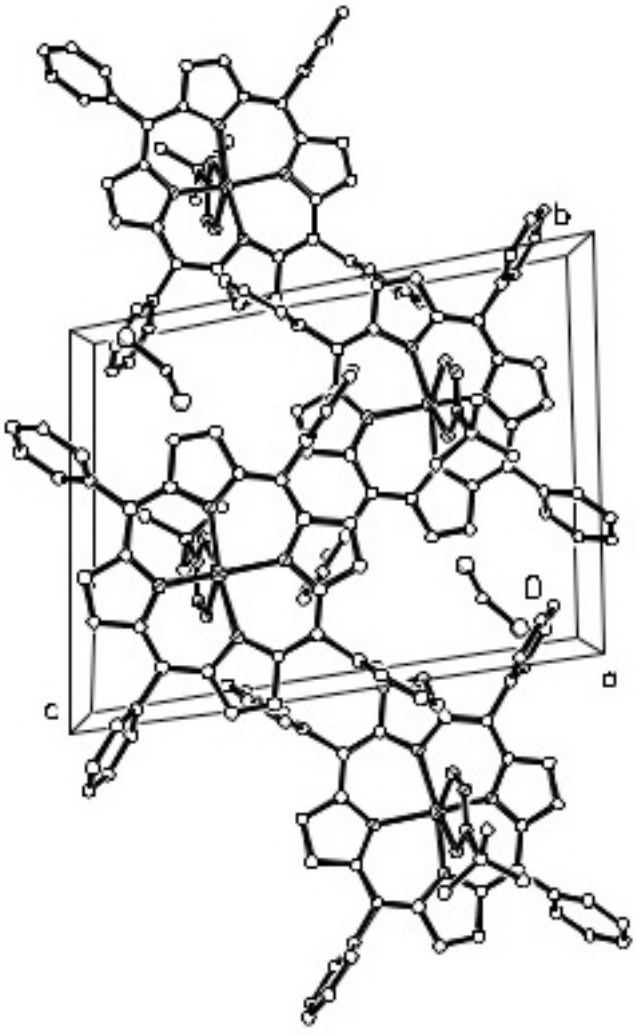

Figure S10. Crystal packing diagram for **2**.CH_2Cl_2.

Table S7. Atomic coordinates and equivalent isotropic displacement parameters for **2**.CH_2Cl_2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0.37891(5)	0.33868(3)	0.70196(3)	0.01301(13)
O(1)	0.2155(2)	0.23960(17)	0.72777(14)	0.0211(5)
O(2)	0.2404(2)	0.42560(18)	0.73179(15)	0.0227(5)
N(1)	0.4082(3)	0.1858(2)	0.66690(15)	0.0144(5)
N(2)	0.3218(3)	0.3444(2)	0.57937(15)	0.0144(5)
N(3)	0.4862(3)	0.4980(2)	0.71338(15)	0.0158(5)
N(4)	0.5403(3)	0.3369(2)	0.80695(15)	0.0144(5)
N(5)	0.1099(3)	0.2753(2)	0.74672(17)	0.0203(6)
N(6)	0.1266(3)	0.3723(2)	0.74775(15)	0.0164(6)
C(1)	0.4434(4)	0.1183(3)	0.72017(19)	0.0183(7)
C(2)	0.3988(4)	0.0129(3)	0.67831(18)	0.0202(7)
C(3)	0.3363(3)	0.0162(3)	0.6014(2)	0.0191(7)
C(4)	0.3397(3)	0.1238(2)	0.59388(18)	0.0153(6)
C(5)	0.2779(3)	0.1592(2)	0.52308(18)	0.0156(6)
C(6)	0.2728(3)	0.2627(2)	0.51717(18)	0.0158(6)
C(7)	0.2213(3)	0.3002(3)	0.44311(19)	0.0185(7)
C(8)	0.2371(3)	0.4041(3)	0.46068(19)	0.0196(7)
C(9)	0.3015(3)	0.4324(2)	0.54511(18)	0.0163(6)
C(10)	0.3446(3)	0.5345(2)	0.58441(19)	0.0167(6)
C(11)	0.4339(3)	0.5642(2)	0.66243(19)	0.0180(7)
C(12)	0.4821(4)	0.6697(3)	0.7024(2)	0.0247(8)
C(13)	0.5610(4)	0.6677(3)	0.7779(2)	0.0247(8)
C(14)	0.5618(3)	0.5599(2)	0.78525(19)	0.0177(7)
C(15)	0.6220(3)	0.5253(2)	0.85637(19)	0.0171(7)
C(16)	0.6136(3)	0.4209(2)	0.86543(18)	0.0159(6)
C(17)	0.6846(3)	0.3848(3)	0.93699(19)	0.0189(7)
C(18)	0.6535(4)	0.2803(2)	0.92200(19)	0.0208(7)
C(19)	0.5657(3)	0.2498(3)	0.84055(19)	0.0175(7)
C(20)	0.5155(4)	0.1472(2)	0.80228(17)	0.0192(7)
C(21)	0.2156(3)	0.0822(2)	0.44765(18)	0.0161(6)
C(22)	0.0659(4)	0.0500(3)	0.4147(2)	0.0232(7)
C(23)	0.0095(4)	-0.0181(3)	0.3434(2)	0.0248(8)
C(24)	0.1015(4)	-0.0553(3)	0.3045(2)	0.0237(7)
C(25)	0.2505(4)	-0.0247(3)	0.3369(2)	0.0256(8)
C(26)	0.3073(4)	0.0438(3)	0.4088(2)	0.0223(7)
C(27)	0.2912(3)	0.6164(2)	0.53830(18)	0.0163(6)
C(28)	0.1519(4)	0.6315(3)	0.5323(2)	0.0266(8)
C(29)	0.0989(4)	0.7057(3)	0.4888(2)	0.0299(8)

C(30)	0.1844(4)	0.7648(3)	0.4511(2)	0.0227(7)
C(31)	0.3227(4)	0.7492(3)	0.4563(2)	0.0294(8)
C(32)	0.3756(4)	0.6758(3)	0.5001(2)	0.0271(8)
C(33)	0.7004(3)	0.6057(2)	0.92855(19)	0.0177(7)
C(34)	0.6355(4)	0.6249(3)	0.9885(2)	0.0218(7)
C(35)	0.7070(4)	0.6998(3)	1.0553(2)	0.0254(8)
C(36)	0.8434(4)	0.7565(3)	1.0622(2)	0.0249(8)
C(37)	0.9093(4)	0.7389(3)	1.0025(2)	0.0282(8)
C(38)	0.8381(4)	0.6641(3)	0.9360(2)	0.0250(8)
C(39)	0.5332(3)	0.0589(2)	0.84905(14)	0.0240(8)
C(40)	0.4125(5)	-0.0023(3)	0.8631(2)	0.0306(8)
C(41)	0.4267(5)	-0.0844(3)	0.9057(2)	0.0370(9)
C(42)	0.5632(4)	-0.1061(3)	0.9358(2)	0.0353(9)
C(43)	0.6847(5)	-0.0466(3)	0.9227(2)	0.0332(8)
C(44)	0.6691(5)	0.0356(3)	0.8798(2)	0.0291(8)
C(39')	0.5730(16)	0.0660(6)	0.8477(3)	0.0282(13)
C(40')	0.4680(17)	-0.0002(11)	0.8708(5)	0.0309(12)
C(41')	0.5035(19)	-0.0795(12)	0.9132(7)	0.0333(12)
C(42')	0.646(2)	-0.0910(10)	0.9321(8)	0.0324(14)
C(43')	0.7537(17)	-0.0269(9)	0.9103(10)	0.0323(15)
C(44')	0.7160(16)	0.0518(7)	0.8676(8)	0.0296(13)
C(45)	0.0214(4)	0.4312(3)	0.77021(19)	0.0210(7)
C(46)	-0.0266(4)	0.4927(3)	0.7031(2)	0.0288(8)
C(47)	0.1045(4)	0.5024(3)	0.8484(2)	0.0316(9)
C(48)	-0.1071(4)	0.3550(3)	0.7790(2)	0.0313(9)
Cl(1A)	0.03876(16)	-0.04573(11)	0.88612(9)	0.0504(4)
C(2A)	-0.0740(7)	-0.1436(3)	0.8103(3)	0.0534(13)
Cl(3A)	0.02083(19)	-0.23180(13)	0.77907(9)	0.0596(5)
Cl(1')	0.0988(13)	-0.1253(9)	0.8802(6)	0.086(2)
C(2A')	0.015(2)	-0.171(3)	0.7789(8)	0.067(2)
Cl(3')	0.1338(13)	-0.2197(8)	0.7334(6)	0.084(3)

Table S8. Bond lengths [Å] and angles [°] for **2**.CH_2Cl_2.

Fe(1)-O(2)	2.050(2)	C(15)-C(33)	1.500(4)
Fe(1)-O(1)	2.051(2)	C(16)-C(17)	1.435(4)
Fe(1)-N(2)	2.085(3)	C(17)-C(18)	1.344(5)
Fe(1)-N(4)	2.087(3)	C(17)-H(17)	0.9500
Fe(1)-N(1)	2.141(3)	C(18)-C(19)	1.433(4)
Fe(1)-N(3)	2.144(3)	C(18)-H(18)	0.9500
O(1)-N(5)	1.306(3)	C(19)-C(20)	1.393(4)
O(2)-N(6)	1.313(3)	C(20)-C(39')	1.499(6)
N(1)-C(1)	1.375(4)	C(20)-C(39)	1.500(5)
N(1)-C(4)	1.379(4)	C(21)-C(26)	1.387(5)
N(2)-C(6)	1.375(4)	C(21)-C(22)	1.388(5)
N(2)-C(9)	1.382(4)	C(22)-C(23)	1.384(5)
N(3)-C(14)	1.375(4)	C(22)-H(22)	0.9500
N(3)-C(11)	1.377(4)	C(23)-C(24)	1.383(5)
N(4)-C(19)	1.376(4)	C(23)-H(23)	0.9500
N(4)-C(16)	1.378(4)	C(24)-C(25)	1.380(5)
N(5)-N(6)	1.261(4)	C(24)-H(24)	0.9500
N(6)-C(45)	1.495(4)	C(25)-C(26)	1.394(5)
C(1)-C(20)	1.405(4)	C(25)-H(25)	0.9500
C(1)-C(2)	1.442(4)	C(26)-H(26)	0.9500
C(2)-C(3)	1.333(5)	C(27)-C(32)	1.379(5)
C(2)-H(2)	0.9500	C(27)-C(28)	1.382(5)
C(3)-C(4)	1.437(4)	C(28)-C(29)	1.390(5)
C(3)-H(3)	0.9500	C(28)-H(28)	0.9500
C(4)-C(5)	1.394(4)	C(29)-C(30)	1.379(5)
C(5)-C(6)	1.390(5)	C(29)-H(29)	0.9500
C(5)-C(21)	1.498(4)	C(30)-C(31)	1.378(5)
C(6)-C(7)	1.434(4)	C(30)-H(30)	0.9500
C(7)-C(8)	1.349(5)	C(31)-C(32)	1.383(5)
C(7)-H(7)	0.9500	C(31)-H(31)	0.9500
C(8)-C(9)	1.428(4)	C(32)-H(32)	0.9500
C(8)-H(8)	0.9500	C(33)-C(34)	1.384(5)
C(9)-C(10)	1.391(5)	C(33)-C(38)	1.389(5)
C(10)-C(11)	1.388(4)	C(34)-C(35)	1.389(5)
C(10)-C(27)	1.499(4)	C(34)-H(34)	0.9500
C(11)-C(12)	1.435(5)	C(35)-C(36)	1.373(5)
C(12)-C(13)	1.350(5)	C(35)-H(35)	0.9500
C(12)-H(12)	0.9500	C(36)-C(37)	1.383(5)
C(13)-C(14)	1.444(5)	C(36)-H(36)	0.9500
C(13)-H(13)	0.9500	C(37)-C(38)	1.385(5)
C(14)-C(15)	1.389(5)	C(37)-H(37)	0.9500
C(15)-C(16)	1.396(5)	C(38)-H(38)	0.9500

C(39)-C(44)	1.392(4)	C(44')-H(44')	0.9500
C(39)-C(40)	1.395(4)	C(45)-C(48)	1.513(5)
C(40)-C(41)	1.384(4)	C(45)-C(46)	1.517(5)
C(40)-H(40)	0.9500	C(45)-C(47)	1.520(5)
C(41)-C(42)	1.386(4)	C(46)-H(46A)	0.9800
C(41)-H(41)	0.9500	C(46)-H(46B)	0.9800
C(42)-C(43)	1.384(4)	C(46)-H(46C)	0.9800
C(42)-H(42)	0.9500	C(47)-H(47A)	0.9800
C(43)-C(44)	1.389(4)	C(47)-H(47B)	0.9800
C(43)-H(43)	0.9500	C(47)-H(47C)	0.9800
C(44)-H(44)	0.9500	C(48)-H(48A)	0.9800
C(39')-C(40')	1.394(5)	C(48)-H(48B)	0.9800
C(39')-C(44')	1.394(5)	C(48)-H(48C)	0.9800
C(40')-C(41')	1.385(5)	Cl(1A)-C(2A)	1.741(4)
C(40')-H(40')	0.9500	C(2A)-Cl(3A)	1.739(4)
C(41')-C(42')	1.381(5)	C(2A)-H(2A1)	0.9900
C(41')-H(41')	0.9500	C(2A)-H(2A2)	0.9900
C(42')-C(43')	1.383(5)	Cl(1')-C(2A')	1.741(5)
C(42')-H(42')	0.9500	C(2A')-Cl(3')	1.742(5)
C(43')-C(44')	1.387(5)	C(2A')-H(2A3)	0.9900
C(43')-H(43')	0.9500	C(2A')-H(2A4)	0.9900

O(2)-Fe(1)-O(1)	72.31(9)	C(14)-N(3)-C(11)	105.9(3)
O(2)-Fe(1)-N(2)	97.97(10)	C(14)-N(3)-Fe(1)	124.1(2)
O(1)-Fe(1)-N(2)	109.17(10)	C(11)-N(3)-Fe(1)	122.8(2)
O(2)-Fe(1)-N(4)	107.43(10)	C(19)-N(4)-C(16)	106.1(3)
O(1)-Fe(1)-N(4)	96.13(10)	C(19)-N(4)-Fe(1)	125.5(2)
N(2)-Fe(1)-N(4)	148.61(10)	C(16)-N(4)-Fe(1)	126.4(2)
O(2)-Fe(1)-N(1)	146.06(10)	N(6)-N(5)-O(1)	111.8(3)
O(1)-Fe(1)-N(1)	74.99(9)	N(5)-N(6)-O(2)	120.8(3)
N(2)-Fe(1)-N(1)	84.26(10)	N(5)-N(6)-C(45)	121.4(3)
N(4)-Fe(1)-N(1)	84.72(10)	O(2)-N(6)-C(45)	117.7(3)
O(2)-Fe(1)-N(3)	74.14(10)	N(1)-C(1)-C(20)	125.5(3)
O(1)-Fe(1)-N(3)	145.08(10)	N(1)-C(1)-C(2)	109.5(3)
N(2)-Fe(1)-N(3)	84.76(10)	C(20)-C(1)-C(2)	125.0(3)
N(4)-Fe(1)-N(3)	84.77(10)	C(3)-C(2)-C(1)	107.9(3)
N(1)-Fe(1)-N(3)	139.52(10)	C(3)-C(2)-H(2)	126.0
N(5)-O(1)-Fe(1)	120.02(19)	C(1)-C(2)-H(2)	126.0
N(6)-O(2)-Fe(1)	115.01(18)	C(2)-C(3)-C(4)	106.8(3)
C(1)-N(1)-C(4)	105.4(3)	C(2)-C(3)-H(3)	126.6
C(1)-N(1)-Fe(1)	123.2(2)	C(4)-C(3)-H(3)	126.6
C(4)-N(1)-Fe(1)	126.0(2)	N(1)-C(4)-C(5)	125.3(3)
C(6)-N(2)-C(9)	105.8(2)	N(1)-C(4)-C(3)	110.3(3)
C(6)-N(2)-Fe(1)	128.2(2)	C(5)-C(4)-C(3)	124.3(3)
C(9)-N(2)-Fe(1)	125.2(2)	C(6)-C(5)-C(4)	124.2(3)

C(6)-C(5)-C(21)	117.2(3)	C(19)-C(20)-C(39')	116.3(4)
C(4)-C(5)-C(21)	118.6(3)	C(1)-C(20)-C(39')	118.0(3)
N(2)-C(6)-C(5)	126.0(3)	C(19)-C(20)-C(39)	120.4(2)
N(2)-C(6)-C(7)	109.9(3)	C(1)-C(20)-C(39)	115.5(2)
C(5)-C(6)-C(7)	124.0(3)	C(26)-C(21)-C(22)	119.1(3)
C(8)-C(7)-C(6)	107.1(3)	C(26)-C(21)-C(5)	120.2(3)
C(8)-C(7)-H(7)	126.5	C(22)-C(21)-C(5)	120.7(3)
C(6)-C(7)-H(7)	126.5	C(23)-C(22)-C(21)	120.2(3)
C(7)-C(8)-C(9)	107.5(3)	C(23)-C(22)-H(22)	119.9
C(7)-C(8)-H(8)	126.3	C(21)-C(22)-H(22)	119.9
C(9)-C(8)-H(8)	126.3	C(24)-C(23)-C(22)	120.4(3)
N(2)-C(9)-C(10)	126.3(3)	C(24)-C(23)-H(23)	119.8
N(2)-C(9)-C(8)	109.7(3)	C(22)-C(23)-H(23)	119.8
C(10)-C(9)-C(8)	123.9(3)	C(25)-C(24)-C(23)	120.0(3)
C(11)-C(10)-C(9)	124.0(3)	C(25)-C(24)-H(24)	120.0
C(11)-C(10)-C(27)	118.9(3)	C(23)-C(24)-H(24)	120.0
C(9)-C(10)-C(27)	117.0(3)	C(24)-C(25)-C(26)	119.6(3)
N(3)-C(11)-C(10)	125.8(3)	C(24)-C(25)-H(25)	120.2
N(3)-C(11)-C(12)	110.0(3)	C(26)-C(25)-H(25)	120.2
C(10)-C(11)-C(12)	124.2(3)	C(21)-C(26)-C(25)	120.7(3)
C(13)-C(12)-C(11)	107.3(3)	C(21)-C(26)-H(26)	119.7
C(13)-C(12)-H(12)	126.4	C(25)-C(26)-H(26)	119.7
C(11)-C(12)-H(12)	126.4	C(32)-C(27)-C(28)	118.9(3)
C(12)-C(13)-C(14)	107.0(3)	C(32)-C(27)-C(10)	122.1(3)
C(12)-C(13)-H(13)	126.5	C(28)-C(27)-C(10)	119.1(3)
C(14)-C(13)-H(13)	126.5	C(27)-C(28)-C(29)	120.2(3)
N(3)-C(14)-C(15)	125.9(3)	C(27)-C(28)-H(28)	119.9
N(3)-C(14)-C(13)	109.8(3)	C(29)-C(28)-H(28)	119.9
C(15)-C(14)-C(13)	124.1(3)	C(30)-C(29)-C(28)	120.4(3)
C(14)-C(15)-C(16)	124.5(3)	C(30)-C(29)-H(29)	119.8
C(14)-C(15)-C(33)	117.7(3)	C(28)-C(29)-H(29)	119.8
C(16)-C(15)-C(33)	117.7(3)	C(31)-C(30)-C(29)	119.5(3)
N(4)-C(16)-C(15)	125.7(3)	C(31)-C(30)-H(30)	120.3
N(4)-C(16)-C(17)	109.6(3)	C(29)-C(30)-H(30)	120.3
C(15)-C(16)-C(17)	124.7(3)	C(30)-C(31)-C(32)	120.0(3)
C(18)-C(17)-C(16)	107.2(3)	C(30)-C(31)-H(31)	120.0
C(18)-C(17)-H(17)	126.4	C(32)-C(31)-H(31)	120.0
C(16)-C(17)-H(17)	126.4	C(27)-C(32)-C(31)	121.1(3)
C(17)-C(18)-C(19)	107.5(3)	C(27)-C(32)-H(32)	119.5
C(17)-C(18)-H(18)	126.2	C(31)-C(32)-H(32)	119.5
C(19)-C(18)-H(18)	126.2	C(34)-C(33)-C(38)	118.5(3)
N(4)-C(19)-C(20)	126.0(3)	C(34)-C(33)-C(15)	120.6(3)
N(4)-C(19)-C(18)	109.6(3)	C(38)-C(33)-C(15)	121.0(3)
C(20)-C(19)-C(18)	124.4(3)	C(33)-C(34)-C(35)	120.9(3)
C(19)-C(20)-C(1)	124.1(3)	C(33)-C(34)-H(34)	119.6

C(35)-C(34)-H(34)	119.6	C(42')-C(43')-C(44')	118.6(7)
C(36)-C(35)-C(34)	120.1(3)	C(42')-C(43')-H(43')	120.7
C(36)-C(35)-H(35)	120.0	C(44')-C(43')-H(43')	120.7
C(34)-C(35)-H(35)	120.0	C(43')-C(44')-C(39')	120.3(7)
C(35)-C(36)-C(37)	119.8(3)	C(43')-C(44')-H(44')	119.8
C(35)-C(36)-H(36)	120.1	C(39')-C(44')-H(44')	119.8
C(37)-C(36)-H(36)	120.1	N(6)-C(45)-C(48)	109.2(3)
C(36)-C(37)-C(38)	120.1(3)	N(6)-C(45)-C(46)	106.7(3)
C(36)-C(37)-H(37)	120.0	C(48)-C(45)-C(46)	110.8(3)
C(38)-C(37)-H(37)	120.0	N(6)-C(45)-C(47)	106.5(3)
C(37)-C(38)-C(33)	120.7(3)	C(48)-C(45)-C(47)	111.9(3)
C(37)-C(38)-H(38)	119.7	C(46)-C(45)-C(47)	111.5(3)
C(33)-C(38)-H(38)	119.7	C(45)-C(46)-H(46A)	109.5
C(44)-C(39)-C(40)	118.1(4)	C(45)-C(46)-H(46B)	109.5
C(44)-C(39)-C(20)	121.5(3)	H(46A)-C(46)-H(46B)	109.5
C(40)-C(39)-C(20)	120.5(3)	C(45)-C(46)-H(46C)	109.5
C(41)-C(40)-C(39)	121.2(4)	H(46A)-C(46)-H(46C)	109.5
C(41)-C(40)-H(40)	119.4	H(46B)-C(46)-H(46C)	109.5
C(39)-C(40)-H(40)	119.4	C(45)-C(47)-H(47A)	109.5
C(40)-C(41)-C(42)	119.6(4)	C(45)-C(47)-H(47B)	109.5
C(40)-C(41)-H(41)	120.2	H(47A)-C(47)-H(47B)	109.5
C(42)-C(41)-H(41)	120.2	C(45)-C(47)-H(47C)	109.5
C(43)-C(42)-C(41)	120.3(4)	H(47A)-C(47)-H(47C)	109.5
C(43)-C(42)-H(42)	119.9	H(47B)-C(47)-H(47C)	109.5
C(41)-C(42)-H(42)	119.9	C(45)-C(48)-H(48A)	109.5
C(42)-C(43)-C(44)	119.6(4)	C(45)-C(48)-H(48B)	109.5
C(42)-C(43)-H(43)	120.2	H(48A)-C(48)-H(48B)	109.5
C(44)-C(43)-H(43)	120.2	C(45)-C(48)-H(48C)	109.5
C(43)-C(44)-C(39)	121.2(4)	H(48A)-C(48)-H(48C)	109.5
C(43)-C(44)-H(44)	119.4	H(48B)-C(48)-H(48C)	109.5
C(39)-C(44)-H(44)	119.4	Cl(3A)-C(2A)-Cl(1A)	112.2(3)
C(40')-C(39')-C(44')	119.3(7)	Cl(3A)-C(2A)-H(2A1)	109.2
C(40')-C(39')-C(20)	114.0(9)	Cl(1A)-C(2A)-H(2A1)	109.2
C(44')-C(39')-C(20)	126.7(10)	Cl(3A)-C(2A)-H(2A2)	109.2
C(41')-C(40')-C(39')	121.2(7)	Cl(1A)-C(2A)-H(2A2)	109.2
C(41')-C(40')-H(40')	119.4	H(2A1)-C(2A)-H(2A2)	107.9
C(39')-C(40')-H(40')	119.4	Cl(1')-C(2A')-Cl(3')	111.1(6)
C(42')-C(41')-C(40')	117.9(7)	Cl(1')-C(2A')-H(2A3)	109.4
C(42')-C(41')-H(41')	121.0	Cl(3')-C(2A')-H(2A3)	109.4
C(40')-C(41')-H(41')	121.0	Cl(1')-C(2A')-H(2A4)	109.4
C(41')-C(42')-C(43')	122.7(8)	Cl(3')-C(2A')-H(2A4)	109.4
C(41')-C(42')-H(42')	118.7	H(2A3)-C(2A')-H(2A4)	108.0
C(43')-C(42')-H(42')	118.7		

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**.CH_2Cl_2. 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}
Fe(1)	13(1)	12(1)	13(1)	1(1)	2(1)	3(1)
O(1)	18(1)	15(1)	33(1)	0(1)	12(1)	5(1)
O(2)	22(1)	15(1)	35(1)	4(1)	14(1)	5(1)
N(1)	15(1)	15(1)	13(1)	1(1)	3(1)	5(1)
N(2)	14(1)	13(1)	15(1)	1(1)	2(1)	4(1)
N(3)	16(1)	15(1)	14(1)	2(1)	2(1)	2(1)
N(4)	14(1)	13(1)	15(1)	-1(1)	3(1)	3(1)
N(5)	19(1)	18(2)	24(2)	-2(1)	8(1)	4(1)
N(6)	16(1)	18(2)	14(1)	-1(1)	3(1)	5(1)
C(1)	22(2)	16(2)	18(2)	2(1)	6(1)	9(1)
C(2)	27(2)	12(2)	21(2)	1(1)	5(1)	6(1)
C(3)	19(2)	15(2)	22(2)	-2(1)	5(1)	4(1)
C(4)	13(1)	15(2)	17(2)	1(1)	3(1)	4(1)
C(5)	11(1)	18(2)	17(2)	0(1)	3(1)	3(1)
C(6)	13(1)	20(2)	14(2)	0(1)	3(1)	5(1)
C(7)	19(2)	19(2)	13(2)	-1(1)	0(1)	3(1)
C(8)	19(2)	22(2)	16(2)	4(1)	0(1)	5(1)
C(9)	16(2)	18(2)	16(2)	5(1)	5(1)	5(1)
C(10)	18(2)	15(2)	20(2)	6(1)	7(1)	4(1)
C(11)	19(2)	15(2)	19(2)	2(1)	6(1)	2(1)
C(12)	31(2)	14(2)	24(2)	5(1)	1(2)	1(1)
C(13)	29(2)	16(2)	23(2)	-1(1)	0(1)	0(1)
C(14)	17(2)	16(2)	18(2)	1(1)	4(1)	0(1)
C(15)	15(2)	18(2)	17(2)	-1(1)	4(1)	2(1)
C(16)	15(2)	19(2)	14(2)	-2(1)	5(1)	4(1)
C(17)	17(2)	22(2)	15(2)	-1(1)	2(1)	5(1)
C(18)	24(2)	23(2)	16(2)	2(1)	3(1)	10(1)
C(19)	19(2)	20(2)	16(2)	5(1)	4(1)	9(1)
C(20)	23(2)	19(2)	17(2)	3(1)	4(1)	12(1)
C(21)	20(2)	11(2)	16(2)	2(1)	4(1)	3(1)
C(22)	21(2)	23(2)	25(2)	1(1)	5(1)	5(1)
C(23)	21(2)	20(2)	27(2)	2(1)	-1(1)	-1(1)
C(24)	30(2)	17(2)	17(2)	-2(1)	2(1)	-3(1)
C(25)	32(2)	24(2)	21(2)	-2(1)	11(2)	6(2)
C(26)	20(2)	21(2)	22(2)	-4(1)	5(1)	0(1)
C(27)	18(2)	12(2)	15(2)	0(1)	1(1)	1(1)

C(28)	28(2)	29(2)	32(2)	17(2)	14(2)	13(2)
C(29)	30(2)	33(2)	37(2)	17(2)	15(2)	18(2)
C(30)	31(2)	16(2)	20(2)	5(1)	1(1)	8(1)
C(31)	25(2)	28(2)	33(2)	16(2)	6(2)	-2(2)
C(32)	15(2)	32(2)	35(2)	14(2)	6(1)	4(1)
C(33)	19(2)	16(2)	15(2)	3(1)	0(1)	4(1)
C(34)	21(2)	20(2)	23(2)	2(1)	5(1)	4(1)
C(35)	33(2)	24(2)	18(2)	1(1)	3(1)	11(2)
C(36)	33(2)	14(2)	21(2)	0(1)	-4(1)	8(1)
C(37)	23(2)	23(2)	31(2)	0(2)	2(2)	-3(2)
C(38)	23(2)	26(2)	24(2)	1(2)	7(1)	2(1)
C(39)	35(2)	22(2)	17(1)	1(1)	5(1)	16(1)
C(40)	38(2)	28(2)	25(2)	9(1)	3(1)	11(2)
C(41)	46(2)	31(2)	31(2)	10(2)	2(2)	8(2)
C(42)	49(2)	28(2)	27(2)	6(2)	1(2)	16(2)
C(43)	45(2)	30(2)	25(2)	5(1)	2(1)	18(2)
C(44)	38(2)	28(2)	22(1)	2(1)	5(1)	16(1)
C(39')	38(2)	25(2)	21(2)	4(2)	4(2)	15(2)
C(40')	40(2)	27(2)	25(2)	6(2)	4(2)	13(2)
C(41')	43(2)	29(2)	27(2)	7(2)	3(2)	14(2)
C(42')	43(2)	28(2)	25(2)	5(2)	3(2)	16(2)
C(43')	43(3)	29(2)	24(2)	3(2)	3(2)	16(2)
C(44')	40(2)	27(2)	22(2)	3(2)	3(2)	17(2)
C(45)	21(2)	26(2)	19(2)	0(1)	6(1)	14(1)
C(46)	34(2)	32(2)	25(2)	5(2)	7(2)	21(2)
C(47)	38(2)	33(2)	23(2)	-5(2)	1(2)	19(2)
C(48)	24(2)	43(2)	34(2)	8(2)	16(2)	15(2)
Cl(1A)	52(1)	41(1)	50(1)	-2(1)	15(1)	-6(1)
C(2A)	62(3)	36(2)	52(3)	7(2)	6(2)	1(2)
Cl(3A)	82(1)	45(1)	47(1)	0(1)	14(1)	13(1)
Cl(1')	87(4)	78(4)	80(4)	6(4)	16(4)	-1(4)
C(2A')	78(4)	47(4)	61(4)	5(3)	5(3)	1(3)
Cl(3')	99(5)	60(4)	71(4)	-5(4)	4(4)	-4(4)

Table S10. Hydrogen coordinates and isotropic displacement parameters for **2**.CH_2Cl_2.

	x	y	z	U(eq)
H(2)	0.4116	-0.0480	0.7015	0.024
H(3)	0.2972	-0.0415	0.5596	0.023
H(7)	0.1831	0.2596	0.3914	0.022
H(8)	0.2103	0.4500	0.4237	0.024
H(12)	0.4623	0.7299	0.6799	0.030
H(13)	0.6071	0.7260	0.8185	0.030
H(17)	0.7428	0.4269	0.9859	0.023
H(18)	0.6842	0.2349	0.9587	0.025
H(22)	0.0020	0.0749	0.4412	0.028
H(23)	-0.0931	-0.0395	0.3210	0.030
H(24)	0.0621	-0.1019	0.2555	0.028
H(25)	0.3140	-0.0501	0.3104	0.031
H(26)	0.4099	0.0644	0.4315	0.027
H(28)	0.0922	0.5910	0.5581	0.032
H(29)	0.0032	0.7157	0.4850	0.036
H(30)	0.1483	0.8160	0.4218	0.027
H(31)	0.3818	0.7888	0.4297	0.035
H(32)	0.4716	0.6662	0.5041	0.033
H(34)	0.5409	0.5863	0.9840	0.026
H(35)	0.6614	0.7118	1.0961	0.031
H(36)	0.8924	0.8076	1.1079	0.030
H(37)	1.0036	0.7782	1.0070	0.034
H(38)	0.8838	0.6526	0.8951	0.030
H(40)	0.3189	0.0127	0.8430	0.037
H(41)	0.3433	-0.1257	0.9143	0.044
H(42)	0.5735	-0.1620	0.9655	0.042
H(43)	0.7781	-0.0619	0.9429	0.040
H(44)	0.7528	0.0766	0.8714	0.035
H(40')	0.3705	0.0093	0.8573	0.037
H(41')	0.4318	-0.1247	0.9288	0.040
H(42')	0.6721	-0.1451	0.9612	0.039
H(43')	0.8511	-0.0367	0.9243	0.039
H(44')	0.7881	0.0963	0.8519	0.036
H(46A)	0.0587	0.5393	0.6969	0.043
H(46B)	-0.0944	0.5339	0.7159	0.043
H(46C)	-0.0752	0.4448	0.6530	0.043
H(47A)	0.1384	0.4605	0.8898	0.047
H(47B)	0.0402	0.5438	0.8652	0.047

H(47C)	0.1885	0.5490	0.8408	0.047
H(48A)	-0.1518	0.3060	0.7291	0.047
H(48B)	-0.1789	0.3930	0.7907	0.047
H(48C)	-0.0738	0.3166	0.8230	0.047
H(2A1)	-0.1522	-0.1812	0.8299	0.064
H(2A2)	-0.1204	-0.1118	0.7641	0.064
H(2A3)	-0.0177	-0.1129	0.7521	0.080
H(2A4)	-0.0721	-0.2259	0.7727	0.080

Table S11. Torsion angles [°] for **2**.CH_2Cl_2.

Fe(1)-O(1)-N(5)-N(6)	-1.2(3)	C(8)-C(9)-C(10)-C(27)	13.5(5)
O(1)-N(5)-N(6)-O(2)	-0.6(4)	C(14)-N(3)-C(11)-C(10)	-176.4(3)
O(1)-N(5)-N(6)-C(45)	-178.2(3)	Fe(1)-N(3)-C(11)-C(10)	-24.9(4)
Fe(1)-O(2)-N(6)-N(5)	2.2(4)	C(14)-N(3)-C(11)-C(12)	2.1(4)
Fe(1)-O(2)-N(6)-C(45)	179.80(19)	Fe(1)-N(3)-C(11)-C(12)	153.6(2)
C(4)-N(1)-C(1)-C(20)	179.8(3)	C(9)-C(10)-C(11)-N(3)	-3.6(5)
Fe(1)-N(1)-C(1)-C(20)	-24.8(4)	C(27)-C(10)-C(11)-N(3)	177.0(3)
C(4)-N(1)-C(1)-C(2)	1.5(3)	C(9)-C(10)-C(11)-C(12)	178.0(3)
Fe(1)-N(1)-C(1)-C(2)	156.9(2)	C(27)-C(10)-C(11)-C(12)	-1.3(5)
N(1)-C(1)-C(2)-C(3)	-0.7(4)	N(3)-C(11)-C(12)-C(13)	-1.3(4)
C(20)-C(1)-C(2)-C(3)	-178.9(3)	C(10)-C(11)-C(12)-C(13)	177.3(3)
C(1)-C(2)-C(3)-C(4)	-0.5(4)	C(11)-C(12)-C(13)-C(14)	-0.1(4)
C(1)-N(1)-C(4)-C(5)	176.2(3)	C(11)-N(3)-C(14)-C(15)	173.6(3)
Fe(1)-N(1)-C(4)-C(5)	21.6(4)	Fe(1)-N(3)-C(14)-C(15)	22.6(4)
C(1)-N(1)-C(4)-C(3)	-1.8(3)	C(11)-N(3)-C(14)-C(13)	-2.2(4)
Fe(1)-N(1)-C(4)-C(3)	-156.4(2)	Fe(1)-N(3)-C(14)-C(13)	-153.2(2)
C(2)-C(3)-C(4)-N(1)	1.5(4)	C(12)-C(13)-C(14)-N(3)	1.4(4)
C(2)-C(3)-C(4)-C(5)	-176.6(3)	C(12)-C(13)-C(14)-C(15)	-174.5(3)
N(1)-C(4)-C(5)-C(6)	-2.2(5)	N(3)-C(14)-C(15)-C(16)	-0.4(5)
C(3)-C(4)-C(5)-C(6)	175.5(3)	C(13)-C(14)-C(15)-C(16)	174.9(3)
N(1)-C(4)-C(5)-C(21)	176.3(3)	N(3)-C(14)-C(15)-C(33)	-179.9(3)
C(3)-C(4)-C(5)-C(21)	-6.0(5)	C(13)-C(14)-C(15)-C(33)	-4.6(5)
C(9)-N(2)-C(6)-C(5)	177.0(3)	C(19)-N(4)-C(16)-C(15)	177.6(3)
Fe(1)-N(2)-C(6)-C(5)	-13.4(4)	Fe(1)-N(4)-C(16)-C(15)	-17.9(4)
C(9)-N(2)-C(6)-C(7)	0.0(3)	C(19)-N(4)-C(16)-C(17)	-0.6(3)
Fe(1)-N(2)-C(6)-C(7)	169.6(2)	Fe(1)-N(4)-C(16)-C(17)	164.0(2)
C(4)-C(5)-C(6)-N(2)	-2.6(5)	C(14)-C(15)-C(16)-N(4)	-2.7(5)
C(21)-C(5)-C(6)-N(2)	178.9(3)	C(33)-C(15)-C(16)-N(4)	176.7(3)
C(4)-C(5)-C(6)-C(7)	174.0(3)	C(14)-C(15)-C(16)-C(17)	175.1(3)
C(21)-C(5)-C(6)-C(7)	-4.5(4)	C(33)-C(15)-C(16)-C(17)	-5.4(5)
N(2)-C(6)-C(7)-C(8)	-0.9(4)	N(4)-C(16)-C(17)-C(18)	-0.5(4)
C(5)-C(6)-C(7)-C(8)	-178.0(3)	C(15)-C(16)-C(17)-C(18)	-178.6(3)
C(6)-C(7)-C(8)-C(9)	1.4(4)	C(16)-C(17)-C(18)-C(19)	1.3(4)
C(6)-N(2)-C(9)-C(10)	-175.3(3)	C(16)-N(4)-C(19)-C(20)	-178.3(3)
Fe(1)-N(2)-C(9)-C(10)	14.6(4)	Fe(1)-N(4)-C(19)-C(20)	16.9(4)
C(6)-N(2)-C(9)-C(8)	0.9(3)	C(16)-N(4)-C(19)-C(18)	1.4(3)
Fe(1)-N(2)-C(9)-C(8)	-169.1(2)	Fe(1)-N(4)-C(19)-C(18)	-163.4(2)
C(7)-C(8)-C(9)-N(2)	-1.4(4)	C(17)-C(18)-C(19)-N(4)	-1.7(4)
C(7)-C(8)-C(9)-C(10)	174.9(3)	C(17)-C(18)-C(19)-C(20)	178.0(3)
N(2)-C(9)-C(10)-C(11)	9.9(5)	N(4)-C(19)-C(20)-C(1)	7.1(5)
C(8)-C(9)-C(10)-C(11)	-165.8(3)	C(18)-C(19)-C(20)-C(1)	-172.6(3)
N(2)-C(9)-C(10)-C(27)	-170.8(3)	N(4)-C(19)-C(20)-C(39')	172.4(7)

C(18)-C(19)-C(20)-C(39')	-7.3(7)	C(15)-C(33)-C(34)-C(35)	-179.5(3)
N(4)-C(19)-C(20)-C(39)	-171.3(3)	C(33)-C(34)-C(35)-C(36)	0.4(5)
C(18)-C(19)-C(20)-C(39)	9.0(5)	C(34)-C(35)-C(36)-C(37)	0.1(5)
N(1)-C(1)-C(20)-C(19)	-2.2(5)	C(35)-C(36)-C(37)-C(38)	-0.2(5)
C(2)-C(1)-C(20)-C(19)	175.8(3)	C(36)-C(37)-C(38)-C(33)	-0.2(5)
N(1)-C(1)-C(20)-C(39')	-167.3(7)	C(34)-C(33)-C(38)-C(37)	0.7(5)
C(2)-C(1)-C(20)-C(39')	10.7(8)	C(15)-C(33)-C(38)-C(37)	179.4(3)
N(1)-C(1)-C(20)-C(39)	176.2(3)	C(19)-C(20)-C(39)-C(44)	-71.2(3)
C(2)-C(1)-C(20)-C(39)	-5.7(5)	C(1)-C(20)-C(39)-C(44)	110.3(3)
C(6)-C(5)-C(21)-C(26)	103.3(4)	C(19)-C(20)-C(39)-C(40)	108.6(3)
C(4)-C(5)-C(21)-C(26)	-75.3(4)	C(1)-C(20)-C(39)-C(40)	-69.9(3)
C(6)-C(5)-C(21)-C(22)	-75.3(4)	C(44)-C(39)-C(40)-C(41)	-0.5(3)
C(4)-C(5)-C(21)-C(22)	106.1(4)	C(20)-C(39)-C(40)-C(41)	179.6(2)
C(26)-C(21)-C(22)-C(23)	-1.1(5)	C(39)-C(40)-C(41)-C(42)	0.6(4)
C(5)-C(21)-C(22)-C(23)	177.5(3)	C(40)-C(41)-C(42)-C(43)	-0.6(5)
C(21)-C(22)-C(23)-C(24)	0.4(5)	C(41)-C(42)-C(43)-C(44)	0.6(5)
C(22)-C(23)-C(24)-C(25)	0.2(5)	C(42)-C(43)-C(44)-C(39)	-0.5(5)
C(23)-C(24)-C(25)-C(26)	0.0(5)	C(40)-C(39)-C(44)-C(43)	0.5(4)
C(22)-C(21)-C(26)-C(25)	1.2(5)	C(20)-C(39)-C(44)-C(43)	-179.6(2)
C(5)-C(21)-C(26)-C(25)	-177.4(3)	C(19)-C(20)-C(39')-C(40')	112.7(5)
C(24)-C(25)-C(26)-C(21)	-0.7(5)	C(1)-C(20)-C(39')-C(40')	-81.1(6)
C(11)-C(10)-C(27)-C(32)	81.9(4)	C(19)-C(20)-C(39')-C(44')	-67.5(5)
C(9)-C(10)-C(27)-C(32)	-97.5(4)	C(1)-C(20)-C(39')-C(44')	98.8(6)
C(11)-C(10)-C(27)-C(28)	-99.5(4)	C(44')-C(39')-C(40')-C(41')	0.0(3)
C(9)-C(10)-C(27)-C(28)	81.1(4)	C(20)-C(39')-C(40')-C(41')	179.9(2)
C(32)-C(27)-C(28)-C(29)	-0.2(5)	C(39')-C(40')-C(41')-C(42')	0.2(5)
C(10)-C(27)-C(28)-C(29)	-178.9(3)	C(40')-C(41')-C(42')-C(43')	-0.1(7)
C(27)-C(28)-C(29)-C(30)	0.1(6)	C(41')-C(42')-C(43')-C(44')	-0.2(7)
C(28)-C(29)-C(30)-C(31)	0.6(6)	C(42')-C(43')-C(44')-C(39')	0.4(7)
C(29)-C(30)-C(31)-C(32)	-1.1(6)	C(40')-C(39')-C(44')-C(43')	-0.3(5)
C(28)-C(27)-C(32)-C(31)	-0.3(5)	C(20)-C(39')-C(44')-C(43')	179.8(3)
C(10)-C(27)-C(32)-C(31)	178.4(3)	N(5)-N(6)-C(45)-C(48)	-7.2(4)
C(30)-C(31)-C(32)-C(27)	0.9(6)	O(2)-N(6)-C(45)-C(48)	175.1(3)
C(14)-C(15)-C(33)-C(34)	103.9(4)	N(5)-N(6)-C(45)-C(46)	-127.1(3)
C(16)-C(15)-C(33)-C(34)	-75.6(4)	O(2)-N(6)-C(45)-C(46)	55.3(4)
C(14)-C(15)-C(33)-C(38)	-74.7(4)	N(5)-N(6)-C(45)-C(47)	113.7(3)
C(16)-C(15)-C(33)-C(38)	105.8(4)	O(2)-N(6)-C(45)-C(47)	-63.9(4)
C(38)-C(33)-C(34)-C(35)	-0.8(5)		

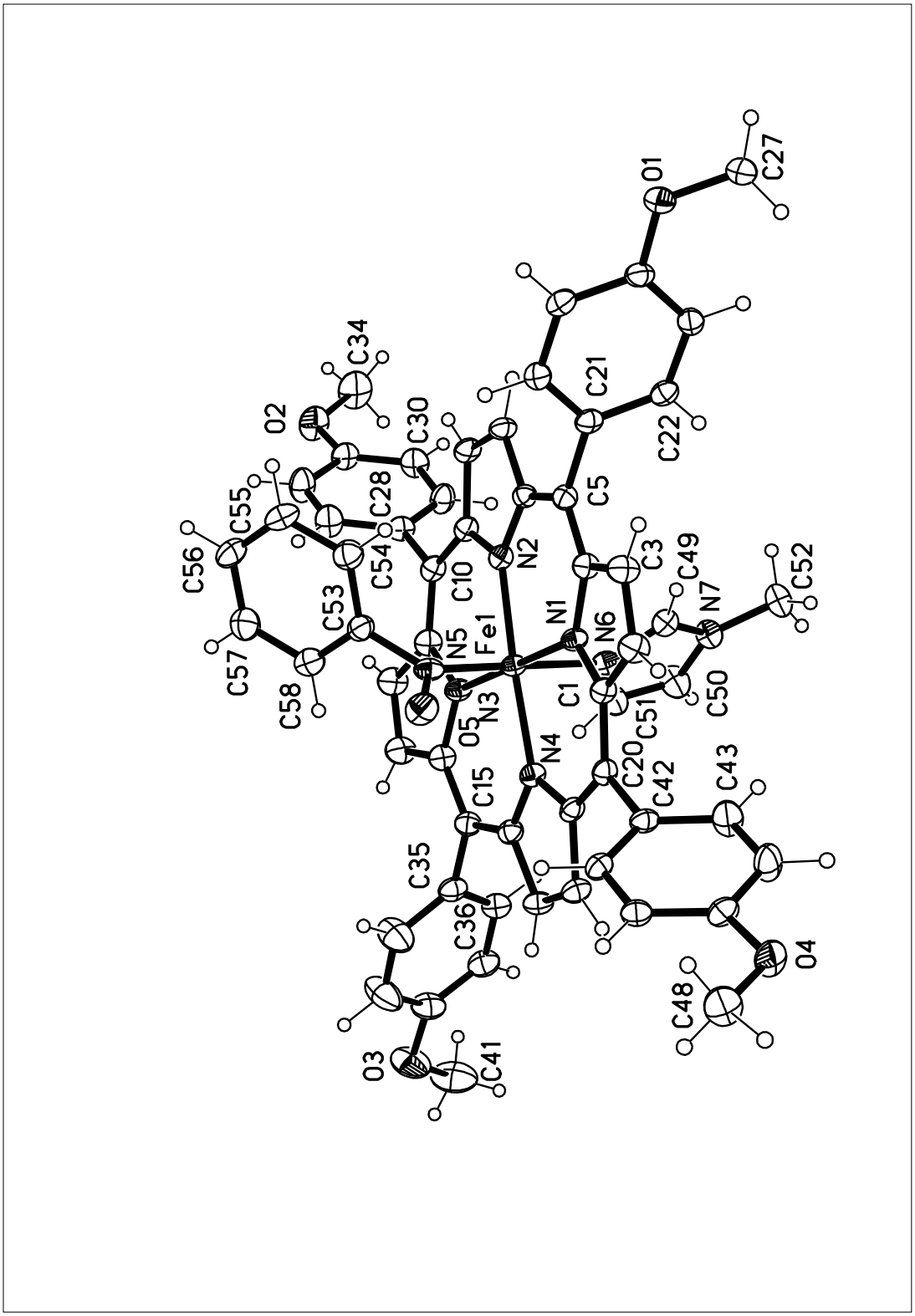

Figure S11. Molecular structure of **6**.

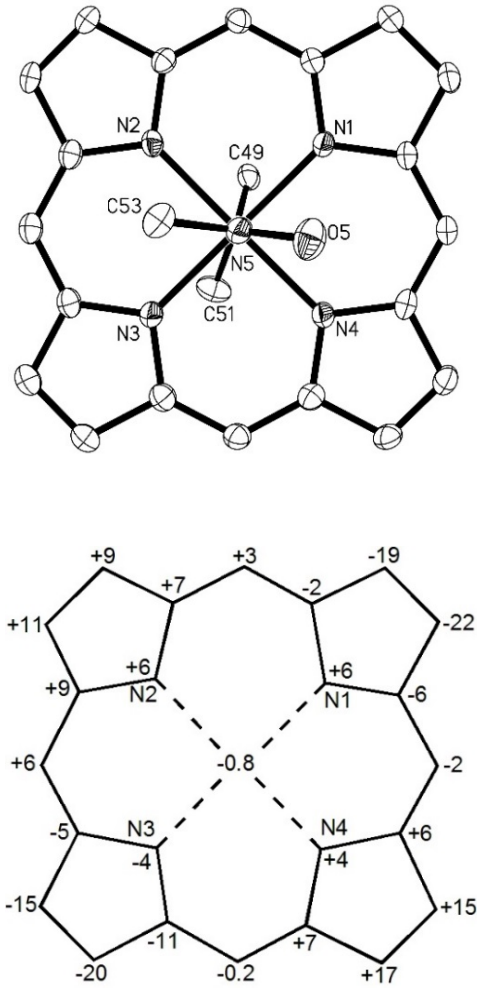

Figure S12. (*Top*) Top view of the axial ligand orientations in **6**. (*Bottom*) Perpendicular atom displacements of the porphyrin atoms from the porphyrin mean plane in **6**.

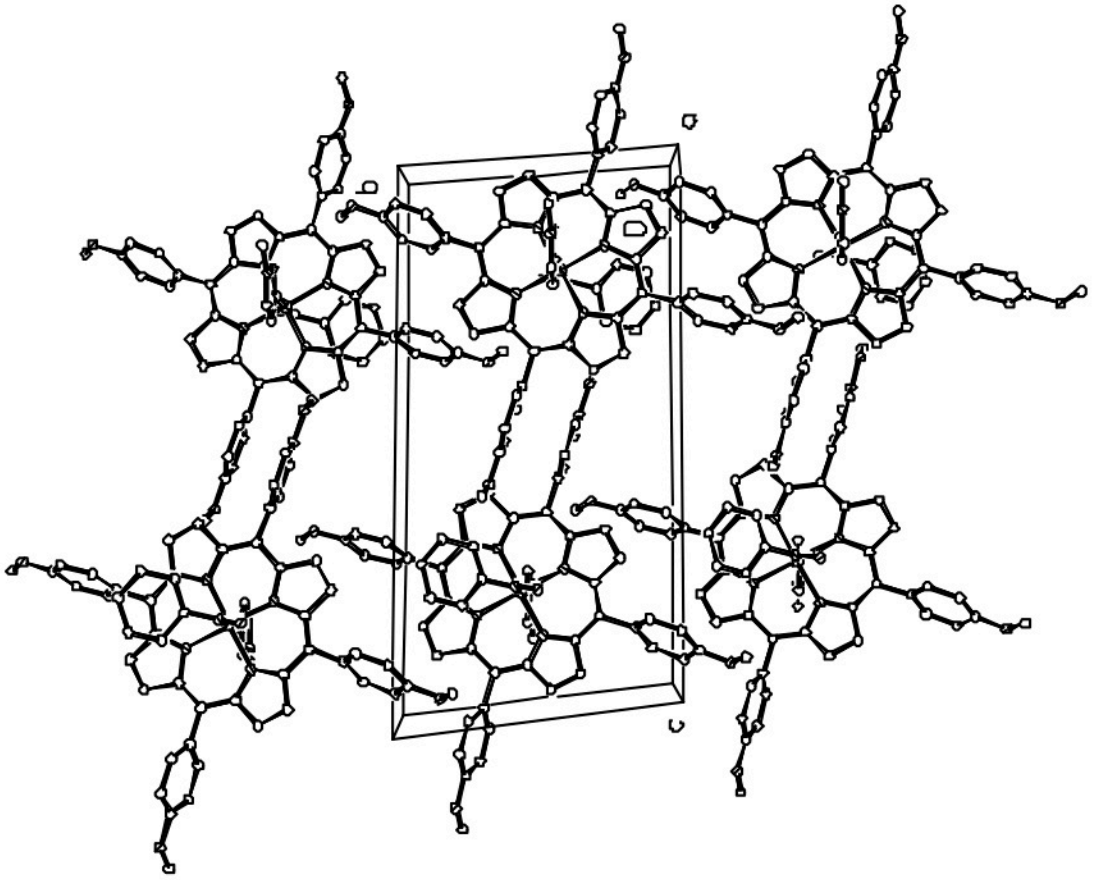

Figure S13. Packing diagram for **6**.

Table S12. Atomic coordinates and equivalent isotropic displacement parameters for **6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0.28135(3)	0.42996(3)	0.21971(2)	0.01621(9)
O(1)	0.38304(18)	0.20544(14)	-0.14883(7)	0.0290(4)
O(2)	0.65591(18)	-0.31409(14)	0.36246(8)	0.0367(4)
O(3)	0.2063(2)	0.67503(19)	0.58066(8)	0.0468(5)
O(4)	-0.10142(17)	1.16139(13)	0.06337(7)	0.0305(4)
O(5)	-0.00490(17)	0.49294(14)	0.22641(8)	0.0309(4)
N(1)	0.24797(18)	0.50900(15)	0.13970(8)	0.0178(4)
N(2)	0.36093(18)	0.27770(15)	0.18517(8)	0.0178(4)
N(3)	0.31807(19)	0.35109(15)	0.29952(8)	0.0200(4)
N(4)	0.21327(18)	0.58427(15)	0.25267(8)	0.0182(4)
N(5)	0.10244(19)	0.41133(15)	0.23351(8)	0.0204(4)
N(6)	0.48493(19)	0.45124(15)	0.20585(8)	0.0199(4)
N(7)	0.70180(19)	0.46476(17)	0.16479(8)	0.0245(4)
C(1)	0.1799(2)	0.62358(18)	0.12627(9)	0.0183(5)
C(2)	0.1520(2)	0.6417(2)	0.06649(10)	0.0240(5)
C(3)	0.2043(2)	0.5391(2)	0.04343(10)	0.0245(5)
C(4)	0.2640(2)	0.45630(19)	0.08898(9)	0.0193(5)
C(5)	0.3251(2)	0.33944(19)	0.08163(9)	0.0187(5)
C(6)	0.3696(2)	0.25690(18)	0.12749(9)	0.0179(5)
C(7)	0.4297(2)	0.13562(18)	0.12066(10)	0.0218(5)
C(8)	0.4586(2)	0.08365(19)	0.17389(10)	0.0221(5)
C(9)	0.4158(2)	0.17184(18)	0.21438(10)	0.0198(5)
C(10)	0.4241(2)	0.15026(19)	0.27454(10)	0.0216(5)
C(11)	0.3739(2)	0.23476(19)	0.31403(10)	0.0225(5)
C(12)	0.3754(3)	0.2127(2)	0.37678(10)	0.0280(5)
C(13)	0.3223(3)	0.3152(2)	0.39974(10)	0.0283(5)
C(14)	0.2883(2)	0.4024(2)	0.35154(10)	0.0225(5)
C(15)	0.2419(2)	0.52174(19)	0.35702(10)	0.0211(5)
C(16)	0.2083(2)	0.60540(19)	0.30999(10)	0.0202(5)
C(17)	0.1593(2)	0.72865(19)	0.31543(10)	0.0234(5)
C(18)	0.1312(2)	0.78042(19)	0.26219(10)	0.0238(5)
C(19)	0.1631(2)	0.69082(18)	0.22324(10)	0.0196(5)
C(20)	0.1432(2)	0.71075(18)	0.16417(10)	0.0186(5)
C(21)	0.3429(2)	0.30208(18)	0.02092(10)	0.0198(5)
C(22)	0.4573(2)	0.32008(18)	-0.02152(10)	0.0204(5)
C(23)	0.4755(2)	0.28851(18)	-0.07837(10)	0.0210(5)
C(24)	0.3772(2)	0.23792(19)	-0.09380(10)	0.0217(5)
C(25)	0.2615(3)	0.2194(2)	-0.05174(10)	0.0257(5)

C(26)	0.2446(3)	0.2522(2)	0.00457(10)	0.0245(5)
C(27)	0.4992(3)	0.2266(2)	-0.19300(11)	0.0333(6)
C(28)	0.4880(2)	0.02793(19)	0.29806(10)	0.0216(5)
C(29)	0.6340(3)	-0.0187(2)	0.28716(11)	0.0282(5)
C(30)	0.6955(3)	-0.1324(2)	0.30761(11)	0.0294(6)
C(31)	0.6082(3)	-0.2010(2)	0.34008(10)	0.0260(5)
C(32)	0.4626(3)	-0.1553(2)	0.35178(12)	0.0341(6)
C(33)	0.4032(3)	-0.0424(2)	0.33069(11)	0.0314(6)
C(34)	0.8038(3)	-0.3673(2)	0.34695(14)	0.0472(8)
C(35)	0.2331(3)	0.56302(19)	0.41591(10)	0.0239(5)
C(36)	0.3531(3)	0.5813(2)	0.43245(11)	0.0276(5)
C(37)	0.3492(3)	0.6189(2)	0.48704(11)	0.0303(6)
C(38)	0.2243(3)	0.6388(2)	0.52536(11)	0.0329(6)
C(39)	0.1019(3)	0.6234(3)	0.50934(13)	0.0493(8)
C(40)	0.1070(3)	0.5858(3)	0.45500(12)	0.0436(7)
C(41)	0.3278(3)	0.6953(3)	0.59875(14)	0.0539(9)
C(42)	0.0762(2)	0.83143(18)	0.13954(10)	0.0198(5)
C(43)	0.1557(3)	0.8946(2)	0.09789(11)	0.0310(6)
C(44)	0.0937(3)	1.0036(2)	0.07308(12)	0.0335(6)
C(45)	-0.0506(2)	1.05209(19)	0.08941(10)	0.0231(5)
C(46)	-0.1320(2)	0.98919(18)	0.12973(10)	0.0209(5)
C(47)	-0.0677(2)	0.87940(18)	0.15457(9)	0.0197(5)
C(48)	-0.2509(3)	1.2070(2)	0.07491(12)	0.0365(6)
C(49)	0.5735(2)	0.45568(19)	0.15561(10)	0.0215(5)
C(50)	0.6946(3)	0.4647(2)	0.22438(11)	0.0320(6)
C(51)	0.5618(3)	0.4568(2)	0.24929(11)	0.0308(6)
C(52)	0.8258(3)	0.4723(2)	0.11964(11)	0.0307(6)
C(53)	0.0672(2)	0.3002(2)	0.25338(10)	0.0239(5)
C(54)	0.0595(3)	0.2293(2)	0.21232(11)	0.0288(5)
C(55)	0.0225(3)	0.1243(2)	0.23208(12)	0.0356(6)
C(56)	-0.0064(3)	0.0918(2)	0.29228(12)	0.0364(6)
C(57)	0.0019(3)	0.1629(2)	0.33248(12)	0.0374(6)
C(58)	0.0386(3)	0.2681(2)	0.31316(11)	0.0330(6)

Table S13. Bond lengths [Å] and angles [°] for **6**.

Fe(1)-N(5)	1.7947(19)	C(8)-H(8)	0.9500
Fe(1)-N(1)	2.0009(18)	C(9)-C(10)	1.394(3)
Fe(1)-N(3)	2.0034(18)	C(10)-C(11)	1.392(3)
Fe(1)-N(4)	2.0035(18)	C(10)-C(28)	1.504(3)
Fe(1)-N(2)	2.0043(18)	C(11)-C(12)	1.441(3)
Fe(1)-N(6)	2.0440(19)	C(12)-C(13)	1.347(3)
O(1)-C(24)	1.371(3)	C(12)-H(12)	0.9500
O(1)-C(27)	1.433(3)	C(13)-C(14)	1.441(3)
O(2)-C(31)	1.373(3)	C(13)-H(13)	0.9500
O(2)-C(34)	1.428(3)	C(14)-C(15)	1.399(3)
O(3)-C(38)	1.375(3)	C(15)-C(16)	1.397(3)
O(3)-C(41)	1.425(3)	C(15)-C(35)	1.495(3)
O(4)-C(45)	1.370(3)	C(16)-C(17)	1.445(3)
O(4)-C(48)	1.417(3)	C(17)-C(18)	1.342(3)
O(5)-N(5)	1.258(2)	C(17)-H(17)	0.9500
N(1)-C(4)	1.375(3)	C(18)-C(19)	1.434(3)
N(1)-C(1)	1.382(3)	C(18)-H(18)	0.9500
N(2)-C(6)	1.376(3)	C(19)-C(20)	1.396(3)
N(2)-C(9)	1.377(3)	C(20)-C(42)	1.504(3)
N(3)-C(11)	1.377(3)	C(21)-C(22)	1.389(3)
N(3)-C(14)	1.378(3)	C(21)-C(26)	1.392(3)
N(4)-C(19)	1.374(3)	C(22)-C(23)	1.387(3)
N(4)-C(16)	1.375(3)	C(22)-H(22)	0.9500
N(5)-C(53)	1.452(3)	C(23)-C(24)	1.388(3)
N(6)-C(49)	1.320(3)	C(23)-H(23)	0.9500
N(6)-C(51)	1.385(3)	C(24)-C(25)	1.395(3)
N(7)-C(49)	1.352(3)	C(25)-C(26)	1.382(3)
N(7)-C(50)	1.368(3)	C(25)-H(25)	0.9500
N(7)-C(52)	1.463(3)	C(26)-H(26)	0.9500
C(1)-C(20)	1.391(3)	C(27)-H(27A)	0.9800
C(1)-C(2)	1.436(3)	C(27)-H(27B)	0.9800
C(2)-C(3)	1.348(3)	C(27)-H(27C)	0.9800
C(2)-H(2)	0.9500	C(28)-C(29)	1.387(3)
C(3)-C(4)	1.439(3)	C(28)-C(33)	1.387(3)
C(3)-H(3)	0.9500	C(29)-C(30)	1.394(3)
C(4)-C(5)	1.394(3)	C(29)-H(29)	0.9500
C(5)-C(6)	1.396(3)	C(30)-C(31)	1.388(3)
C(5)-C(21)	1.500(3)	C(30)-H(30)	0.9500
C(6)-C(7)	1.439(3)	C(31)-C(32)	1.384(3)
C(7)-C(8)	1.345(3)	C(32)-C(33)	1.384(3)
C(7)-H(7)	0.9500	C(32)-H(32)	0.9500
C(8)-C(9)	1.440(3)	C(33)-H(33)	0.9500

C(34)-H(34A)	0.9800	C(46)-H(46)	0.9500
C(34)-H(34B)	0.9800	C(47)-H(47)	0.9500
C(34)-H(34C)	0.9800	C(48)-H(48A)	0.9800
C(35)-C(40)	1.381(4)	C(48)-H(48B)	0.9800
C(35)-C(36)	1.383(3)	C(48)-H(48C)	0.9800
C(36)-C(37)	1.391(3)	C(49)-H(49)	0.9500
C(36)-H(36)	0.9500	C(50)-C(51)	1.346(3)
C(37)-C(38)	1.361(4)	C(50)-H(50)	0.9500
C(37)-H(37)	0.9500	C(51)-H(51)	0.9500
C(38)-C(39)	1.387(4)	C(52)-H(52A)	0.9800
C(39)-C(40)	1.383(4)	C(52)-H(52B)	0.9800
C(39)-H(39)	0.9500	C(52)-H(52C)	0.9800
C(40)-H(40)	0.9500	C(53)-C(58)	1.379(3)
C(41)-H(41A)	0.9800	C(53)-C(54)	1.385(3)
C(41)-H(41B)	0.9800	C(54)-C(55)	1.391(4)
C(41)-H(41C)	0.9800	C(54)-H(54)	0.9500
C(42)-C(47)	1.380(3)	C(55)-C(56)	1.389(4)
C(42)-C(43)	1.390(3)	C(55)-H(55)	0.9500
C(43)-C(44)	1.382(3)	C(56)-C(57)	1.374(4)
C(43)-H(43)	0.9500	C(56)-H(56)	0.9500
C(44)-C(45)	1.389(3)	C(57)-C(58)	1.391(4)
C(44)-H(44)	0.9500	C(57)-H(57)	0.9500
C(45)-C(46)	1.383(3)	C(58)-H(58)	0.9500
C(46)-C(47)	1.396(3)		

N(5)-Fe(1)-N(1)	89.13(8)	C(4)-N(1)-Fe(1)	126.68(14)
N(5)-Fe(1)-N(3)	91.81(8)	C(1)-N(1)-Fe(1)	126.96(14)
N(1)-Fe(1)-N(3)	179.06(8)	C(6)-N(2)-C(9)	105.67(17)
N(5)-Fe(1)-N(4)	90.43(8)	C(6)-N(2)-Fe(1)	127.09(14)
N(1)-Fe(1)-N(4)	89.48(7)	C(9)-N(2)-Fe(1)	127.22(15)
N(3)-Fe(1)-N(4)	90.56(7)	C(11)-N(3)-C(14)	106.02(18)
N(5)-Fe(1)-N(2)	92.97(8)	C(11)-N(3)-Fe(1)	127.33(15)
N(1)-Fe(1)-N(2)	90.08(7)	C(14)-N(3)-Fe(1)	126.63(15)
N(3)-Fe(1)-N(2)	89.83(7)	C(19)-N(4)-C(16)	105.53(18)
N(4)-Fe(1)-N(2)	176.57(7)	C(19)-N(4)-Fe(1)	127.75(15)
N(5)-Fe(1)-N(6)	178.80(8)	C(16)-N(4)-Fe(1)	126.72(15)
N(1)-Fe(1)-N(6)	91.92(7)	O(5)-N(5)-C(53)	113.21(18)
N(3)-Fe(1)-N(6)	87.14(7)	O(5)-N(5)-Fe(1)	123.42(15)
N(4)-Fe(1)-N(6)	89.02(7)	C(53)-N(5)-Fe(1)	123.36(14)
N(2)-Fe(1)-N(6)	87.60(7)	C(49)-N(6)-C(51)	105.40(19)
C(24)-O(1)-C(27)	116.78(18)	C(49)-N(6)-Fe(1)	128.63(15)
C(31)-O(2)-C(34)	117.4(2)	C(51)-N(6)-Fe(1)	125.86(15)
C(38)-O(3)-C(41)	117.2(2)	C(49)-N(7)-C(50)	107.15(19)
C(45)-O(4)-C(48)	116.38(18)	C(49)-N(7)-C(52)	126.6(2)
C(4)-N(1)-C(1)	105.38(17)	C(50)-N(7)-C(52)	126.3(2)

N(1)-C(1)-C(20)	125.9(2)	N(4)-C(16)-C(15)	126.1(2)
N(1)-C(1)-C(2)	110.26(18)	N(4)-C(16)-C(17)	109.87(19)
C(20)-C(1)-C(2)	123.81(19)	C(15)-C(16)-C(17)	124.0(2)
C(3)-C(2)-C(1)	106.99(19)	C(18)-C(17)-C(16)	107.0(2)
C(3)-C(2)-H(2)	126.5	C(18)-C(17)-H(17)	126.5
C(1)-C(2)-H(2)	126.5	C(16)-C(17)-H(17)	126.5
C(2)-C(3)-C(4)	107.2(2)	C(17)-C(18)-C(19)	107.2(2)
C(2)-C(3)-H(3)	126.4	C(17)-C(18)-H(18)	126.4
C(4)-C(3)-H(3)	126.4	C(19)-C(18)-H(18)	126.4
N(1)-C(4)-C(5)	126.26(19)	N(4)-C(19)-C(20)	125.65(19)
N(1)-C(4)-C(3)	110.20(19)	N(4)-C(19)-C(18)	110.34(19)
C(5)-C(4)-C(3)	123.5(2)	C(20)-C(19)-C(18)	124.0(2)
C(4)-C(5)-C(6)	123.4(2)	C(1)-C(20)-C(19)	123.35(19)
C(4)-C(5)-C(21)	117.44(19)	C(1)-C(20)-C(42)	117.27(19)
C(6)-C(5)-C(21)	119.12(19)	C(19)-C(20)-C(42)	119.37(19)
N(2)-C(6)-C(5)	125.93(19)	C(22)-C(21)-C(26)	117.9(2)
N(2)-C(6)-C(7)	110.20(18)	C(22)-C(21)-C(5)	120.3(2)
C(5)-C(6)-C(7)	123.9(2)	C(26)-C(21)-C(5)	121.8(2)
C(8)-C(7)-C(6)	106.93(19)	C(23)-C(22)-C(21)	121.8(2)
C(8)-C(7)-H(7)	126.5	C(23)-C(22)-H(22)	119.1
C(6)-C(7)-H(7)	126.5	C(21)-C(22)-H(22)	119.1
C(7)-C(8)-C(9)	107.37(19)	C(24)-C(23)-C(22)	119.6(2)
C(7)-C(8)-H(8)	126.3	C(24)-C(23)-H(23)	120.2
C(9)-C(8)-H(8)	126.3	C(22)-C(23)-H(23)	120.2
N(2)-C(9)-C(10)	125.9(2)	O(1)-C(24)-C(23)	124.6(2)
N(2)-C(9)-C(8)	109.82(19)	O(1)-C(24)-C(25)	116.1(2)
C(10)-C(9)-C(8)	124.2(2)	C(23)-C(24)-C(25)	119.3(2)
C(11)-C(10)-C(9)	123.7(2)	C(26)-C(25)-C(24)	120.2(2)
C(11)-C(10)-C(28)	118.5(2)	C(26)-C(25)-H(25)	119.9
C(9)-C(10)-C(28)	117.80(19)	C(24)-C(25)-H(25)	119.9
N(3)-C(11)-C(10)	125.8(2)	C(25)-C(26)-C(21)	121.2(2)
N(3)-C(11)-C(12)	109.80(19)	C(25)-C(26)-H(26)	119.4
C(10)-C(11)-C(12)	124.4(2)	C(21)-C(26)-H(26)	119.4
C(13)-C(12)-C(11)	107.2(2)	O(1)-C(27)-H(27A)	109.5
C(13)-C(12)-H(12)	126.4	O(1)-C(27)-H(27B)	109.4
C(11)-C(12)-H(12)	126.4	H(27A)-C(27)-H(27B)	109.5
C(12)-C(13)-C(14)	107.3(2)	O(1)-C(27)-H(27C)	109.5
C(12)-C(13)-H(13)	126.4	H(27A)-C(27)-H(27C)	109.5
C(14)-C(13)-H(13)	126.4	H(27B)-C(27)-H(27C)	109.5
N(3)-C(14)-C(15)	125.9(2)	C(29)-C(28)-C(33)	117.8(2)
N(3)-C(14)-C(13)	109.69(19)	C(29)-C(28)-C(10)	120.9(2)
C(15)-C(14)-C(13)	124.3(2)	C(33)-C(28)-C(10)	121.3(2)
C(16)-C(15)-C(14)	123.7(2)	C(28)-C(29)-C(30)	122.0(2)
C(16)-C(15)-C(35)	117.8(2)	C(28)-C(29)-H(29)	119.0
C(14)-C(15)-C(35)	118.4(2)	C(30)-C(29)-H(29)	119.0

C(31)-C(30)-C(29)	119.0(2)	C(44)-C(43)-C(42)	121.2(2)
C(31)-C(30)-H(30)	120.5	C(44)-C(43)-H(43)	119.4
C(29)-C(30)-H(30)	120.5	C(42)-C(43)-H(43)	119.4
O(2)-C(31)-C(32)	115.9(2)	C(43)-C(44)-C(45)	120.2(2)
O(2)-C(31)-C(30)	124.5(2)	C(43)-C(44)-H(44)	119.9
C(32)-C(31)-C(30)	119.6(2)	C(45)-C(44)-H(44)	119.9
C(31)-C(32)-C(33)	120.5(2)	O(4)-C(45)-C(46)	124.8(2)
C(31)-C(32)-H(32)	119.7	O(4)-C(45)-C(44)	115.9(2)
C(33)-C(32)-H(32)	119.7	C(46)-C(45)-C(44)	119.3(2)
C(32)-C(33)-C(28)	121.0(2)	C(45)-C(46)-C(47)	119.8(2)
C(32)-C(33)-H(33)	119.5	C(45)-C(46)-H(46)	120.1
C(28)-C(33)-H(33)	119.5	C(47)-C(46)-H(46)	120.1
O(2)-C(34)-H(34A)	109.5	C(42)-C(47)-C(46)	121.4(2)
O(2)-C(34)-H(34B)	109.5	C(42)-C(47)-H(47)	119.3
H(34A)-C(34)-H(34B)	109.5	C(46)-C(47)-H(47)	119.3
O(2)-C(34)-H(34C)	109.5	O(4)-C(48)-H(48A)	109.5
H(34A)-C(34)-H(34C)	109.5	O(4)-C(48)-H(48B)	109.5
H(34B)-C(34)-H(34C)	109.5	H(48A)-C(48)-H(48B)	109.5
C(40)-C(35)-C(36)	117.8(2)	O(4)-C(48)-H(48C)	109.5
C(40)-C(35)-C(15)	122.1(2)	H(48A)-C(48)-H(48C)	109.5
C(36)-C(35)-C(15)	120.1(2)	H(48B)-C(48)-H(48C)	109.5
C(35)-C(36)-C(37)	121.8(2)	N(6)-C(49)-N(7)	111.2(2)
C(35)-C(36)-H(36)	119.1	N(6)-C(49)-H(49)	124.4
C(37)-C(36)-H(36)	119.1	N(7)-C(49)-H(49)	124.4
C(38)-C(37)-C(36)	119.5(2)	C(51)-C(50)-N(7)	106.6(2)
C(38)-C(37)-H(37)	120.3	C(51)-C(50)-H(50)	126.7
C(36)-C(37)-H(37)	120.3	N(7)-C(50)-H(50)	126.7
C(37)-C(38)-O(3)	125.3(2)	C(50)-C(51)-N(6)	109.7(2)
C(37)-C(38)-C(39)	119.9(2)	C(50)-C(51)-H(51)	125.2
O(3)-C(38)-C(39)	114.8(2)	N(6)-C(51)-H(51)	125.2
C(40)-C(39)-C(38)	120.2(3)	N(7)-C(52)-H(52A)	109.5
C(40)-C(39)-H(39)	119.9	N(7)-C(52)-H(52B)	109.5
C(38)-C(39)-H(39)	119.9	H(52A)-C(52)-H(52B)	109.5
C(35)-C(40)-C(39)	120.9(3)	N(7)-C(52)-H(52C)	109.5
C(35)-C(40)-H(40)	119.5	H(52A)-C(52)-H(52C)	109.5
C(39)-C(40)-H(40)	119.5	H(52B)-C(52)-H(52C)	109.5
O(3)-C(41)-H(41A)	109.5	C(58)-C(53)-C(54)	121.0(2)
O(3)-C(41)-H(41B)	109.5	C(58)-C(53)-N(5)	119.2(2)
H(41A)-C(41)-H(41B)	109.5	C(54)-C(53)-N(5)	119.8(2)
O(3)-C(41)-H(41C)	109.5	C(53)-C(54)-C(55)	119.1(2)
H(41A)-C(41)-H(41C)	109.5	C(53)-C(54)-H(54)	120.4
H(41B)-C(41)-H(41C)	109.5	C(55)-C(54)-H(54)	120.4
C(47)-C(42)-C(43)	118.1(2)	C(56)-C(55)-C(54)	120.0(2)
C(47)-C(42)-C(20)	121.0(2)	C(56)-C(55)-H(55)	120.0
C(43)-C(42)-C(20)	120.75(19)	C(54)-C(55)-H(55)	120.0

C(57)-C(56)-C(55)	120.2(2)	C(58)-C(57)-H(57)	119.9
C(57)-C(56)-H(56)	119.9	C(53)-C(58)-C(57)	119.5(2)
C(55)-C(56)-H(56)	119.9	C(53)-C(58)-H(58)	120.3
C(56)-C(57)-C(58)	120.2(3)	C(57)-C(58)-H(58)	120.3
C(56)-C(57)-H(57)	119.9		

Table S14. 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}
Fe(1)	17(1)	13(1)	17(1)	-1(1)	-6(1)	0(1)
O(1)	38(1)	30(1)	21(1)	-7(1)	-1(1)	-13(1)
O(2)	33(1)	19(1)	50(1)	10(1)	-10(1)	2(1)
O(3)	47(1)	67(1)	32(1)	-24(1)	-9(1)	-11(1)
O(4)	28(1)	18(1)	38(1)	8(1)	-3(1)	1(1)
O(5)	23(1)	25(1)	43(1)	-3(1)	-8(1)	-1(1)
N(1)	19(1)	14(1)	20(1)	-2(1)	-5(1)	-1(1)
N(2)	17(1)	15(1)	20(1)	1(1)	-6(1)	-2(1)
N(3)	23(1)	16(1)	20(1)	-2(1)	-6(1)	-1(1)
N(4)	20(1)	16(1)	19(1)	-1(1)	-6(1)	-2(1)
N(5)	24(1)	17(1)	19(1)	-4(1)	-7(1)	1(1)
N(6)	20(1)	16(1)	24(1)	-2(1)	-8(1)	0(1)
N(7)	20(1)	27(1)	25(1)	-1(1)	-6(1)	-3(1)
C(1)	18(1)	15(1)	21(1)	1(1)	-5(1)	-1(1)
C(2)	26(1)	19(1)	23(1)	2(1)	-7(1)	1(1)
C(3)	31(1)	22(1)	20(1)	-1(1)	-8(1)	-1(1)
C(4)	21(1)	18(1)	18(1)	-1(1)	-5(1)	-2(1)
C(5)	20(1)	19(1)	18(1)	-1(1)	-4(1)	-5(1)
C(6)	16(1)	17(1)	21(1)	-3(1)	-3(1)	-3(1)
C(7)	25(1)	15(1)	25(1)	-5(1)	-3(1)	-1(1)
C(8)	24(1)	12(1)	28(1)	-1(1)	-5(1)	1(1)
C(9)	16(1)	16(1)	26(1)	-1(1)	-4(1)	-2(1)
C(10)	20(1)	17(1)	26(1)	1(1)	-6(1)	-2(1)
C(11)	22(1)	19(1)	24(1)	2(1)	-8(1)	0(1)
C(12)	34(1)	24(1)	23(1)	3(1)	-10(1)	-1(1)
C(13)	38(1)	26(1)	19(1)	0(1)	-9(1)	-5(1)
C(14)	23(1)	22(1)	22(1)	-1(1)	-7(1)	-3(1)
C(15)	22(1)	22(1)	20(1)	-3(1)	-5(1)	-4(1)
C(16)	19(1)	20(1)	23(1)	-4(1)	-5(1)	-5(1)
C(17)	27(1)	22(1)	23(1)	-8(1)	-6(1)	-4(1)
C(18)	27(1)	16(1)	28(1)	-3(1)	-5(1)	-2(1)
C(19)	18(1)	13(1)	27(1)	-1(1)	-4(1)	-3(1)
C(20)	18(1)	14(1)	21(1)	2(1)	-4(1)	-2(1)
C(21)	25(1)	13(1)	20(1)	0(1)	-6(1)	-1(1)
C(22)	19(1)	17(1)	26(1)	-3(1)	-7(1)	-2(1)
C(23)	20(1)	17(1)	23(1)	-1(1)	-1(1)	-2(1)

C(24)	29(1)	16(1)	19(1)	-3(1)	-4(1)	-3(1)
C(25)	30(1)	24(1)	28(1)	-6(1)	-5(1)	-12(1)
C(26)	30(1)	24(1)	21(1)	-3(1)	-1(1)	-10(1)
C(27)	48(2)	30(1)	23(1)	-8(1)	4(1)	-17(1)
C(28)	26(1)	17(1)	20(1)	2(1)	-8(1)	0(1)
C(29)	28(1)	22(1)	34(1)	4(1)	-5(1)	-7(1)
C(30)	22(1)	26(1)	35(1)	1(1)	-6(1)	1(1)
C(31)	31(1)	19(1)	26(1)	4(1)	-9(1)	-2(1)
C(32)	29(1)	27(1)	41(2)	10(1)	-5(1)	-5(1)
C(33)	24(1)	25(1)	39(2)	4(1)	-4(1)	0(1)
C(34)	39(2)	24(1)	66(2)	11(1)	-10(2)	8(1)
C(35)	32(1)	17(1)	22(1)	-1(1)	-8(1)	-3(1)
C(36)	30(1)	26(1)	28(1)	-6(1)	-6(1)	-5(1)
C(37)	32(1)	29(1)	33(1)	-6(1)	-13(1)	-6(1)
C(38)	42(2)	35(2)	23(1)	-9(1)	-11(1)	-6(1)
C(39)	36(2)	80(2)	36(2)	-27(2)	2(1)	-14(2)
C(40)	34(2)	69(2)	34(2)	-20(1)	-5(1)	-16(1)
C(41)	54(2)	63(2)	50(2)	-27(2)	-26(2)	1(2)
C(42)	23(1)	14(1)	21(1)	-2(1)	-5(1)	-1(1)
C(43)	22(1)	24(1)	38(2)	6(1)	-1(1)	2(1)
C(44)	29(1)	24(1)	40(2)	9(1)	2(1)	-3(1)
C(45)	25(1)	14(1)	28(1)	1(1)	-7(1)	-1(1)
C(46)	20(1)	18(1)	24(1)	-3(1)	-5(1)	0(1)
C(47)	24(1)	17(1)	20(1)	0(1)	-6(1)	-6(1)
C(48)	31(1)	23(1)	43(2)	9(1)	-4(1)	7(1)
C(49)	21(1)	20(1)	23(1)	1(1)	-8(1)	-3(1)
C(50)	27(1)	48(2)	25(1)	-4(1)	-9(1)	-13(1)
C(51)	26(1)	46(2)	23(1)	-4(1)	-7(1)	-11(1)
C(52)	26(1)	40(2)	25(1)	2(1)	-2(1)	-9(1)
C(53)	19(1)	21(1)	32(1)	-6(1)	-2(1)	-5(1)
C(54)	30(1)	30(1)	28(1)	-4(1)	-6(1)	-10(1)
C(55)	44(2)	29(1)	40(2)	-13(1)	-5(1)	-15(1)
C(56)	42(2)	19(1)	49(2)	-6(1)	1(1)	-11(1)
C(57)	43(2)	32(2)	35(2)	-1(1)	3(1)	-12(1)
C(58)	40(2)	29(1)	32(1)	-7(1)	-1(1)	-12(1)

Table S15. Hydrogen coordinates and isotropic displacement parameters for **6**.

	x	y	z	U(eq)
H(2)	0.1055	0.7126	0.0469	0.029
H(3)	0.2022	0.5241	0.0044	0.029
H(7)	0.4459	0.0992	0.0853	0.026
H(8)	0.4997	0.0035	0.1831	0.027
H(12)	0.4078	0.1395	0.3980	0.034
H(13)	0.3097	0.3278	0.4402	0.034
H(17)	0.1489	0.7660	0.3501	0.028
H(18)	0.0966	0.8613	0.2522	0.029
H(22)	0.5249	0.3550	-0.0113	0.024
H(23)	0.5549	0.3014	-0.1066	0.025
H(25)	0.1941	0.1842	-0.0618	0.031
H(26)	0.1644	0.2405	0.0326	0.029
H(27A)	0.4980	0.3094	-0.1974	0.050
H(27B)	0.4895	0.2038	-0.2307	0.050
H(27C)	0.5895	0.1811	-0.1811	0.050
H(29)	0.6938	0.0284	0.2651	0.034
H(30)	0.7957	-0.1625	0.2994	0.035
H(32)	0.4028	-0.2018	0.3745	0.041
H(33)	0.3029	-0.0127	0.3387	0.038
H(34A)	0.8607	-0.3256	0.3623	0.071
H(34B)	0.8288	-0.3643	0.3038	0.071
H(34C)	0.8233	-0.4484	0.3640	0.071
H(36)	0.4404	0.5679	0.4058	0.033
H(37)	0.4331	0.6305	0.4975	0.036
H(39)	0.0143	0.6388	0.5357	0.059
H(40)	0.0226	0.5755	0.4444	0.052
H(41A)	0.3576	0.7600	0.5732	0.081
H(41B)	0.4059	0.6252	0.5957	0.081
H(41C)	0.3036	0.7144	0.6398	0.081
H(43)	0.2545	0.8624	0.0863	0.037
H(44)	0.1500	1.0454	0.0448	0.040
H(46)	-0.2313	1.0206	0.1405	0.025
H(47)	-0.1242	0.8369	0.1824	0.024
H(48A)	-0.2816	1.2105	0.1175	0.055
H(48B)	-0.2992	1.1567	0.0607	0.055
H(48C)	-0.2752	1.2852	0.0544	0.055
H(49)	0.5502	0.4528	0.1179	0.026
H(50)	0.7688	0.4692	0.2443	0.038
H(51)	0.5263	0.4554	0.2904	0.037

H(52A)	0.7961	0.5303	0.0872	0.046
H(52B)	0.8675	0.3965	0.1044	0.046
H(52C)	0.8967	0.4952	0.1370	0.046
H(54)	0.0793	0.2522	0.1712	0.035
H(55)	0.0169	0.0749	0.2044	0.043
H(56)	-0.0319	0.0201	0.3057	0.044
H(57)	-0.0176	0.1401	0.3736	0.045
H(58)	0.0439	0.3175	0.3409	0.040

Table 16. Torsion angles [°] for **6**.

N(1)-Fe(1)-N(5)-O(5)	-51.39(17)	N(2)-C(9)-C(10)-C(11)	1.4(4)
N(3)-Fe(1)-N(5)-O(5)	128.65(17)	C(8)-C(9)-C(10)-C(11)	-175.6(2)
N(4)-Fe(1)-N(5)-O(5)	38.08(17)	N(2)-C(9)-C(10)-C(28)	180.0(2)
N(2)-Fe(1)-N(5)-O(5)	-141.43(17)	C(8)-C(9)-C(10)-C(28)	2.9(3)
N(1)-Fe(1)-N(5)-C(53)	127.91(17)	C(14)-N(3)-C(11)-C(10)	-177.4(2)
N(3)-Fe(1)-N(5)-C(53)	-52.05(17)	Fe(1)-N(3)-C(11)-C(10)	4.3(3)
N(4)-Fe(1)-N(5)-C(53)	-142.62(17)	C(14)-N(3)-C(11)-C(12)	1.5(3)
N(2)-Fe(1)-N(5)-C(53)	37.87(17)	Fe(1)-N(3)-C(11)-C(12)	-176.73(15)
C(4)-N(1)-C(1)-C(20)	-179.0(2)	C(9)-C(10)-C(11)-N(3)	-4.3(4)
Fe(1)-N(1)-C(1)-C(20)	11.8(3)	C(28)-C(10)-C(11)-N(3)	177.1(2)
C(4)-N(1)-C(1)-C(2)	0.6(2)	C(9)-C(10)-C(11)-C(12)	176.9(2)
Fe(1)-N(1)-C(1)-C(2)	-168.61(15)	C(28)-C(10)-C(11)-C(12)	-1.7(3)
N(1)-C(1)-C(2)-C(3)	-0.7(3)	N(3)-C(11)-C(12)-C(13)	-0.6(3)
C(20)-C(1)-C(2)-C(3)	178.9(2)	C(10)-C(11)-C(12)-C(13)	178.3(2)
C(1)-C(2)-C(3)-C(4)	0.5(3)	C(11)-C(12)-C(13)-C(14)	-0.5(3)
C(1)-N(1)-C(4)-C(5)	-178.8(2)	C(11)-N(3)-C(14)-C(15)	173.8(2)
Fe(1)-N(1)-C(4)-C(5)	-9.5(3)	Fe(1)-N(3)-C(14)-C(15)	-7.9(3)
C(1)-N(1)-C(4)-C(3)	-0.3(2)	C(11)-N(3)-C(14)-C(13)	-1.8(3)
Fe(1)-N(1)-C(4)-C(3)	168.95(15)	Fe(1)-N(3)-C(14)-C(13)	176.45(15)
C(2)-C(3)-C(4)-N(1)	-0.1(3)	C(12)-C(13)-C(14)-N(3)	1.5(3)
C(2)-C(3)-C(4)-C(5)	178.4(2)	C(12)-C(13)-C(14)-C(15)	-174.3(2)
N(1)-C(4)-C(5)-C(6)	5.1(4)	N(3)-C(14)-C(15)-C(16)	5.4(4)
C(3)-C(4)-C(5)-C(6)	-173.2(2)	C(13)-C(14)-C(15)-C(16)	-179.6(2)
N(1)-C(4)-C(5)-C(21)	-175.0(2)	N(3)-C(14)-C(15)-C(35)	-172.1(2)
C(3)-C(4)-C(5)-C(21)	6.7(3)	C(13)-C(14)-C(15)-C(35)	2.9(3)
C(9)-N(2)-C(6)-C(5)	179.6(2)	C(19)-N(4)-C(16)-C(15)	176.3(2)
Fe(1)-N(2)-C(6)-C(5)	0.7(3)	Fe(1)-N(4)-C(16)-C(15)	-4.2(3)
C(9)-N(2)-C(6)-C(7)	0.5(2)	C(19)-N(4)-C(16)-C(17)	-2.4(2)
Fe(1)-N(2)-C(6)-C(7)	-178.36(14)	Fe(1)-N(4)-C(16)-C(17)	177.17(14)
C(4)-C(5)-C(6)-N(2)	-0.4(3)	C(14)-C(15)-C(16)-N(4)	1.0(4)
C(21)-C(5)-C(6)-N(2)	179.7(2)	C(35)-C(15)-C(16)-N(4)	178.5(2)
C(4)-C(5)-C(6)-C(7)	178.5(2)	C(14)-C(15)-C(16)-C(17)	179.5(2)
C(21)-C(5)-C(6)-C(7)	-1.4(3)	C(35)-C(15)-C(16)-C(17)	-3.0(3)
N(2)-C(6)-C(7)-C(8)	-0.6(3)	N(4)-C(16)-C(17)-C(18)	1.8(3)
C(5)-C(6)-C(7)-C(8)	-179.7(2)	C(15)-C(16)-C(17)-C(18)	-176.9(2)
C(6)-C(7)-C(8)-C(9)	0.4(2)	C(16)-C(17)-C(18)-C(19)	-0.4(3)
C(6)-N(2)-C(9)-C(10)	-177.7(2)	C(16)-N(4)-C(19)-C(20)	-177.0(2)
Fe(1)-N(2)-C(9)-C(10)	1.2(3)	Fe(1)-N(4)-C(19)-C(20)	3.5(3)
C(6)-N(2)-C(9)-C(8)	-0.3(2)	C(16)-N(4)-C(19)-C(18)	2.1(2)
Fe(1)-N(2)-C(9)-C(8)	178.60(14)	Fe(1)-N(4)-C(19)-C(18)	-177.39(15)
C(7)-C(8)-C(9)-N(2)	-0.1(3)	C(17)-C(18)-C(19)-N(4)	-1.1(3)
C(7)-C(8)-C(9)-C(10)	177.4(2)	C(17)-C(18)-C(19)-C(20)	178.1(2)

N(1)-C(1)-C(20)-C(19)	-4.4(4)	C(15)-C(35)-C(36)-C(37)	-179.5(2)
C(2)-C(1)-C(20)-C(19)	176.0(2)	C(35)-C(36)-C(37)-C(38)	-0.3(4)
N(1)-C(1)-C(20)-C(42)	176.9(2)	C(36)-C(37)-C(38)-O(3)	179.4(2)
C(2)-C(1)-C(20)-C(42)	-2.7(3)	C(36)-C(37)-C(38)-C(39)	-1.1(4)
N(4)-C(19)-C(20)-C(1)	-3.6(4)	C(41)-O(3)-C(38)-C(37)	1.2(4)
C(18)-C(19)-C(20)-C(1)	177.4(2)	C(41)-O(3)-C(38)-C(39)	-178.3(3)
N(4)-C(19)-C(20)-C(42)	175.1(2)	C(37)-C(38)-C(39)-C(40)	1.2(5)
C(18)-C(19)-C(20)-C(42)	-3.9(3)	O(3)-C(38)-C(39)-C(40)	-179.2(3)
C(4)-C(5)-C(21)-C(22)	80.7(3)	C(36)-C(35)-C(40)-C(39)	-1.3(4)
C(6)-C(5)-C(21)-C(22)	-99.4(3)	C(15)-C(35)-C(40)-C(39)	179.7(3)
C(4)-C(5)-C(21)-C(26)	-97.2(3)	C(38)-C(39)-C(40)-C(35)	0.0(5)
C(6)-C(5)-C(21)-C(26)	82.7(3)	C(1)-C(20)-C(42)-C(47)	105.6(2)
C(26)-C(21)-C(22)-C(23)	-0.8(3)	C(19)-C(20)-C(42)-C(47)	-73.2(3)
C(5)-C(21)-C(22)-C(23)	-178.82(19)	C(1)-C(20)-C(42)-C(43)	-70.0(3)
C(21)-C(22)-C(23)-C(24)	0.3(3)	C(19)-C(20)-C(42)-C(43)	111.2(3)
C(27)-O(1)-C(24)-C(23)	-0.4(3)	C(47)-C(42)-C(43)-C(44)	1.4(4)
C(27)-O(1)-C(24)-C(25)	178.4(2)	C(20)-C(42)-C(43)-C(44)	177.2(2)
C(22)-C(23)-C(24)-O(1)	178.7(2)	C(42)-C(43)-C(44)-C(45)	-0.1(4)
C(22)-C(23)-C(24)-C(25)	-0.1(3)	C(48)-O(4)-C(45)-C(46)	-6.3(3)
O(1)-C(24)-C(25)-C(26)	-178.3(2)	C(48)-O(4)-C(45)-C(44)	173.7(2)
C(23)-C(24)-C(25)-C(26)	0.6(3)	C(43)-C(44)-C(45)-O(4)	178.6(2)
C(24)-C(25)-C(26)-C(21)	-1.2(4)	C(43)-C(44)-C(45)-C(46)	-1.4(4)
C(22)-C(21)-C(26)-C(25)	1.3(3)	O(4)-C(45)-C(46)-C(47)	-178.4(2)
C(5)-C(21)-C(26)-C(25)	179.2(2)	C(44)-C(45)-C(46)-C(47)	1.6(3)
C(11)-C(10)-C(28)-C(29)	-106.9(3)	C(43)-C(42)-C(47)-C(46)	-1.2(3)
C(9)-C(10)-C(28)-C(29)	74.5(3)	C(20)-C(42)-C(47)-C(46)	-176.9(2)
C(11)-C(10)-C(28)-C(33)	73.9(3)	C(45)-C(46)-C(47)-C(42)	-0.3(3)
C(9)-C(10)-C(28)-C(33)	-104.7(3)	C(51)-N(6)-C(49)-N(7)	-0.5(2)
C(33)-C(28)-C(29)-C(30)	0.4(4)	Fe(1)-N(6)-C(49)-N(7)	-176.86(14)
C(10)-C(28)-C(29)-C(30)	-178.9(2)	C(50)-N(7)-C(49)-N(6)	0.8(3)
C(28)-C(29)-C(30)-C(31)	-0.3(4)	C(52)-N(7)-C(49)-N(6)	-179.7(2)
C(34)-O(2)-C(31)-C(32)	174.7(2)	C(49)-N(7)-C(50)-C(51)	-0.7(3)
C(34)-O(2)-C(31)-C(30)	-5.5(4)	C(52)-N(7)-C(50)-C(51)	179.8(2)
C(29)-C(30)-C(31)-O(2)	179.9(2)	N(7)-C(50)-C(51)-N(6)	0.4(3)
C(29)-C(30)-C(31)-C(32)	-0.3(4)	C(49)-N(6)-C(51)-C(50)	0.1(3)
O(2)-C(31)-C(32)-C(33)	-179.3(2)	Fe(1)-N(6)-C(51)-C(50)	176.55(17)
C(30)-C(31)-C(32)-C(33)	0.9(4)	O(5)-N(5)-C(53)-C(58)	-90.1(3)
C(31)-C(32)-C(33)-C(28)	-0.8(4)	Fe(1)-N(5)-C(53)-C(58)	90.5(2)
C(29)-C(28)-C(33)-C(32)	0.2(4)	O(5)-N(5)-C(53)-C(54)	88.4(2)
C(10)-C(28)-C(33)-C(32)	179.4(2)	Fe(1)-N(5)-C(53)-C(54)	-91.0(2)
C(16)-C(15)-C(35)-C(40)	85.5(3)	C(58)-C(53)-C(54)-C(55)	-0.1(4)
C(14)-C(15)-C(35)-C(40)	-96.9(3)	N(5)-C(53)-C(54)-C(55)	-178.5(2)
C(16)-C(15)-C(35)-C(36)	-93.5(3)	C(53)-C(54)-C(55)-C(56)	0.1(4)
C(14)-C(15)-C(35)-C(36)	84.1(3)	C(54)-C(55)-C(56)-C(57)	-0.2(4)
C(40)-C(35)-C(36)-C(37)	1.4(4)	C(55)-C(56)-C(57)-C(58)	0.3(4)

C(54)-C(53)-C(58)-C(57)	0.2(4)
N(5)-C(53)-C(58)-C(57)	178.7(2)
C(56)-C(57)-C(58)-C(53)	-0.3(4)

Table S17. Hydrogen bonds for **6** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...O(1)#1	0.95	2.64	3.491(3)	150.0
C(50)-H(50)...O(5)#2	0.95	2.27	3.071(3)	141.4
C(52)-H(52C)...O(5)#2	0.98	2.44	3.297(3)	146.3

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