Supplementary Material

for

Synthesis, Structure, and Characterization of Dichloro-(1-Benzyl-4-Acetato-1,4,7-Triazacyclononane)Iron(III)

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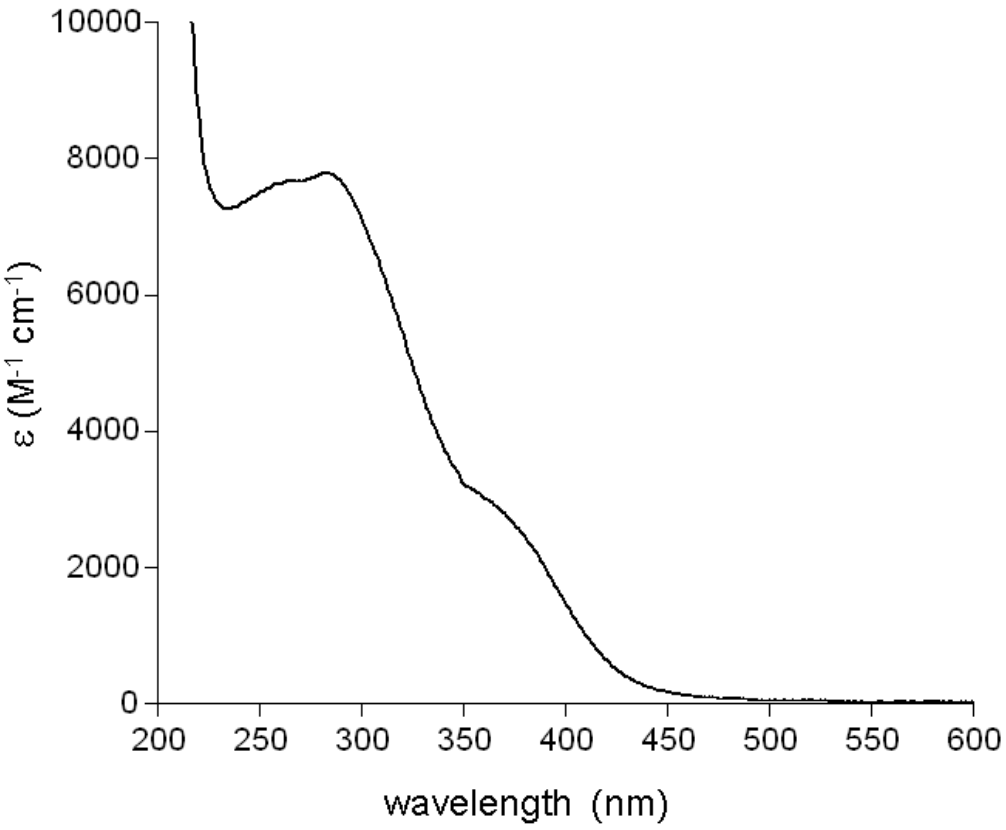

Fig. S1. UV-vis spectrum of $[FeL^1Cl_2]$ (**1)** in acetonitrile.

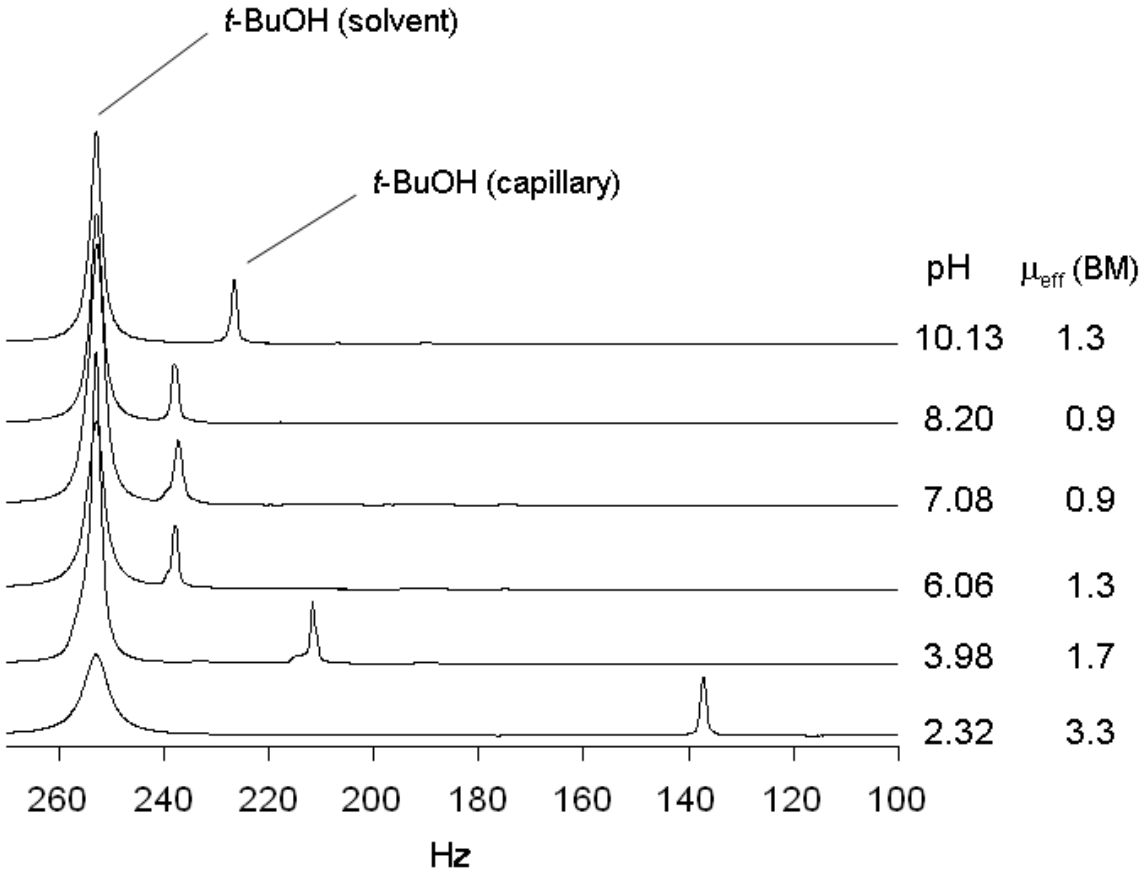

Fig. S2. Evans Method: pH dependent ^{1}H NMR spectra (200 MHz) of **1** in D_2O containing *t*-BuOH (5%) at 25 °C.

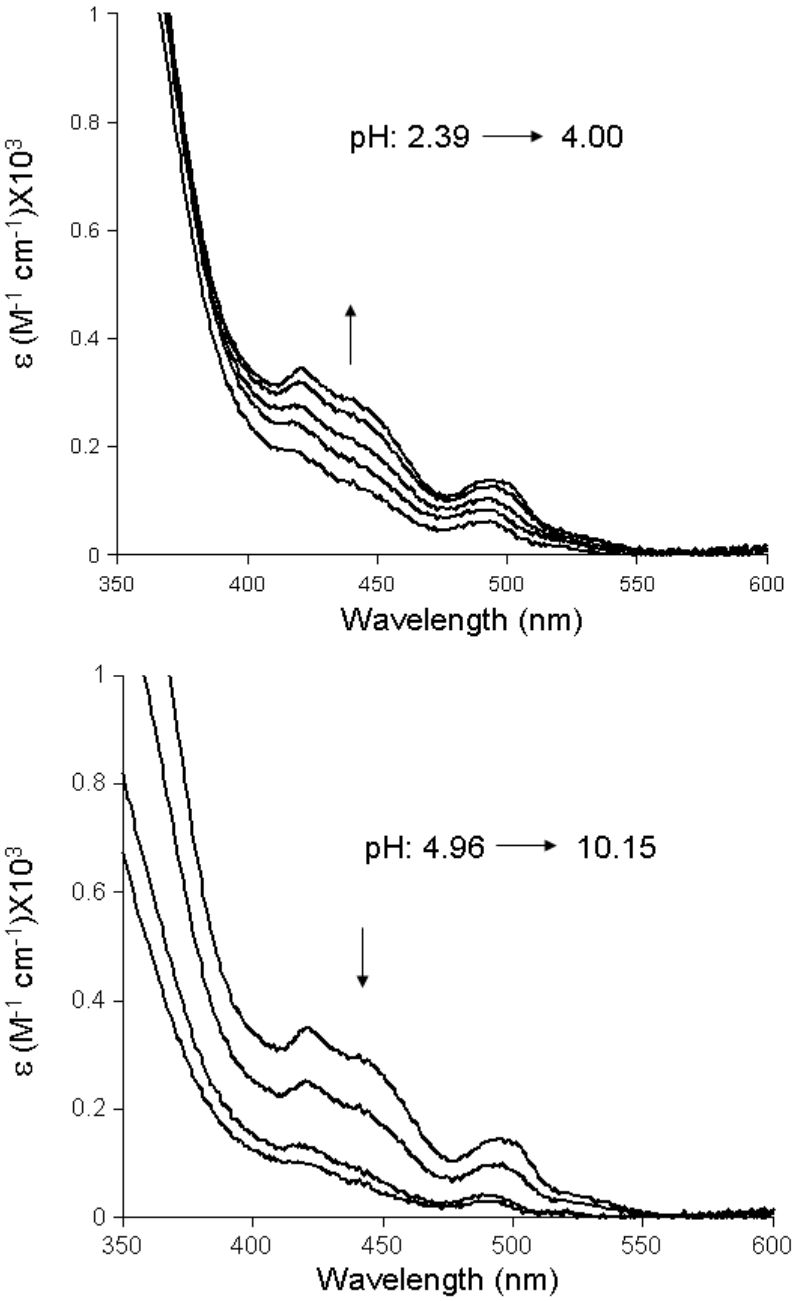

Fig. S3. Progressive changes in the UV-vis spectra of **1** (0.14 mM) in water at varying pHs (25 °C).

Crystallographic Data for $FeL^1Cl_2 \cdot 0.5CH_3CN$ ($1 \cdot 0.5CH_3CN$)

Data collection

A crystal (approximate dimensions 0.36 x 0.32 x 0.05 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker SMART Platform CCD diffractometer for a data collection at 173(2) K. A preliminary set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 69 reflections. The data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 25 seconds and a detector distance of 4.94 cm. A randomly oriented region of reciprocal space was surveyed to the extent of 1.5 hemispheres and to a resolution of 0.84 Å. Three major sections of frames were collected with 0.30º steps in ω at three different ϕ settings and a detector position of -28º in 2θ. The intensity data were corrected for absorption and decay (SADABS).[1] Final cell constants were calculated from the xyz centroids of 1663 strong reflections from the actual data collection after integration (SAINT).[2] Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SIR97[3] and refined using SHELXL-97.[4] The space group *Aba*2 was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters, except those belonging to the disordered solvent acetonitrile (see below), which could not be modeled as such. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0302$ and $wR2 = 0.0763$ (F^2, all data).

Structure description

The structure is similar to the one suggested. The iron atom is coordinated by two chloride ligands in addition to the TACN ligand. There is also one half of an acetonitrile solvent molecule per iron molecule, doubly disordered over a two-fold axis (50:50, 54:46).

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1)include William W. Brennessel as a coauthor or 2)acknowledge William W. Brennessel, Victor G. Young, Jr., and the X-Ray Crystallographic Laboratory.

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[1] An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38 (1995).

[2] SAINT V6.2, Bruker Analytical X-Ray Systems, Madison, WI (2001).

[3] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna. Sir97: a new tool for crystal structure determination and refinement. *J. Appl. Cryst.* **32**, 115-119 (1998).

[4] SHELXTL V6.10, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

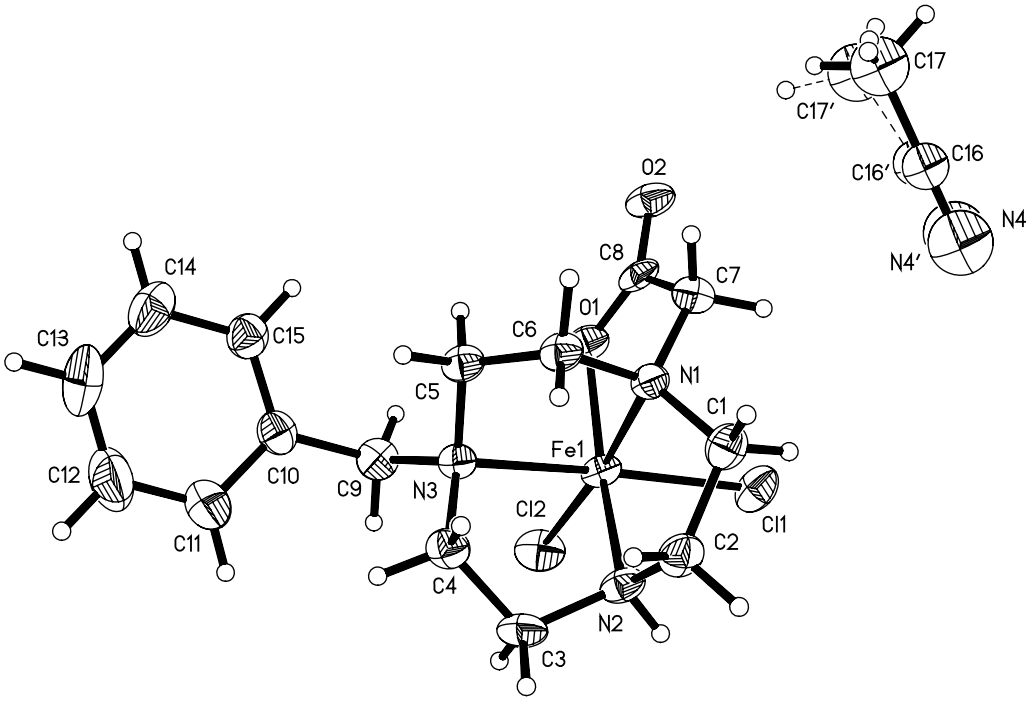
$$R_{int} = \Sigma\ |F_o^2 - < F_o^2 >| \ / \ \Sigma|F_o{}^2|$$

$$R_1 = \Sigma||F_o|-|F_c|| \ / \ \Sigma|F_o|$$

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

$$\text{where } w = q \ / \ [\sigma^2\ (F_o^2) + (a*P)^2 + b*P + d + e*\sin(\theta)]$$

$$\text{GooF} = S = [\Sigma[w(F_o^2-F_c{}^2)^2] \ / \ (n-p)]^{1/2}$$


C17
C17′
C16
C16′
N4
N4′
O2
C8
C7
O1
C6
C5
N1
C1
C14
C13
C15
Fe1
C12
C10
C9
N3
Cl2
Cl1
C11
C2
C4
N2
C3

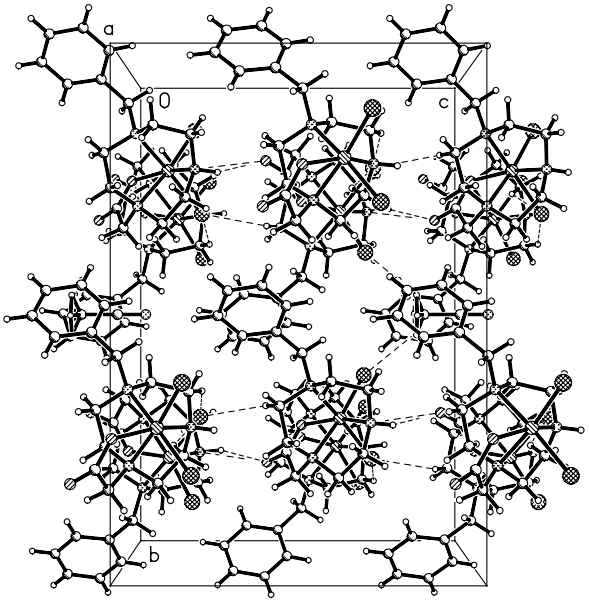

a
O
c
b

Table S1. Crystal data and structure refinement for $FeL^1Cl_2 \cdot 0.5CH_3CN$ (**1**·$0.5CH_3CN$).

Identification code	03117	
Empirical formula	C16 H22.50 Cl2 Fe N3.50 O2	
Formula weight	422.63	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*Aba*2	
Unit cell dimensions	a = 13.716(2) Å	α = 90°
	b = 19.975(3) Å	β = 90°
	c = 13.863(2) Å	γ = 90°
Volume	3798(1) $Å^3$	
Z	8	
Density (calculated)	1.478 Mg/m^3	
Absorption coefficient	1.091 mm^{-1}	
F(000)	1752	
Crystal color, morphology	yellow, plate	
Crystal size	0.36 x 0.32 x 0.05 mm^3	
Theta range for data collection	2.04 to 25.03°	
Index ranges	$-15 \le h \le 16$, $-23 \le k \le 23$, $-16 \le l \le 16$	
Reflections collected	13005	
Independent reflections	3338 [R(int) = 0.0453]	
Observed reflections	2912	
Completeness to theta = 25.03°	100.0%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000000 and 0.825731	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3338 / 10 / 285	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	$R1$ = 0.0302, $wR2$ = 0.0689	
R indices (all data)	$R1$ = 0.0415, $wR2$ = 0.0763	
Absolute structure parameter	0.282(19)	
Largest diff. peak and hole	0.404 and -0.278 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $FeL^1Cl_2 \cdot 0.5CH_3CN$ (**1**·$0.5CH_3CN$). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Fe1	9795(1)	2097(1)	6222(2)	24(1)
Cl1	10447(1)	2945(1)	7167(2)	39(1)
Cl2	10601(1)	1242(1)	6941(2)	41(1)
N1	8924(2)	2846(1)	5402(3)	26(1)
N2	8504(2)	2136(1)	7062(3)	29(1)
N3	8788(2)	1415(1)	5357(3)	25(1)
C1	8350(3)	3212(2)	6147(4)	33(1)
C2	7853(3)	2711(2)	6815(4)	35(1)
C3	8021(3)	1476(2)	6972(4)	34(1)
C4	7875(3)	1303(2)	5920(4)	32(1)
C5	8595(3)	1807(2)	4466(3)	28(1)
C6	8278(3)	2509(2)	4691(3)	29(1)
O1	10646(2)	2264(1)	5096(3)	29(1)
C7	9671(3)	3253(2)	4920(4)	33(1)
C8	10555(3)	2830(2)	4652(3)	29(1)
O2	11146(2)	3052(1)	4072(3)	38(1)
C9	9292(3)	770(2)	5110(4)	34(1)
C10	8780(3)	337(2)	4373(3)	33(1)
C11	8159(4)	-174(2)	4663(5)	57(1)
C12	7695(4)	-566(3)	3984(5)	75(2)
C13	7848(4)	-462(2)	3014(5)	62(1)
C14	8480(3)	20(2)	2715(4)	50(1)
C15	8949(3)	422(2)	3394(4)	37(1)
N4	10000	5000	5549(6)	82(4)
C16	10000	5000	4730(6)	41(2)
C17	10000	5000	3670(6)	65(4)
N4'	10545(15)	4954(9)	5544(8)	82(4)
C16'	10453(11)	4917(7)	4731(7)	41(2)
C17'	10473(15)	4804(10)	3683(8)	65(4)

Table S3. Bond lengths [Å] and angles [°] $FeL^1Cl_2 \cdot 0.5CH_3CN$ (**1**·$0.5CH_3CN$).

Fe(1)-O(1)	1.977(2)	C(9)-C(10)	1.512(5)
Fe(1)-N(2)	2.122(3)	C(9)-H(9A)	1.01(4)
Fe(1)-N(1)	2.226(3)	C(9)-H(9B)	0.97(4)
Fe(1)-Cl(2)	2.2656(10)	C(10)-C(15)	1.387(5)
Fe(1)-N(3)	2.281(3)	C(10)-C(11)	1.390(6)
Fe(1)-Cl(1)	2.3212(10)	C(11)-C(12)	1.380(7)
N(1)-C(7)	1.469(4)	C(11)-H(11A)	0.96(5)
N(1)-C(6)	1.487(4)	C(12)-C(13)	1.377(8)
N(1)-C(1)	1.490(4)	C(12)-H(12A)	0.91(6)
N(2)-C(3)	1.480(5)	C(13)-C(14)	1.359(7)
N(2)-C(2)	1.494(5)	C(13)-H(13A)	0.9500
N(3)-C(5)	1.487(4)	C(14)-C(15)	1.393(6)
N(3)-C(4)	1.492(4)	C(14)-H(14A)	0.95(5)
N(3)-C(9)	1.501(5)	C(15)-H(15A)	0.99(4)
C(1)-C(2)	1.525(5)	N(4)-C(16)	1.1357(10)
C(1)-H(1A)	0.92(4)	C(16)-C(17)	1.4696(10)
C(1)-H(1B)	0.95(4)	C(17)-H(17D)	0.9800
C(2)-H(2A)	0.97(4)	C(17)-H(17E)	0.9800
C(2)-H(2B)	1.00(4)	C(17)-H(17F)	0.9800
C(3)-C(4)	1.512(5)	N(4')-C(16')	1.1371(10)
C(3)-H(3A)	1.03(4)	C(16')-C(17')	1.4709(10)
C(3)-H(3B)	0.97(4)	C(17')-H(17A)	0.9800
C(4)-H(4A)	0.99(4)	C(17')-H(17B)	0.9800
C(4)-H(4B)	0.90(4)	C(17')-H(17C)	0.9800
C(5)-C(6)	1.501(5)	O(1)-Fe(1)-N(2)	156.98(10)
C(5)-H(5A)	1.03(4)	O(1)-Fe(1)-N(1)	78.53(10)
C(5)-H(5B)	0.93(4)	N(2)-Fe(1)-N(1)	78.91(10)
C(6)-H(6A)	0.96(4)	O(1)-Fe(1)-Cl(2)	100.71(8)
C(6)-H(6B)	0.91(4)	N(2)-Fe(1)-Cl(2)	101.15(8)
O(1)-C(8)	1.294(4)	N(1)-Fe(1)-Cl(2)	173.21(8)
C(7)-C(8)	1.524(5)	O(1)-Fe(1)-N(3)	92.47(10)
C(7)-H(7A)	1.00(4)	N(2)-Fe(1)-N(3)	78.75(10)
C(7)-H(7B)	1.03(4)	N(1)-Fe(1)-N(3)	78.97(10)
C(8)-O(2)	1.225(4)	Cl(2)-Fe(1)-N(3)	94.35(7)

O(1)-Fe(1)-Cl(1)	95.49(8)	C(4)-C(3)-H(3B)	110(2)
N(2)-Fe(1)-Cl(1)	89.13(8)	H(3A)-C(3)-H(3B)	110(3)
N(1)-Fe(1)-Cl(1)	90.26(7)	N(3)-C(4)-C(3)	111.0(3)
Cl(2)-Fe(1)-Cl(1)	96.53(4)	N(3)-C(4)-H(4A)	110(2)
N(3)-Fe(1)-Cl(1)	165.08(7)	C(3)-C(4)-H(4A)	111(2)
C(7)-N(1)-C(6)	111.4(3)	N(3)-C(4)-H(4B)	105(3)
C(7)-N(1)-C(1)	114.3(3)	C(3)-C(4)-H(4B)	110(2)
C(6)-N(1)-C(1)	111.5(3)	H(4A)-C(4)-H(4B)	109(3)
C(7)-N(1)-Fe(1)	103.3(2)	N(3)-C(5)-C(6)	111.8(3)
C(6)-N(1)-Fe(1)	110.7(2)	N(3)-C(5)-H(5A)	110(2)
C(1)-N(1)-Fe(1)	105.1(2)	C(6)-C(5)-H(5A)	108.8(19)
C(3)-N(2)-C(2)	113.4(3)	N(3)-C(5)-H(5B)	110(2)
C(3)-N(2)-Fe(1)	107.1(2)	C(6)-C(5)-H(5B)	109(2)
C(2)-N(2)-Fe(1)	113.6(2)	H(5A)-C(5)-H(5B)	107(3)
C(5)-N(3)-C(4)	111.3(3)	N(1)-C(6)-C(5)	112.8(3)
C(5)-N(3)-C(9)	110.2(3)	N(1)-C(6)-H(6A)	108(2)
C(4)-N(3)-C(9)	112.2(3)	C(5)-C(6)-H(6A)	111(2)
C(5)-N(3)-Fe(1)	103.3(2)	N(1)-C(6)-H(6B)	103(2)
C(4)-N(3)-Fe(1)	108.8(2)	C(5)-C(6)-H(6B)	113(2)
C(9)-N(3)-Fe(1)	110.8(2)	H(6A)-C(6)-H(6B)	108(3)
N(1)-C(1)-C(2)	109.5(3)	C(8)-O(1)-Fe(1)	117.7(2)
N(1)-C(1)-H(1A)	112(2)	N(1)-C(7)-C(8)	111.0(3)
C(2)-C(1)-H(1A)	109(2)	N(1)-C(7)-H(7A)	108(2)
N(1)-C(1)-H(1B)	107(2)	C(8)-C(7)-H(7A)	113(2)
C(2)-C(1)-H(1B)	115(2)	N(1)-C(7)-H(7B)	116(2)
H(1A)-C(1)-H(1B)	104(3)	C(8)-C(7)-H(7B)	109(2)
N(2)-C(2)-C(1)	112.2(3)	H(7A)-C(7)-H(7B)	99(3)
N(2)-C(2)-H(2A)	110(2)	O(2)-C(8)-O(1)	124.3(3)
C(1)-C(2)-H(2A)	109(2)	O(2)-C(8)-C(7)	119.1(3)
N(2)-C(2)-H(2B)	111(2)	O(1)-C(8)-C(7)	116.5(3)
C(1)-C(2)-H(2B)	110(2)	N(3)-C(9)-C(10)	115.5(3)
H(2A)-C(2)-H(2B)	104(3)	N(3)-C(9)-H(9A)	104(2)
N(2)-C(3)-C(4)	110.2(3)	C(10)-C(9)-H(9A)	111(2)
N(2)-C(3)-H(3A)	116(2)	N(3)-C(9)-H(9B)	103(2)
C(4)-C(3)-H(3A)	105(2)	C(10)-C(9)-H(9B)	114(2)
N(2)-C(3)-H(3B)	105(2)	H(9A)-C(9)-H(9B)	108(3)

C(15)-C(10)-C(11)	118.4(4)	C(10)-C(15)-H(15A)	119(2)
C(15)-C(10)-C(9)	121.0(3)	C(14)-C(15)-H(15A)	120(2)
C(11)-C(10)-C(9)	120.6(4)	N(4)-C(16)-C(17)	180.000(5)
C(12)-C(11)-C(10)	120.2(5)	C(16)-C(17)-H(17D)	109.5
C(12)-C(11)-H(11A)	122(3)	C(16)-C(17)-H(17E)	109.5
C(10)-C(11)-H(11A)	118(3)	H(17D)-C(17)-H(17E)	109.5
C(13)-C(12)-C(11)	120.6(5)	C(16)-C(17)-H(17F)	109.5
C(13)-C(12)-H(12A)	113(4)	H(17D)-C(17)-H(17F)	109.5
C(11)-C(12)-H(12A)	126(4)	H(17E)-C(17)-H(17F)	109.5
C(14)-C(13)-C(12)	120.1(4)	N(4')-C(16')-C(17')	171.0(12)
C(14)-C(13)-H(13A)	119.9	C(16')-C(17')-H(17A)	109.5
C(12)-C(13)-H(13A)	119.9	C(16')-C(17')-H(17B)	109.5
C(13)-C(14)-C(15)	119.8(4)	H(17A)-C(17')-H(17B)	109.5
C(13)-C(14)-H(14A)	133(3)	C(16')-C(17')-H(17C)	109.5
C(15)-C(14)-H(14A)	107(3)	H(17A)-C(17')-H(17C)	109.5
C(10)-C(15)-C(14)	120.9(4)	H(17B)-C(17')-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $FeL^1Cl_2 \cdot 0.5CH_3CN$ (**1**·0.5CH_3CN). 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	16(1)	37(1)	20(1)	1(1)	-1(1)	0(1)
Cl1	27(1)	56(1)	35(1)	-14(1)	-3(1)	-6(1)
Cl2	30(1)	53(1)	39(1)	11(1)	-9(1)	6(1)
N1	25(2)	29(2)	23(1)	0(1)	1(1)	-2(1)
N2	20(1)	41(2)	25(1)	0(1)	1(1)	-2(1)
N3	22(2)	29(2)	25(1)	2(1)	0(1)	0(1)
C1	29(2)	34(2)	36(2)	-5(2)	2(2)	5(2)
C2	28(2)	41(2)	36(2)	-6(2)	10(2)	1(2)
C3	26(2)	47(2)	30(2)	9(2)	4(2)	-4(2)
C4	24(2)	38(2)	34(2)	1(2)	1(2)	-4(2)
C5	23(2)	38(2)	23(2)	4(1)	-4(2)	2(2)
C6	25(2)	38(2)	23(2)	2(2)	-5(2)	-2(2)
O1	22(1)	40(1)	26(1)	1(1)	2(1)	2(1)
C7	34(2)	31(2)	33(2)	5(2)	4(2)	-2(2)
C8	28(2)	45(2)	15(2)	-5(2)	-3(1)	-6(2)
O2	28(1)	62(2)	23(1)	1(1)	2(1)	-11(1)
C9	31(2)	35(2)	35(2)	1(2)	-3(2)	4(2)
C10	32(2)	27(2)	40(2)	-1(2)	1(2)	2(2)
C11	73(4)	42(2)	56(3)	-4(2)	13(3)	-13(2)
C12	78(4)	61(3)	85(5)	-25(3)	25(3)	-35(3)
C13	56(3)	57(3)	73(3)	-30(3)	-13(3)	-7(2)
C14	61(3)	45(3)	43(2)	-11(2)	-8(2)	13(2)
C15	39(2)	33(2)	40(2)	-4(2)	0(2)	4(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $FeL^1Cl_2 \cdot 0.5CH_3CN$ (**1**·$0.5CH_3CN$).

	x	y	z	U(eq)
H1A	7880(30)	3487(18)	5870(30)	40
H1B	8790(30)	3514(17)	6450(30)	40
H2A	7650(30)	2936(18)	7400(30)	42
H2B	7230(30)	2551(18)	6520(30)	42
H3A	7340(30)	1433(18)	7280(30)	41
H3B	8470(30)	1160(20)	7270(30)	41
H4A	7650(30)	837(19)	5840(30)	38
H4B	7430(30)	1578(19)	5660(30)	38
H5A	8060(30)	1579(17)	4060(30)	33
H5B	9150(30)	1825(18)	4090(30)	33
H6A	8260(30)	2779(17)	4120(30)	34
H6B	7680(30)	2528(17)	4980(30)	34
H7A	9840(30)	3640(19)	5350(30)	39
H7B	9450(30)	3512(19)	4320(30)	39
H9A	9360(30)	531(18)	5750(30)	40
H9B	9930(30)	920(20)	4910(30)	40
H11A	8070(40)	-250(20)	5340(40)	69
H12A	7330(40)	-940(30)	4110(40)	89
H13A	7512	-727	2553	74
H14A	8700(30)	160(20)	2100(40)	60
H15A	9430(30)	760(20)	3180(30)	44
H17D	10361	5391	3434	97
H17E	9327	5019	3434	97
H17F	10312	4590	3434	97
H17A	9896	5009	3388	97
H17B	10473	4322	3552	97
H17C	11062	5007	3410	97

Table S6. Torsion angles [°] for $FeL^1Cl_2 \cdot 0.5CH_3CN$ (**1**·0.5CH_3CN).

O1-Fe1-N1-C7	-30.9(2)	Cl1-Fe1-N3-C4	-44.2(4)
N2-Fe1-N1-C7	153.7(2)	O1-Fe1-N3-C9	69.8(2)
Cl2-Fe1-N1-C7	-115.2(6)	N2-Fe1-N3-C9	-131.7(2)
N3-Fe1-N1-C7	-125.7(2)	N1-Fe1-N3-C9	147.6(2)
Cl1-Fe1-N1-C7	64.6(2)	Cl2-Fe1-N3-C9	-31.2(2)
O1-Fe1-N1-C6	88.4(2)	Cl1-Fe1-N3-C9	-167.9(2)
N2-Fe1-N1-C6	-86.9(2)	C7-N1-C1-C2	-161.4(3)
Cl2-Fe1-N1-C6	4.2(8)	C6-N1-C1-C2	71.1(4)
N3-Fe1-N1-C6	-6.4(2)	Fe1-N1-C1-C2	-48.9(3)
Cl1-Fe1-N1-C6	-176.0(2)	C3-N2-C2-C1	-133.3(3)
O1-Fe1-N1-C1	-151.1(2)	Fe1-N2-C2-C1	-10.7(4)
N2-Fe1-N1-C1	33.6(2)	N1-C1-C2-N2	40.9(4)
Cl2-Fe1-N1-C1	124.7(6)	C2-N2-C3-C4	72.3(4)
N3-Fe1-N1-C1	114.1(2)	Fe1-N2-C3-C4	-53.9(3)
Cl1-Fe1-N1-C1	-55.50(19)	C5-N3-C4-C3	-131.3(3)
O1-Fe1-N2-C3	101.7(3)	C9-N3-C4-C3	104.7(3)
N1-Fe1-N2-C3	113.4(2)	Fe1-N3-C4-C3	-18.2(4)
Cl2-Fe1-N2-C3	-59.7(2)	N2-C3-C4-N3	47.9(4)
N3-Fe1-N2-C3	32.6(2)	C4-N3-C5-C6	66.3(4)
Cl1-Fe1-N2-C3	-156.2(2)	C9-N3-C5-C6	-168.6(3)
O1-Fe1-N2-C2	-24.4(4)	Fe1-N3-C5-C6	-50.3(3)
N1-Fe1-N2-C2	-12.7(2)	C7-N1-C6-C5	95.3(3)
Cl2-Fe1-N2-C2	174.2(2)	C1-N1-C6-C5	-135.7(3)
N3-Fe1-N2-C2	-93.5(2)	Fe1-N1-C6-C5	-19.1(3)
Cl1-Fe1-N2-C2	77.7(2)	N3-C5-C6-N1	48.9(4)
O1-Fe1-N3-C5	-48.1(2)	N2-Fe1-O1-C8	36.1(4)
N2-Fe1-N3-C5	110.4(2)	N1-Fe1-O1-C8	24.5(2)
N1-Fe1-N3-C5	29.7(2)	Cl2-Fe1-O1-C8	-162.4(2)
Cl2-Fe1-N3-C5	-149.07(19)	N3-Fe1-O1-C8	102.7(2)
Cl1-Fe1-N3-C5	74.2(4)	Cl1-Fe1-O1-C8	-64.7(2)
O1-Fe1-N3-C4	-166.5(2)	C6-N1-C7-C8	-85.5(3)
N2-Fe1-N3-C4	-7.9(2)	C1-N1-C7-C8	147.1(3)
N1-Fe1-N3-C4	-88.7(2)	Fe1-N1-C7-C8	33.4(3)
Cl2-Fe1-N3-C4	92.6(2)	Fe1-O1-C8-O2	165.5(3)

Fe1-O1-C8-C7	-11.5(4)	C15-C10-C11-C12	-2.8(7)
N1-C7-C8-O2	164.6(3)	C9-C10-C11-C12	179.9(4)
N1-C7-C8-O1	-18.3(4)	C10-C11-C12-C13	0.9(9)
C5-N3-C9-C10	-54.5(4)	C11-C12-C13-C14	1.6(9)
C4-N3-C9-C10	70.1(4)	C12-C13-C14-C15	-2.0(7)
Fe1-N3-C9-C10	-168.1(2)	C11-C10-C15-C14	2.4(6)
N3-C9-C10-C15	88.1(4)	C9-C10-C15-C14	179.7(3)
N3-C9-C10-C11	-94.7(4)	C13-C14-C15-C10	0.0(6)

Symmetry transformations used to generate equivalent atoms: