

{Tris[2-(imidazol-2-ylmethylimino)ethyl]-methylammonium]iron(II) tris(perchlorate) dihydrate

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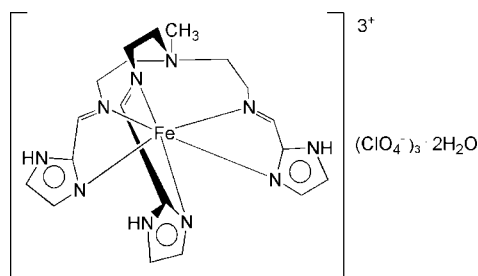
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 19.1.

The title complex, $[\text{Fe}(\text{C}_{19}\text{H}_{27}\text{N}_{10})](\text{ClO}_4)_3 \cdot 2\text{H}_2\text{O}$, is a new polymorph of an iron(II) Schiff base complex of tris(2-aminoethyl)methylammonium with imidazole-2-carboxaldehyde. The octahedral Fe^{II} atom is bound to three facial imidazole N atoms with average $\text{Fe}-\text{N}_{\text{imidazole}}$ and $\text{Fe}-\text{N}_{\text{imine}}$ bond distances of 1.963 (5) and 1.951 (5) Å, respectively. The central N atom of the tripodal ligand is outside the bonding distance at 3.92 Å. The crystal packing is stabilized by the hydrogen-bonding interactions between the two water molecules (acceptor) and two of the three imidazole NH groups (donor). The third imidazole NH group (donor) forms a hydrogen bond to one of the three perchlorate counter-ions (acceptor).

Related literature

For the synthesis, see: Brewer *et al.* (2005). For related structures, see: Brewer *et al.* (2006, 2007).



Experimental

Crystal data

$[\text{Fe}(\text{C}_{19}\text{H}_{27}\text{N}_{10})](\text{ClO}_4)_3 \cdot 2\text{H}_2\text{O}$
 $M_r = 785.74$
Orthorhombic, $Pbca$

$a = 13.9630$ (18) Å
 $b = 11.7810$ (15) Å
 $c = 37.182$ (5) Å

$V = 6116.4$ (14) Å³
 $Z = 8$
Mo $K\alpha$ radiation

$\mu = 0.84$ mm⁻¹
 $T = 173$ K
 $0.54 \times 0.45 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.682$, $T_{\text{max}} = 0.904$
65065 measured reflections
8324 independent reflections
6601 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.108$
 $S = 1.04$
8324 reflections
436 parameters
6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.76$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.62$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1W}-\text{H1W2}\cdots\text{O14}^{\text{i}}$	0.807 (19)	2.29 (4)	2.938 (3)	138 (5)
$\text{O2W}-\text{H2W1}\cdots\text{O14}^{\text{ii}}$	0.820 (17)	2.26 (2)	2.987 (3)	148 (4)
$\text{O2W}-\text{H2W2}\cdots\text{O22}^{\text{iii}}$	0.821 (18)	2.07 (2)	2.861 (3)	160 (4)
$\text{N3A}-\text{H3AB}\cdots\text{O2W}$	0.88	1.91	2.730 (3)	155
$\text{N3B}-\text{H3BB}\cdots\text{O1W}$	0.88	1.95	2.752 (3)	152
$\text{N3C}-\text{H3CB}\cdots\text{O14}$	0.88	2.05	2.907 (3)	163

Symmetry codes: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, z$; (ii) $x, y + 1, z$; (iii) $-x + \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2006); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2214).

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supplementary materials

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{Tris[2-(imidazol-2-ylmethylimino)ethyl]methylammonium}iron(II) tris(perchlorate) dihydrate

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Comment

Iron(II) and iron(III) Schiff base complexes of tris(2-aminoethyl)amine (tren) with imidazole carboxaldehyde have displayed spin crossover behavior (Brewer *et al.*, 2006). Further, it has been demonstrated that the distance between the Fe atom and the central tren-N atom, N_{ap} , is an indicator of spin-state (Brewer *et al.*, 2006). Shorter distances correlate with high spin and longer distances with low spin. Quarternization of N_{ap} , as observed in the title complex, (I), results in an elongated Fe— N_{ap} distance due to both the conformation of the N_{ap} atom (inverted away from the Fe atom) and the repulsive forces between the positively charged atoms (Brewer *et al.*, 2005). Recently, it was shown that (I), without the methyl group on N_{ap} , could serve as a bidentate hydrogen bond donor to the perchlorate anion of potassium perchlorate using the adjacent imidazole-NH and imine-CH H atoms to give supramolecular complexes (Brewer *et al.*, 2007). Since the present molecule possesses this same structural feature, the reaction of it with potassium perchlorate was investigated. The reaction did not yield the desired product but gave (I) as a polymorph (Brewer *et al.*, 2007). The structure of the iron cation differs from the original report in that the three arms of the ligand are not identical. In addition, the hydrogen bonding interactions with coordinated water and perchlorate are significantly different. Investigation of these effects on the spin crossover process and reactivity of the complex will be aided by the structural characterization of this new polymorph. In view of the importance of the spin crossover phenomenon and supramolecular systems, the present paper reports the crystal structure of (I) (Fig. 1).

The octahedral iron(II) atom is bound to three facial imidazole-N atoms whose average Fe—N bond distances for the imidazole- and imine-N atoms are 1.963 (5) Å and 1.951 (5) Å, respectively. The central N atom of the tripodal ligand is outside the bonding distance at 3.92 Å. Crystal packing is stabilized by the hydrogen bonding interactions between the two water molecules (acceptor) and two of the three imidazole NH groups (donor). The third imidazole NH group (donor) hydrogen bonds to one of the three perchlorate counterions (acceptor) (Table 1 & Fig. 2).

Experimental

Complex (I) was synthesized as previously described (Brewer *et al.*, 2005) and was recrystallized from methanol solution in the presence of equimolar potassium perchlorate. The resulting crystals were analyzed by X-ray diffraction.

Refinement

The positional parameters of the water-bound H atoms were refined with $U_{iso}(H) = 1.17-1.49U_{eq}(C,N)$; see Table 1 for distances. The remaining H atoms were included in the riding model approximation with N—H = 0.88 Å and C—H = 0.95 to 0.99 Å, and with $U_{iso}(H) = 1.17-1.49U_{eq}(C,N)$.

Figures

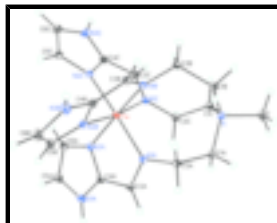


Fig. 1. Molecular structure of the cation in (I), showing atom labeling and 50% probability displacement ellipsoids.

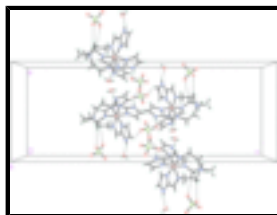


Fig. 2. Partial packing diagram for (I), viewed down the *b* axis. Dashed lines indicate C–H...O (water & perchlorate) hydrogen bonds.

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Crystal data

[Fe(C₁₉H₂₇N₁₀)](ClO₄)₃·2H₂O

M_r = 785.74

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

a = 13.9630 (18) Å

b = 11.7810 (15) Å

c = 37.182 (5) Å

V = 6116.4 (14) Å³

Z = 8

*F*₀₀₀ = 3232

D_x = 1.707 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 9963 reflections

θ = 2.2–28.9°

μ = 0.84 mm⁻¹

T = 173 K

Chunk, dark-red

0.54 × 0.45 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 173 K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

*T*_{min} = 0.682, *T*_{max} = 0.904

65065 measured reflections

8324 independent reflections

6601 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.054

θ_{max} = 29.3°

θ_{min} = 1.8°

h = -19→19

k = -16→13

l = -51→51

Refinement

Refinement on *F*²

Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 5.7069P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
8324 reflections	$(\Delta/\sigma)_{\max} = 0.001$
436 parameters	$\Delta\rho_{\max} = 0.76 \text{ e } \text{\AA}^{-3}$
6 restraints	$\Delta\rho_{\min} = -0.62 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe	0.542493 (19)	0.511159 (2)	0.110991 (7)	0.01627 (7)
Cl1	0.32256 (4)	0.00301 (5)	0.015096 (15)	0.02982 (12)
Cl2	0.24581 (4)	0.63667 (5)	0.208500 (15)	0.02861 (12)
Cl3	0.57715 (4)	0.00513 (5)	0.181644 (16)	0.03151 (13)
O11	0.3162 (2)	0.0909 (2)	-0.01088 (7)	0.0756 (8)
O12	0.23275 (13)	-0.05400 (18)	0.01888 (6)	0.0489 (5)
O13	0.39474 (14)	-0.07620 (18)	0.00529 (6)	0.0526 (5)
O14	0.34756 (14)	0.05377 (19)	0.04951 (5)	0.0494 (5)
O21	0.23376 (18)	0.51820 (17)	0.21519 (7)	0.0598 (6)
O22	0.19608 (18)	0.6630 (2)	0.17533 (6)	0.0610 (6)
O23	0.34507 (13)	0.66157 (19)	0.20374 (6)	0.0505 (5)
O24	0.20629 (13)	0.70357 (17)	0.23716 (5)	0.0437 (5)
O31	0.50024 (19)	-0.0216 (2)	0.15709 (7)	0.0687 (7)
O32	0.61507 (15)	-0.10022 (17)	0.19422 (8)	0.0617 (6)
O33	0.65127 (16)	0.06867 (16)	0.16416 (7)	0.0570 (6)
O34	0.53883 (17)	0.06912 (18)	0.21060 (6)	0.0576 (6)
O1W	0.96601 (19)	0.4969 (3)	0.08139 (9)	0.1023 (13)
H1W1	0.983 (4)	0.562 (3)	0.0904 (16)	0.153*
H1W2	1.003 (4)	0.489 (5)	0.0650 (12)	0.153*
O2W	0.28606 (16)	0.98531 (17)	0.12333 (6)	0.0461 (5)

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H2W1	0.287 (3)	1.024 (3)	0.1051 (6)	0.069*
H2W2	0.304 (3)	1.029 (3)	0.1392 (7)	0.069*
N	0.56728 (13)	0.38916 (15)	0.20854 (4)	0.0215 (3)
N1A	0.54566 (12)	0.61049 (14)	0.15322 (4)	0.0190 (3)
N2A	0.44316 (12)	0.61938 (14)	0.09684 (5)	0.0199 (3)
N3A	0.36892 (13)	0.78081 (16)	0.10830 (5)	0.0269 (4)
H3AB	0.3517	0.8440	0.1192	0.032*
N1B	0.65376 (12)	0.42147 (14)	0.12542 (4)	0.0193 (3)
N2B	0.64328 (12)	0.60169 (14)	0.08733 (4)	0.0198 (3)
N3B	0.79608 (13)	0.61176 (17)	0.07239 (5)	0.0288 (4)
H3BB	0.8573	0.5947	0.0707	0.035*
N1C	0.45107 (12)	0.40472 (14)	0.13101 (4)	0.0192 (3)
N2C	0.52259 (12)	0.41612 (14)	0.06825 (4)	0.0198 (3)
N3C	0.44957 (15)	0.26827 (17)	0.04444 (5)	0.0304 (4)
H3CB	0.4121	0.2086	0.0422	0.036*
C	0.57789 (18)	0.3404 (2)	0.24639 (6)	0.0301 (5)
H0A	0.5769	0.2573	0.2452	0.045*
H0B	0.5248	0.3669	0.2615	0.045*
H0C	0.6388	0.3656	0.2568	0.045*
C1A	0.56992 (16)	0.51802 (17)	0.21406 (5)	0.0236 (4)
H1AA	0.5037	0.5427	0.2195	0.028*
H1AB	0.6084	0.5327	0.2359	0.028*
C2A	0.60808 (15)	0.59560 (17)	0.18461 (5)	0.0220 (4)
H2AA	0.6205	0.6712	0.1952	0.026*
H2AB	0.6702	0.5650	0.1762	0.026*
C3A	0.49249 (15)	0.69994 (17)	0.15189 (5)	0.0214 (4)
H3AA	0.4921	0.7567	0.1701	0.026*
C4A	0.43400 (14)	0.70505 (17)	0.12017 (5)	0.0209 (4)
C5A	0.33456 (16)	0.7412 (2)	0.07621 (6)	0.0301 (5)
H5AA	0.2875	0.7764	0.0615	0.036*
C6A	0.38088 (15)	0.64128 (19)	0.06928 (6)	0.0258 (4)
H6AA	0.3714	0.5947	0.0487	0.031*
C1B	0.65416 (15)	0.34079 (18)	0.18863 (6)	0.0238 (4)
H1BA	0.7086	0.3924	0.1934	0.029*
H1BB	0.6700	0.2674	0.2001	0.029*
C2B	0.65151 (15)	0.32028 (17)	0.14818 (5)	0.0221 (4)
H2BA	0.7068	0.2718	0.1417	0.026*
H2BB	0.5926	0.2771	0.1425	0.026*
C3B	0.73460 (15)	0.45056 (18)	0.11120 (5)	0.0221 (4)
H3BA	0.7922	0.4088	0.1144	0.027*
C4B	0.72866 (14)	0.55230 (18)	0.09009 (5)	0.0219 (4)
C5B	0.65706 (16)	0.69750 (18)	0.06694 (6)	0.0243 (4)
H5BA	0.6089	0.7507	0.0605	0.029*
C6B	0.75165 (17)	0.7035 (2)	0.05749 (6)	0.0300 (5)
H6BA	0.7809	0.7609	0.0433	0.036*
C1C	0.47042 (15)	0.34435 (18)	0.19572 (6)	0.0233 (4)
H1CA	0.4811	0.2670	0.1861	0.028*
H1CB	0.4291	0.3363	0.2172	0.028*
C2C	0.41328 (14)	0.40958 (18)	0.16763 (5)	0.0217 (4)

H2CA	0.3470	0.3797	0.1674	0.026*
H2CB	0.4100	0.4901	0.1751	0.026*
C3C	0.41876 (15)	0.32709 (18)	0.10959 (6)	0.0243 (4)
H3CA	0.3723	0.2723	0.1165	0.029*
C4C	0.46053 (15)	0.33235 (18)	0.07423 (6)	0.0244 (4)
C5C	0.55206 (15)	0.40500 (19)	0.03331 (6)	0.0245 (4)
H5CA	0.5964	0.4533	0.0214	0.029*
C6C	0.50736 (18)	0.3132 (2)	0.01838 (6)	0.0310 (5)
H6CA	0.5150	0.2858	-0.0055	0.037*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe	0.01808 (13)	0.01279 (13)	0.01794 (13)	-0.00035 (10)	0.00077 (10)	-0.00083 (10)
Cl1	0.0326 (3)	0.0217 (3)	0.0352 (3)	0.0011 (2)	-0.0064 (2)	-0.0012 (2)
Cl2	0.0264 (2)	0.0239 (3)	0.0356 (3)	0.00118 (19)	0.0062 (2)	-0.0030 (2)
Cl3	0.0313 (3)	0.0234 (3)	0.0399 (3)	0.0000 (2)	0.0070 (2)	-0.0013 (2)
O11	0.118 (2)	0.0463 (14)	0.0629 (15)	0.0105 (14)	-0.0153 (15)	0.0256 (12)
O12	0.0305 (9)	0.0428 (11)	0.0734 (14)	-0.0057 (8)	-0.0084 (9)	-0.0190 (10)
O13	0.0387 (11)	0.0425 (12)	0.0765 (15)	0.0111 (9)	0.0060 (10)	-0.0037 (10)
O14	0.0471 (11)	0.0592 (13)	0.0418 (11)	-0.0193 (10)	-0.0031 (9)	-0.0152 (10)
O21	0.0761 (16)	0.0259 (10)	0.0775 (16)	-0.0005 (10)	0.0343 (13)	0.0033 (10)
O22	0.0761 (16)	0.0557 (14)	0.0512 (12)	0.0259 (12)	-0.0215 (11)	-0.0124 (10)
O23	0.0311 (9)	0.0589 (13)	0.0615 (13)	-0.0122 (9)	0.0157 (9)	-0.0303 (10)
O24	0.0441 (10)	0.0425 (11)	0.0447 (10)	0.0049 (9)	0.0181 (8)	-0.0097 (8)
O31	0.0615 (15)	0.0787 (18)	0.0660 (16)	-0.0064 (13)	-0.0182 (12)	0.0026 (13)
O32	0.0452 (12)	0.0272 (10)	0.113 (2)	0.0029 (9)	-0.0029 (12)	0.0131 (11)
O33	0.0592 (13)	0.0294 (10)	0.0824 (16)	-0.0085 (9)	0.0369 (12)	-0.0004 (10)
O34	0.0787 (16)	0.0403 (12)	0.0538 (13)	-0.0004 (11)	0.0307 (11)	-0.0083 (10)
O1W	0.0430 (14)	0.185 (4)	0.079 (2)	0.0426 (19)	0.0211 (13)	0.056 (2)
O2W	0.0545 (12)	0.0397 (11)	0.0442 (11)	0.0104 (10)	-0.0002 (10)	-0.0089 (9)
N	0.0263 (8)	0.0185 (8)	0.0196 (8)	-0.0007 (7)	0.0005 (7)	0.0020 (6)
N1A	0.0221 (8)	0.0159 (8)	0.0190 (8)	-0.0029 (6)	0.0008 (6)	0.0002 (6)
N2A	0.0207 (8)	0.0163 (8)	0.0227 (8)	0.0005 (6)	0.0009 (6)	0.0007 (6)
N3A	0.0275 (9)	0.0192 (9)	0.0340 (10)	0.0054 (7)	0.0034 (8)	0.0025 (7)
N1B	0.0221 (8)	0.0155 (8)	0.0203 (8)	0.0013 (6)	0.0020 (6)	-0.0021 (6)
N2B	0.0230 (8)	0.0168 (8)	0.0195 (8)	-0.0023 (6)	0.0008 (6)	-0.0013 (6)
N3B	0.0237 (9)	0.0324 (10)	0.0304 (9)	-0.0048 (8)	0.0048 (7)	0.0049 (8)
N1C	0.0198 (8)	0.0161 (8)	0.0218 (8)	-0.0002 (6)	0.0013 (6)	0.0000 (6)
N2C	0.0227 (8)	0.0158 (8)	0.0209 (8)	0.0024 (6)	0.0001 (6)	-0.0013 (6)
N3C	0.0373 (10)	0.0250 (10)	0.0288 (9)	-0.0055 (8)	-0.0040 (8)	-0.0109 (8)
C	0.0424 (13)	0.0268 (11)	0.0212 (10)	-0.0012 (10)	-0.0011 (9)	0.0066 (8)
C1A	0.0323 (10)	0.0193 (10)	0.0193 (9)	-0.0004 (8)	-0.0019 (8)	-0.0014 (7)
C2A	0.0267 (10)	0.0177 (9)	0.0217 (9)	-0.0037 (8)	-0.0044 (8)	-0.0026 (7)
C3A	0.0268 (10)	0.0150 (9)	0.0224 (9)	-0.0010 (7)	0.0047 (8)	-0.0023 (7)
C4A	0.0212 (9)	0.0170 (9)	0.0243 (10)	0.0005 (7)	0.0040 (7)	0.0015 (7)
C5A	0.0277 (11)	0.0297 (12)	0.0329 (12)	0.0038 (9)	-0.0022 (9)	0.0069 (9)
C6A	0.0246 (10)	0.0276 (11)	0.0251 (10)	-0.0010 (8)	-0.0022 (8)	0.0025 (8)

supplementary materials

C1B	0.0246 (10)	0.0214 (10)	0.0254 (10)	0.0031 (8)	-0.0014 (8)	0.0038 (8)
C2B	0.0254 (10)	0.0163 (9)	0.0245 (10)	0.0025 (8)	0.0021 (8)	0.0021 (7)
C3B	0.0213 (9)	0.0220 (10)	0.0231 (9)	0.0014 (8)	0.0009 (8)	-0.0022 (8)
C4B	0.0218 (9)	0.0231 (10)	0.0209 (9)	-0.0026 (8)	0.0033 (7)	-0.0012 (8)
C5B	0.0301 (10)	0.0191 (10)	0.0236 (10)	-0.0033 (8)	-0.0012 (8)	0.0022 (8)
C6B	0.0344 (12)	0.0275 (12)	0.0279 (10)	-0.0087 (9)	0.0032 (9)	0.0049 (9)
C1C	0.0250 (10)	0.0211 (10)	0.0238 (10)	-0.0045 (8)	0.0026 (8)	0.0025 (8)
C2C	0.0199 (9)	0.0213 (10)	0.0241 (10)	-0.0008 (8)	0.0039 (8)	-0.0003 (8)
C3C	0.0240 (10)	0.0195 (10)	0.0293 (10)	-0.0046 (8)	0.0004 (8)	-0.0019 (8)
C4C	0.0273 (10)	0.0197 (10)	0.0261 (10)	-0.0011 (8)	-0.0039 (8)	-0.0056 (8)
C5C	0.0292 (10)	0.0229 (10)	0.0213 (9)	0.0046 (8)	-0.0007 (8)	-0.0019 (8)
C6C	0.0384 (12)	0.0309 (12)	0.0236 (10)	0.0044 (10)	-0.0027 (9)	-0.0080 (9)

Geometric parameters (Å, °)

Fe—N1C	1.9414 (17)	N1C—C3C	1.294 (3)
Fe—N2A	1.9528 (17)	N1C—C2C	1.461 (3)
Fe—N1A	1.9559 (17)	N2C—C4C	1.332 (3)
Fe—N1B	1.9567 (17)	N2C—C5C	1.369 (3)
Fe—N2C	1.9665 (17)	N3C—C4C	1.349 (3)
Fe—N2B	1.9701 (17)	N3C—C6C	1.368 (3)
Cl1—O11	1.418 (2)	N3C—H3CB	0.8800
Cl1—O13	1.421 (2)	C—H0A	0.9800
Cl1—O12	1.4295 (19)	C—H0B	0.9800
Cl1—O14	1.4548 (19)	C—H0C	0.9800
Cl2—O23	1.4277 (18)	C1A—C2A	1.523 (3)
Cl2—O21	1.428 (2)	C1A—H1AA	0.9900
Cl2—O24	1.4357 (18)	C1A—H1AB	0.9900
Cl2—O22	1.449 (2)	C2A—H2AA	0.9900
Cl3—O34	1.419 (2)	C2A—H2AB	0.9900
Cl3—O32	1.428 (2)	C3A—C4A	1.436 (3)
Cl3—O33	1.4330 (19)	C3A—H3AA	0.9500
Cl3—O31	1.444 (2)	C5A—C6A	1.368 (3)
O1W—H1W1	0.866 (19)	C5A—H5AA	0.9500
O1W—H1W2	0.807 (19)	C6A—H6AA	0.9500
O2W—H2W1	0.820 (17)	C1B—C2B	1.524 (3)
O2W—H2W2	0.821 (18)	C1B—H1BA	0.9900
N—C	1.527 (3)	C1B—H1BB	0.9900
N—C1C	1.528 (3)	C2B—H2BA	0.9900
N—C1B	1.531 (3)	C2B—H2BB	0.9900
N—C1A	1.532 (3)	C3B—C4B	1.435 (3)
N1A—C3A	1.290 (3)	C3B—H3BA	0.9500
N1A—C2A	1.467 (2)	C5B—C6B	1.369 (3)
N2A—C4A	1.337 (3)	C5B—H5BA	0.9500
N2A—C6A	1.368 (3)	C6B—H6BA	0.9500
N3A—C4A	1.348 (3)	C1C—C2C	1.523 (3)
N3A—C5A	1.368 (3)	C1C—H1CA	0.9900
N3A—H3AB	0.8800	C1C—H1CB	0.9900
N1B—C3B	1.293 (3)	C2C—H2CA	0.9900

Fig. 1

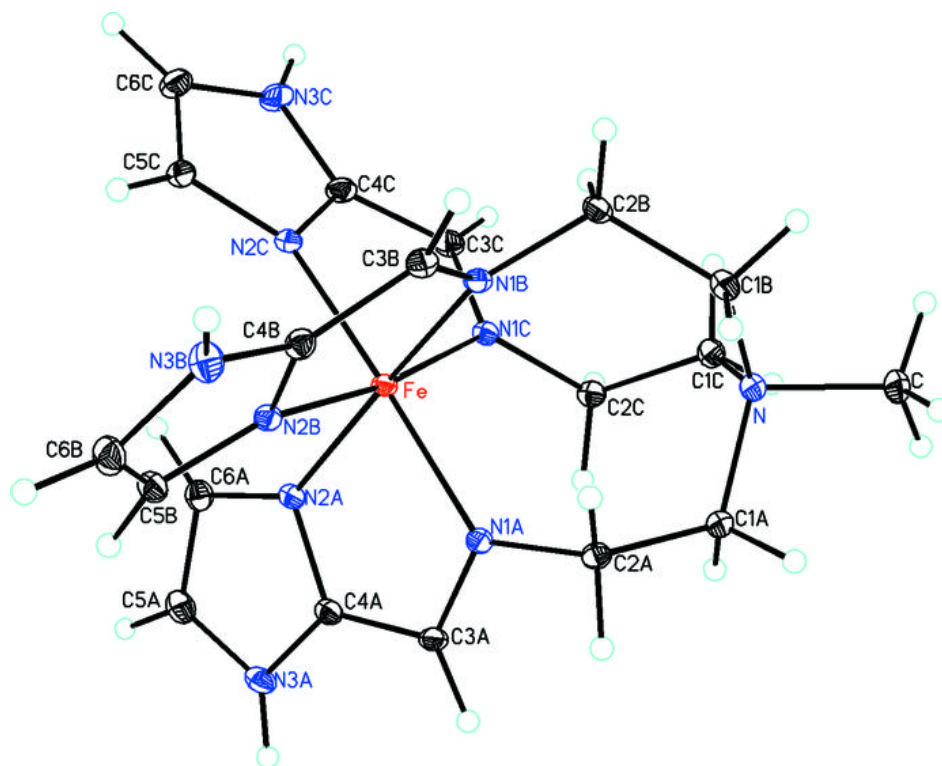


Fig. 2

