

Poly[[diaquatetrakis(μ_2 -benzene-1,4-dicarbonitrile- κ^2 N:N')iron(II)] bis[tetrachloridoferrate(III)] nitromethane tetrasolvate]

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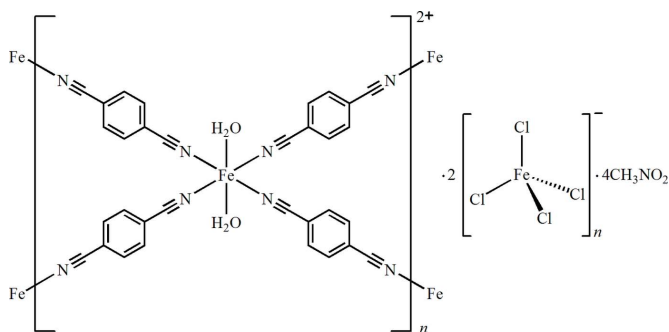
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.032; wR factor = 0.073; data-to-parameter ratio = 18.9.

In the title compound, $\{[\text{Fe}^{\text{II}}(\text{C}_8\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2][\text{Fe}^{\text{III}}\text{Cl}_4]_2 \cdot 4\text{CH}_3\text{NO}_2\}_n$, the Fe^{II} and Fe^{III} ions are hexa- and tetra-coordinated, respectively. Each unique benzene-1,4-dicarbonitrile molecule lies across a crystallographic inversion centre and bridges two Fe^{II} ions (each situated on an inversion centre), generating two-dimensional (4,4) square grid layers. The tetrachloridoferrate(III) anions and nitromethane solvent molecules lie between the square grid layers and are further link to the adjacent layers into a three-dimensional supra-molecular structure through $\text{O}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For background to Fe^{II} spin-crossover complexes, see: Kahn & Martinez (1998); Neville *et al.* (2007, 2008); Murray (2008). For the use of two connecting organodinitrile ligands for the development of magnetism, see: Chainok *et al.* (2010, 2012). For the synthesis, see: Chainok *et al.* (2012).



Experimental

Crystal data

$[\text{Fe}(\text{C}_8\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2][\text{FeCl}_4]_2 \cdot 4\text{CH}_3\text{NO}_2$	$\beta = 102.466$ (1) $^\circ$
$M_r = 987.62$	$V = 1989.9$ (3) Å 3
Monoclinic, $P2_1/n$	$Z = 2$
$a = 12.1307$ (9) Å	Mo $K\alpha$ radiation
$b = 12.1554$ (9) Å	$\mu = 1.67$ mm $^{-1}$
$c = 13.8209$ (10) Å	$T = 100$ K
	$0.27 \times 0.27 \times 0.24$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	11573 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	4397 independent reflections
$T_{\text{min}} = 0.661$, $T_{\text{max}} = 0.690$	3541 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.073$	$\Delta\rho_{\text{max}} = 0.76$ e Å $^{-3}$
$S = 1.03$	$\Delta\rho_{\text{min}} = -0.50$ e Å $^{-3}$
4397 reflections	
233 parameters	
3 restraints	

Table 1

Selected bond lengths (Å).

Fe1—O1	2.0884 (15)	Fe2—Cl2	2.1811 (6)
Fe1—N21	2.1309 (17)	Fe2—Cl3	2.1968 (6)
Fe1—N11	2.1649 (17)	Fe2—Cl4	2.1996 (6)
Cl1—Fe2	2.2070 (6)		

Table 2

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1—H1 \cdots O2	0.87 (2)	1.99 (2)	2.804 (2)	155 (3)
O1—H1 \cdots O4	0.87 (2)	2.57 (3)	3.074 (3)	118 (2)
O1—H2 \cdots Cl1	0.84 (2)	2.43 (2)	3.2731 (16)	177 (3)

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5052).

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supporting information

Acta Cryst. (2012). E68, m211–m212 [doi:10.1107/S1600536812002486]

Poly[[diaquatetrakis(μ_2 -benzene-1,4-dicarbonitrile- κ^2 N:N')iron(II)] bis-tetrachloridoferrate(III)] nitromethane tetrasolvate]

Pimonrat Prommon, Pinyada Promseenong and Kittipong Chainok

S1. Comment

The d^6 Fe(II) complexes exhibiting spin-crossover (SCO) transitions between a 1A_1 low spin ($S = 0$) and a 5T_2 high spin ($S = 2$) states are of interest due to their possible applications as molecular switches or materials for information storage (Kahn & Martinez 1998). Although the fundamental origin of the SCO phenomenon is molecular, SCO transitions in the crystal structure can be reversibly switched by external stimuli such as light, temperature and pressure as well as the existence of long or short range supramolecular interactions (Neville *et al.* 2007, 2008; Murray 2008). The title compound was obtained as a minor product in another an earlier from part of further study of how the nature of the two-connecting organodinitrile bridging ligands affect the SCO phenomenon in the Fe(II) complexes (Chainok *et al.* 2010).

A fragment containing the asymmetric unit with atom numbering and coordination environments of the metal centre of the title compound is shown in Fig. 1. The asymmetric unit contains one iron(II) cation (half-occupancy), one coordinated water molecule, half of two independent benzene-1,4-dicarbonitrile ligand, one tetrachloridoferrate(III) anion, and two nitromethane solvent molecules. The Fe^{II} ion resides in an inversion center and is octahedrally coordinated by four nitrogen atoms from benzene-1,4-dicarbonitrile ligands in the equatorial plane and two equivalent terminal water molecules occupying the axial positions. The Fe—N and Fe—O bond lengths in the title compound, Table 1, are comparable to that observed for a high spin species in the corresponding Fe(II) complex containing the two-connecting organodinitrile ligands such as [Fe^{II}(AIBN)(H₂O)][Fe^{III}Cl₄]₂ (Fe—N = 2.144 (1)–2.171 (1) Å and Fe—O = 2.084 (1) Å), AIBN = 2,2'-azobisisobutyronitrile (Chainok *et al.* 2010). Each benzene-1,4-dicarbonitrile ligand has crystallographically imposed inversion symmetry and is bound to two neighboring Fe^{II} ions generating two-dimensional approximate square grid layers with (4,4) topology perpendicular to the *c* axis, with the dimension of 12.1307 (9) × 12.1554 (9) Å (Fe^{II}...Fe^{II} distances across the benzene-1,4-dicarbonitrile ligand), Fig. 2. The layers are packed to each other with an interlayer separation of 6.0777 (5) Å.

The Fe^{III} atom is a tetrahedrally coordinated to four chloride anions. The bond lengths and angles around the Fe(III) ions are within the common ranges for this type of coordination environment (Chainok *et al.* 2010). The tetrachloridoferrate(III) anions and the nitromethane solvent molecules all lie in general position in the structure, and are included in the layers by eschewing the interpenetration of the networks. These guest molecules are then further linked to the adjacent two-dimensional layers into a three-dimensional supramolecular structure through O—H...Cl and O—H...O hydrogen bonds formed between the apically water molecules coordinated to the metal ions and Cl and O atoms of the guest molecules, Table 2.

S2. Experimental

Single crystals of the title compound were obtained as the minor product during the synthesis of $[\text{Fe}^{\text{II}}(\text{C}_8\text{H}_4\text{N}_2)_2][\text{Fe}^{\text{III}}\text{Cl}_4]_2$ (Chainok *et al.* 2012) when traces of air and moisture are presented. Typically, FeCl_2 (62 mg, 0.5 mmol) and FeCl_3 (163 mg, 1 mmol) were dissolved in 3 ml of CH_3NO_2 to form a yellow brown solution and this was pipetted into one side of the H-tube. Benzene-1,4-dicarbonitrile (192 mg, 1.5 mmol) was dissolved in 3 ml of CH_3NO_2 to give a colorless solution and this was pipetted into the other side arm of the H-tube. The H-tube was then carefully filled with CH_3NO_2 . Upon slow diffusion for two weeks, yellow block-shaped of the major product (*ca.* 60% yield based on FeCl_2) and pale yellow plate of the minor product (*ca.* 5% yield based on FeCl_2) single crystals were formed in the iron-containing side of the H-tube.

S3. Refinement

The hydrogen atoms were placed in the geometrically idealized positions and constrained to ride on their parent atom positions with a C–H distances of 0.95 and 0.99 Å $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and 0.98 Å for CH_3 [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$]. The hydrogen atoms attached to oxygen atoms of the water molecules were located in a difference Fourier map and refined being in their as-found positions with a *DFIX* restraint of O–H distance at 0.90 Å, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

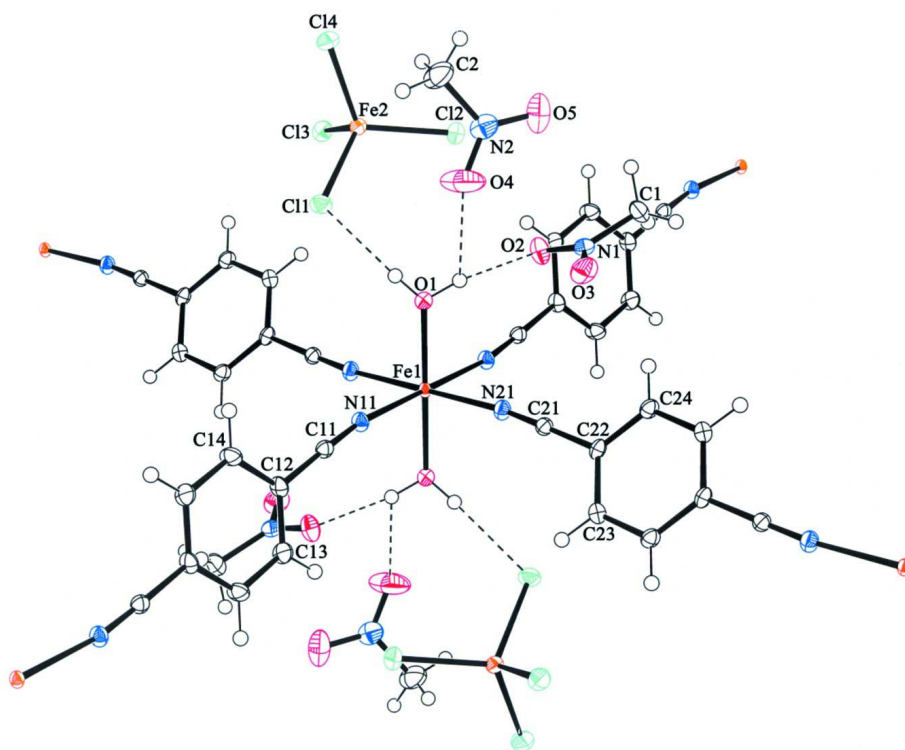


Figure 1

Displacement ellipsoid plot of a fragment at the 50% probability level containing the asymmetric unit with atom numbering and coordination environments of the metal centers of the title compound.

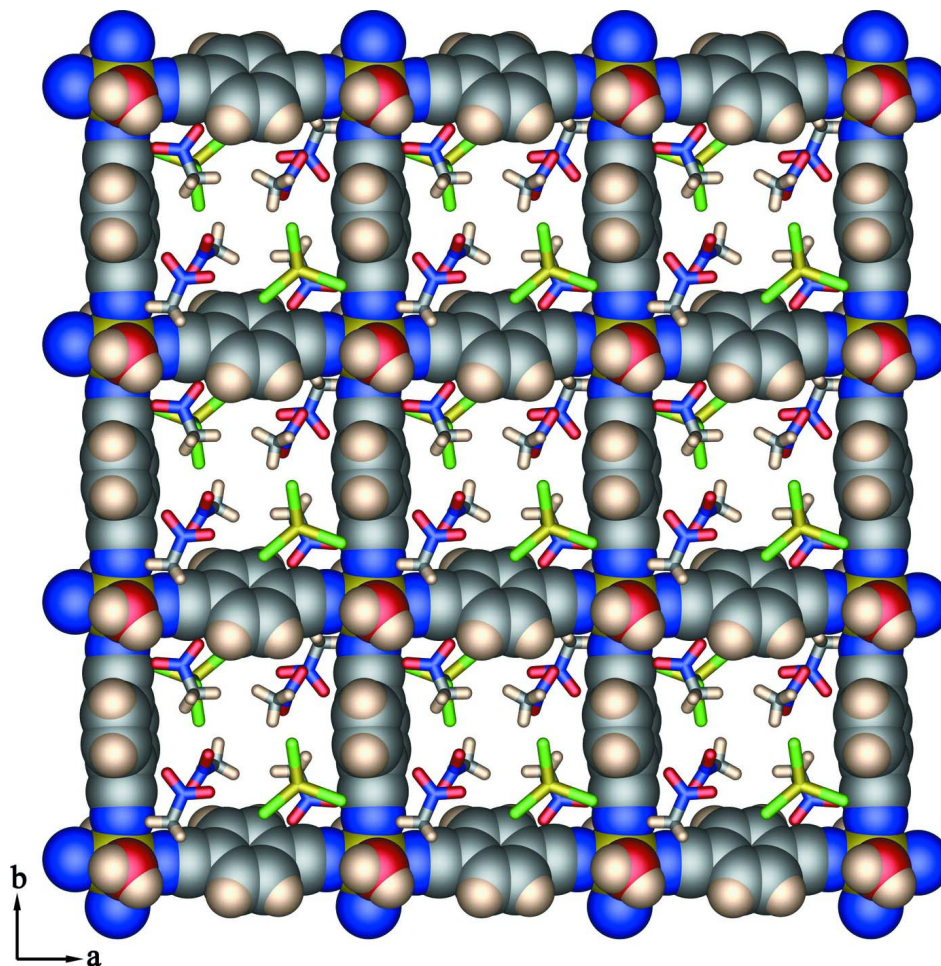


Figure 2

Inclusion of tetrachloridoferrate(III) anions and nitromethane molecules in the square grid networks of the title compound.

Poly[[diaquatetrakis(μ_2 -benzene-1,4-dicarbonitrile- $\kappa^2N:N'$)iron(II)] bis[tetrachloroferrate(III)] nitromethane tetrasolvate]

Crystal data

$[\text{Fe}(\text{C}_8\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2][\text{FeCl}_4]_2 \cdot 4\text{CH}_3\text{NO}_2$

$M_r = 987.62$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 12.1307(9) \text{ \AA}$

$b = 12.1554(9) \text{ \AA}$

$c = 13.8209(10) \text{ \AA}$

$\beta = 102.466(1)^\circ$

$V = 1989.9(3) \text{ \AA}^3$

$Z = 2$

$F(000) = 988$

$D_x = 1.648 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3583 reflections

$\theta = 2.4\text{--}27.4^\circ$

$\mu = 1.67 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, yellow

$0.27 \times 0.27 \times 0.24 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm⁻¹
 ω and φ scans
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.661$, $T_{\max} = 0.690$

11573 measured reflections
4397 independent reflections
3541 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\max} = 28.1^\circ$, $\theta_{\min} = 2.0^\circ$
 $h = -15 \rightarrow 16$
 $k = -12 \rightarrow 15$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.073$
 $S = 1.03$
4397 reflections
233 parameters
3 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.042P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.76 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.50 \text{ e } \text{\AA}^{-3}$

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 $F^2 > \sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.5000	0.5000	0.5000	0.01056 (10)
Cl1	0.31456 (5)	0.45491 (4)	0.76369 (4)	0.02217 (13)
O1	0.52584 (13)	0.46637 (12)	0.65141 (11)	0.0173 (3)
N1	0.74782 (15)	0.26095 (15)	0.71549 (13)	0.0200 (4)
C1	0.7964 (2)	0.15057 (19)	0.74355 (17)	0.0270 (5)
H1A	0.7828	0.1301	0.8086	0.040*
H1B	0.8778	0.1522	0.7465	0.040*
H1C	0.7606	0.0965	0.6941	0.040*
H1	0.576 (2)	0.417 (2)	0.676 (2)	0.052 (9)*
Fe2	0.29049 (3)	0.29511 (2)	0.83208 (2)	0.01702 (9)
Cl2	0.42489 (5)	0.18565 (5)	0.80885 (4)	0.02811 (14)
O2	0.64553 (13)	0.26786 (12)	0.68614 (12)	0.0259 (4)
N2	0.67018 (18)	0.34984 (17)	0.93557 (15)	0.0297 (5)
C2	0.6206 (3)	0.3774 (2)	1.0194 (2)	0.0437 (7)
H2A	0.6721	0.3550	1.0810	0.066*

H2B	0.5485	0.3388	1.0131	0.066*
H2C	0.6080	0.4570	1.0205	0.066*
H2	0.4716 (18)	0.466 (2)	0.6803 (19)	0.043 (9)*
Cl3	0.12062 (5)	0.23479 (4)	0.76444 (4)	0.02225 (13)
O3	0.81115 (14)	0.33973 (14)	0.72375 (13)	0.0318 (4)
Cl4	0.30172 (5)	0.31921 (5)	0.99164 (4)	0.02609 (14)
O4	0.6489 (2)	0.41206 (17)	0.86466 (15)	0.0661 (7)
O5	0.72545 (17)	0.26586 (17)	0.93885 (17)	0.0515 (6)
N11	0.49078 (14)	0.32436 (14)	0.47352 (13)	0.0159 (4)
C11	0.49325 (17)	0.23044 (17)	0.47862 (15)	0.0151 (4)
C12	0.49595 (17)	0.11201 (16)	0.48873 (15)	0.0164 (4)
C13	0.48332 (19)	0.06644 (17)	0.57797 (16)	0.0203 (5)
H13	0.4724	0.1125	0.6306	0.024*
C14	0.51318 (19)	0.04656 (17)	0.41060 (16)	0.0200 (5)
H14	0.5224	0.0791	0.3503	0.024*
N21	0.32197 (14)	0.50641 (13)	0.48775 (13)	0.0166 (4)
C21	0.22841 (17)	0.50554 (16)	0.48975 (15)	0.0148 (4)
C22	0.11031 (17)	0.50257 (16)	0.49328 (15)	0.0146 (4)
C23	0.07732 (17)	0.42932 (16)	0.55939 (15)	0.0160 (4)
H23	0.1310	0.3821	0.5994	0.019*
C24	0.03464 (17)	0.57343 (17)	0.43427 (15)	0.0164 (4)
H24	0.0595	0.6230	0.3903	0.020*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0092 (2)	0.00766 (19)	0.0156 (2)	0.00009 (14)	0.00442 (15)	0.00041 (15)
Cl1	0.0274 (3)	0.0176 (3)	0.0228 (3)	-0.0022 (2)	0.0083 (2)	0.0030 (2)
O1	0.0169 (8)	0.0178 (8)	0.0186 (8)	0.0021 (6)	0.0067 (6)	0.0021 (6)
N1	0.0243 (11)	0.0234 (10)	0.0130 (9)	0.0027 (8)	0.0053 (8)	0.0015 (7)
C1	0.0316 (14)	0.0252 (13)	0.0236 (12)	0.0121 (10)	0.0046 (10)	0.0056 (10)
Fe2	0.02082 (17)	0.01520 (16)	0.01655 (17)	0.00175 (12)	0.00737 (13)	0.00109 (12)
Cl2	0.0319 (3)	0.0281 (3)	0.0275 (3)	0.0120 (2)	0.0134 (3)	0.0028 (2)
O2	0.0192 (8)	0.0229 (8)	0.0328 (9)	0.0043 (6)	-0.0009 (7)	-0.0019 (7)
N2	0.0383 (13)	0.0251 (11)	0.0270 (11)	-0.0068 (9)	0.0104 (9)	-0.0065 (9)
C2	0.072 (2)	0.0264 (14)	0.0435 (17)	0.0025 (13)	0.0369 (16)	-0.0013 (12)
Cl3	0.0246 (3)	0.0183 (3)	0.0254 (3)	-0.0026 (2)	0.0088 (2)	-0.0022 (2)
O3	0.0274 (10)	0.0317 (10)	0.0394 (10)	-0.0080 (7)	0.0139 (8)	-0.0008 (8)
Cl4	0.0343 (3)	0.0283 (3)	0.0175 (3)	0.0041 (2)	0.0098 (2)	0.0008 (2)
O4	0.132 (2)	0.0412 (13)	0.0303 (11)	-0.0064 (13)	0.0280 (13)	0.0054 (10)
O5	0.0399 (12)	0.0445 (12)	0.0723 (15)	0.0128 (9)	0.0172 (11)	-0.0088 (11)
N11	0.0160 (9)	0.0117 (9)	0.0203 (9)	-0.0003 (6)	0.0046 (7)	-0.0003 (7)
C11	0.0140 (10)	0.0146 (11)	0.0176 (10)	-0.0011 (8)	0.0055 (8)	-0.0002 (8)
C12	0.0167 (10)	0.0095 (9)	0.0228 (11)	-0.0021 (8)	0.0041 (9)	-0.0010 (8)
C13	0.0283 (12)	0.0125 (10)	0.0219 (11)	-0.0007 (8)	0.0097 (9)	-0.0039 (9)
C14	0.0285 (12)	0.0131 (10)	0.0197 (11)	-0.0022 (9)	0.0081 (9)	0.0017 (9)
N21	0.0145 (9)	0.0137 (9)	0.0223 (9)	-0.0001 (7)	0.0058 (7)	-0.0005 (7)
C21	0.0165 (11)	0.0118 (10)	0.0169 (10)	0.0000 (8)	0.0053 (8)	-0.0001 (8)

C22	0.0109 (9)	0.0154 (10)	0.0186 (10)	-0.0018 (7)	0.0054 (8)	-0.0041 (8)
C23	0.0147 (10)	0.0149 (10)	0.0178 (10)	0.0018 (8)	0.0018 (8)	-0.0010 (8)
C24	0.0157 (10)	0.0151 (10)	0.0198 (11)	-0.0022 (8)	0.0071 (9)	-0.0003 (8)

Geometric parameters (Å, °)

Fe1—O1	2.0884 (15)	N2—C2	1.455 (3)
Fe1—O1 ⁱ	2.0884 (15)	C2—H2A	0.9800
Fe1—N21 ⁱ	2.1309 (17)	C2—H2B	0.9800
Fe1—N21	2.1309 (17)	C2—H2C	0.9800
Fe1—N11	2.1649 (17)	N11—C11	1.144 (3)
Fe1—N11 ⁱ	2.1649 (17)	C11—C12	1.446 (3)
C11—Fe2	2.2070 (6)	C12—C13	1.390 (3)
O1—H1	0.872 (17)	C12—C14	1.393 (3)
O1—H2	0.840 (16)	C13—C14 ⁱⁱ	1.382 (3)
N1—O3	1.218 (2)	C13—H13	0.9500
N1—O2	1.222 (2)	C14—C13 ⁱⁱ	1.382 (3)
N1—C1	1.483 (3)	C14—H14	0.9500
C1—H1A	0.9800	N21—C21	1.141 (3)
C1—H1B	0.9800	C21—C22	1.444 (3)
C1—H1C	0.9800	C22—C24	1.388 (3)
Fe2—C12	2.1811 (6)	C22—C23	1.395 (3)
Fe2—C13	2.1968 (6)	C23—C24 ⁱⁱⁱ	1.380 (3)
Fe2—C14	2.1996 (6)	C23—H23	0.9500
N2—O5	1.217 (3)	C24—C23 ⁱⁱⁱ	1.380 (3)
N2—O4	1.221 (3)	C24—H24	0.9500
O1—Fe1—O1 ⁱ	180.0	C14—Fe2—C11	109.08 (2)
O1—Fe1—N21 ⁱ	89.02 (6)	O5—N2—O4	124.7 (2)
O1 ⁱ —Fe1—N21 ⁱ	90.98 (6)	O5—N2—C2	118.9 (2)
O1—Fe1—N21	90.98 (6)	O4—N2—C2	116.4 (2)
O1 ⁱ —Fe1—N21	89.02 (6)	N2—C2—H2A	109.5
N21 ⁱ —Fe1—N21	180.00 (9)	N2—C2—H2B	109.5
O1—Fe1—N11	88.13 (6)	H2A—C2—H2B	109.5
O1 ⁱ —Fe1—N11	91.87 (6)	N2—C2—H2C	109.5
N21 ⁱ —Fe1—N11	89.53 (6)	H2A—C2—H2C	109.5
N21—Fe1—N11	90.47 (6)	H2B—C2—H2C	109.5
O1—Fe1—N11 ⁱ	91.87 (6)	C11—N11—Fe1	166.95 (17)
O1 ⁱ —Fe1—N11 ⁱ	88.13 (6)	N11—C11—C12	177.9 (2)
N21 ⁱ —Fe1—N11 ⁱ	90.47 (6)	C13—C12—C14	121.59 (19)
N21—Fe1—N11 ⁱ	89.53 (6)	C13—C12—C11	118.55 (19)
N11—Fe1—N11 ⁱ	180.0	C14—C12—C11	119.85 (19)
Fe1—O1—H1	118.0 (19)	C14 ⁱⁱ —C13—C12	119.4 (2)
Fe1—O1—H2	120.9 (19)	C14 ⁱⁱ —C13—H13	120.3
H1—O1—H2	111 (2)	C12—C13—H13	120.3
O3—N1—O2	123.50 (19)	C13 ⁱⁱ —C14—C12	119.0 (2)
O3—N1—C1	118.69 (19)	C13 ⁱⁱ —C14—H14	120.5
O2—N1—C1	117.81 (18)	C12—C14—H14	120.5

N1—C1—H1A	109.5	C21—N21—Fe1	173.63 (17)
N1—C1—H1B	109.5	N21—C21—C22	179.0 (2)
H1A—C1—H1B	109.5	C24—C22—C23	122.29 (19)
N1—C1—H1C	109.5	C24—C22—C21	119.98 (19)
H1A—C1—H1C	109.5	C23—C22—C21	117.71 (18)
H1B—C1—H1C	109.5	C24 ⁱⁱⁱ —C23—C22	118.85 (19)
C12—Fe2—C13	113.33 (3)	C24 ⁱⁱⁱ —C23—H23	120.6
C12—Fe2—C14	110.02 (2)	C22—C23—H23	120.6
C13—Fe2—C14	108.69 (2)	C23 ⁱⁱⁱ —C24—C22	118.86 (19)
C12—Fe2—C11	107.56 (2)	C23 ⁱⁱⁱ —C24—H24	120.6
C13—Fe2—C11	108.07 (2)	C22—C24—H24	120.6
O1—Fe1—N11—C11	-10.8 (7)	O1—Fe1—N21—C21	-13.1 (15)
O1 ⁱ —Fe1—N11—C11	169.2 (7)	O1 ⁱ —Fe1—N21—C21	166.9 (15)
N21 ⁱ —Fe1—N11—C11	78.2 (7)	N21 ⁱ —Fe1—N21—C21	141 (2)
N21—Fe1—N11—C11	-101.8 (7)	N11—Fe1—N21—C21	75.1 (15)
N11 ⁱ —Fe1—N11—C11	-43 (18)	N11 ⁱ —Fe1—N21—C21	-104.9 (15)
Fe1—N11—C11—C12	25 (7)	Fe1—N21—C21—C22	-35 (15)
N11—C11—C12—C13	2 (6)	N21—C21—C22—C24	-168 (13)
N11—C11—C12—C14	-177 (100)	N21—C21—C22—C23	14 (14)
C14—C12—C13—C14 ⁱⁱ	-0.6 (4)	C24—C22—C23—C24 ⁱⁱⁱ	0.6 (3)
C11—C12—C13—C14 ⁱⁱ	-179.35 (19)	C21—C22—C23—C24 ⁱⁱⁱ	178.61 (18)
C13—C12—C14—C13 ⁱⁱ	0.6 (4)	C23—C22—C24—C23 ⁱⁱⁱ	-0.6 (3)
C11—C12—C14—C13 ⁱⁱ	179.33 (19)	C21—C22—C24—C23 ⁱⁱⁱ	-178.57 (18)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $-x, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2	0.87 (2)	1.99 (2)	2.804 (2)	155 (3)
O1—H1 \cdots O4	0.87 (2)	2.57 (3)	3.074 (3)	118 (2)
O1—H2 \cdots C11	0.84 (2)	2.43 (2)	3.2731 (16)	177 (3)