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Crystal structure of *catena*-poly[[[tetraaquairon(II)]-*trans*-μ-1,2-bis(pyridin-4-yl)ethene-κ^2N:N'] bis(*p*-toluenesulfonate) methanol disolvate]

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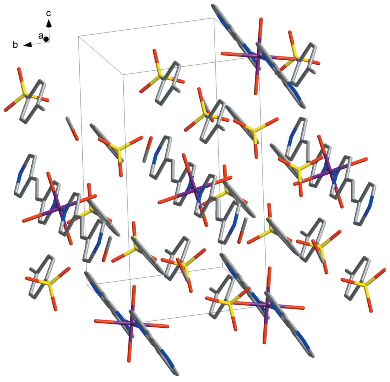
In the title polymeric complex, $\{[Fe(C_{12}H_{10}N_2)_2(H_2O)_4](CH_3C_6H_4SO_3)_2\cdot 2CH_3OH\}_n$, the Fe^{II} cation, located on an inversion centre, is coordinated by four water molecules in the equatorial positions and two 1,2-bis(pyridin-4-yl)ethene molecules in the axial positions. This results in a distorted octahedral geometry for the $[N_2O_4]$ coordination polyhedron. The 1,2-bis(pyridin-4-yl)ethene molecules bridge the Fe^{II} cations, forming polymeric chains running along the *a*-axis direction. Stabilization of the crystal structure is provided by O—H···O hydrogen bonds; these are formed by coordinated water molecules as donors towards the O atoms of the methanol molecules and tosylate anions as acceptors of protons, leading to the formation of a three-dimensional supramolecular network. Weak C—H···O hydrogen bonds are also observed in the crystal.

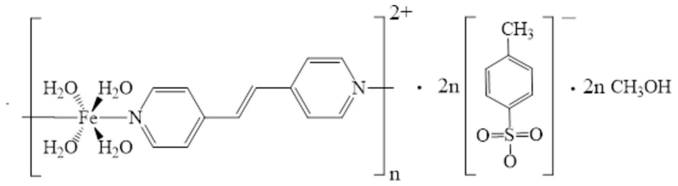


1. Chemical context

Transition metal complexes containing pyridine or substituted pyridines as ligands are of current interest due to their supramolecular arrangements and the probability of being spin-crossover compounds. Spin crossover (SCO), sometimes referred to as a spin transition or a spin equilibrium behaviour, is a phenomenon that occurs in some metal complexes wherein the spin state of a compound changes due to the influence of external stimuli such as temperature, pressure, light irradiation, magnetic field or guest effects (Gütlich & Goodwin, 2004). Bridging N-donor ligands are often used to produce Fe-based SCO complexes; for example, pyrazine is known to form interesting three-dimensional frameworks with remarkable transition characteristics (Muñoz & Real, 2011; Gural'skiy, Golub *et al.*, 2016; Gural'skiy, Shylin *et al.*, 2016).

A variation of the aromatic N-donor ligand can lead to possible spin-state modulation in transition metal complexes (Gütlich & Goodwin, 2004). In recent years, particular attention has been drawn to bridging ligands that able to form analogues of Hoffman clathrates with a large pore size. These ligands include bridge-polydentate derivatives of pyridine and other azine ligands (Muñoz & Real, 2011). Importantly, Fe-based SCO in analogues of Hoffman clathrates is known in complexes with 1,2-bis(pyridin-4-yl)ethene as a bridging N-donor ligand. Its complex with cyanoargentate as a co-ligand shows one of the largest thermal hysteresis (*ca* 95K wide) observed for spin-crossover complexes (Niel *et al.*, 2002).

Here we report on the title new polymeric compound based on 1,2-bis(pyridin-4-yl)ethene in which Fe^{II} ions are stabilized in the high-spin state.



2. Structural commentary

The Fe^{II} cation has a distorted octahedral coordination environment [FeN_2O_4], formed by two N atoms of 1,2-bis(pyridin-4-yl)ethene and by four O atoms of four water molecules (Fig. 1). Two 1,2-bis(pyridin-4-yl)ethene molecules are coordinated at the axial positions [with an Fe—N distance of 2.218 (2) Å]. The equatorial positions of the Fe^{II} cation are occupied by four O-coordinated water molecules with bond lengths Fe1—O1 = 2.114 (2) and Fe1—O2 = 2.077 (2) Å. The small difference in the lengths of the Fe—O bonds of 0.037 Å could be associated with a different participation of the water hydrogen atoms in hydrogen bonding. The metal-to-ligand distances clearly indicate the high-spin nature of the complex described herein.

The Fe^{II} octahedral distortion parameter (the sum of the moduli of the deviations from 90° for all *cis* bond angles) is $\Sigma|90 - \Theta| = 28.15$ (8), where Θ is the *cis*-N—Fe—O and *cis*-O—Fe—O angles in the coordination environment of the Fe^{II} atom. This value indicates a significant polyhedral distortion, which can be explained by the Jahn–Teller effect and the presence of different types of ligands.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O3^{i}	0.83 (2)	1.93 (2)	2.753 (3)	172 (3)
O1—H1B···O3^{ii}	0.84 (2)	1.90 (2)	2.726 (2)	168 (3)
O2—H2A···O6	0.84 (2)	1.82 (2)	2.654 (3)	172 (3)
O2—H2B···O5	0.84 (2)	1.92 (2)	2.752 (3)	170 (3)
O6—H6A···O4^{ii}	0.91 (2)	1.95 (2)	2.823 (3)	161 (3)
C4—H4···O5^{iii}	0.95	2.51	3.406 (3)	157
C13—H13B···O4^{iv}	0.98	2.59	3.562 (4)	172
C13—H13C···O5^{v}	0.98	2.51	3.465 (4)	165

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

3. Supramolecular features

The coordination structure is formed by binding 1,2-bis(pyridin-4-yl)ethene fragments with Fe^{II} cations into polymer chains that propagate along the *a*-axis direction. Stabilization in the crystal structure is ensured by O—H···O hydrogen bonds (Fig. 2, Table 1): (i) H atoms of water molecules and the oxygen atoms of tosylate anions; (ii) H atoms of water molecules and methanol molecules; (iii) H atoms of the hydroxyl group of methanol with the tosylate anion. The compound contains two solvate molecules of methanol per Fe^{II} cation. In the crystal lattice, each tosylate anion is connected with three water molecules of the complex cation, leading to the formation of a three-dimensional supramolecular network

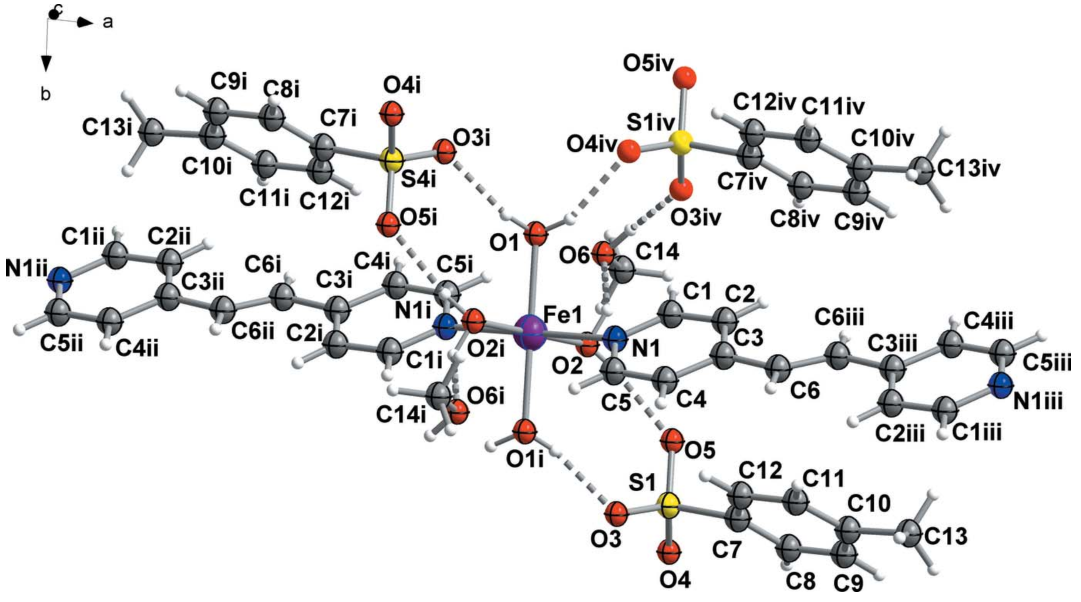


Figure 1
A fragment of the molecular structure of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $-1+x, y, z$; (iii) $1-x, 1-y, 1-z$; (iv) $x, -1+y, z$.]

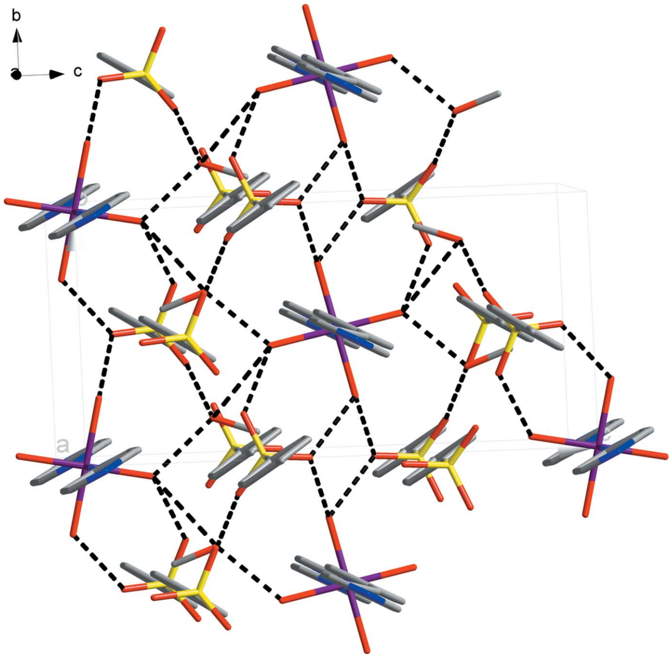


Figure 2
Crystal structure of the title compound, showing hydrogen bonds as dashed lines. Colour key: violet Fe, yellow S, blue N, grey C and red O.

(Fig. 2). In addition, weak C—H⋯O hydrogen bonds are also observed in the crystal. A view of the packing is shown in Fig. 3.

4. Database survey

A survey of the Cambridge Structural Database confirmed that the structure of the title complex has not been reported previously. 41 structures are known with an Fe cation coordinated by four water O atoms and two N atoms from the pyridine fragment. The survey yielded the structure of one related compound, in which the Fe^{II} cation has a distorted octahedral coordination environment [FeN_2O_4], formed by two N atoms of 1,2-bis(pyridin-4-yl)ethene and by four O atoms of four water molecules; however, it contains 2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-olate as the anion and crystallizes in the orthorhombic *Pbcn* space group. In this analogue, Fe1—N1 = 2.2304 (2), Fe1—O2 = 2.1030 (2) and Fe1—O4 = 2.0908 (2) Å (Garcia *et al.*, 2011), contrary to what is observed in the title compound.

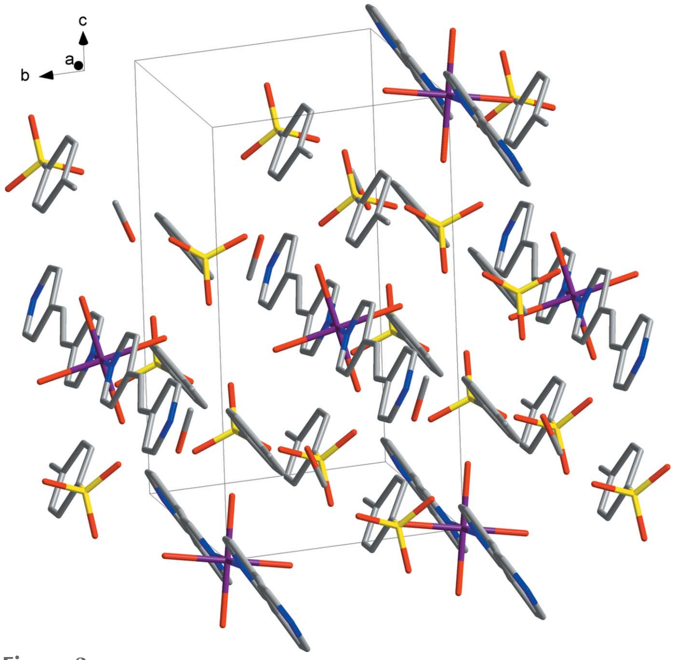


Figure 3
The crystal packing. Colour key: violet Fe, yellow S, blue N, grey C and red O.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_{12}H_{10}N_2)(H_2O)_4](C_7H_7O_3S)_2 \cdot 2CH_4O$
M_r	716.59
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	200
a, b, c (Å)	13.8416 (9), 7.7686 (4), 16.4076 (13)
β (°)	111.845 (9)
V (Å^3)	1637.6 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.65
Crystal size (mm)	0.35 × 0.2 × 0.15
Data collection	
Diffractometer	Rigaku OD Xcalibur, Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.920, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6379, 2857, 2363
R_{int}	0.030
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.097, 1.06
No. of reflections	2857
No. of parameters	227
No. of restraints	7
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.33

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2017* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

5. Synthesis and crystallization

Crystals of the title compound were prepared by the slow diffusion method between three layers in a 10 ml tube. The first layer was a solution of [$Fe(OTs)_2$]·$6H_2O$ (OTs = *p*-toluenesulfonate) (0.1012 g, 0.02 mmol) in water (2.5 ml), the second was a mixture of water/methanol (1:1, 5 ml) and the third layer was a solution of 1,2-bis(pyridin-4-yl)ethene (0.0352 g, 0.02 mmol) in methanol (2.5 ml). After two weeks, red crystals grew in the second layer; these were collected and maintained under the mother solution until measured.

Acta Cryst. (2017). E**73**, 1977–1980 Hiiuk *et al.* • $[Fe(C_{12}H_{10}N_2)(H_2O)_4](C_7H_7O_3S)_2 \cdot 2CH_4O$ **1979**

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All aromatic hydrogens and hydrogen atoms of the CH groups were placed in their expected calculated positions (C—H = 0.95 Å) and refined as riding with $U_{\rm iso}$(H) = 1.2$U_{\rm iso}$(C). Methyl H atoms were placed in their expected calculated positions (C—H = 0.98 Å) and refined as rotating groups with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C). Hydrogen atoms of the water molecules were assigned based on the difference-Fourier map, and the O—H distances and the H—O—H angles were constrained using DFIX (O—H = 0.84 Å) and DANG (H—H = 1.34 Å) instructions. The hydrogen H atom of the solvent methanol molecule was assigned based on the difference-Fourier map, and the O—H distance was constrained using a DFIX (O—H = 0.96 Å) instruction.

Funding information

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Crystal structure of *catena*-poly[[[tetraaquairon(II)]-*trans*-μ-1,2-bis(pyridin-4-yl)ethene-κ^2N:N'] bis(*p*-toluenesulfonate) methanol disolvate]

Volodymyr M. Hiiuk, Diana D. Barakhty, Sergiu Shova, Ruslan A. Polunin and Il'ya A. Gural'skiy

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

catena-Poly[[[tetraaquairon(II)]-*trans*-μ-1,2-bis(pyridin-4-yl)ethene-κ^2N:N'] bis(*p*-toluenesulfonate) methanol disolvate]

Crystal data

$[Fe(C_{12}H_{10}N_2)(H_2O)_4](C_7H_7O_3S)_2\cdot 2CH_4O$
$M_r = 716.59$
Monoclinic, $P2_1/c$
$a = 13.8416$ (9) Å
$b = 7.7686$ (4) Å
$c = 16.4076$ (13) Å
$\beta = 111.845$ (9)°
$V = 1637.6$ (2) Å^3
$Z = 2$
$F(000) = 752$
$D_x = 1.453$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2979 reflections
$\theta = 2.6$–31.1°
$\mu = 0.65$ mm^{-1}
$T = 200$ K
Prism, clear intense red
0.35 × 0.2 × 0.15 mm

Data collection

Rigaku OD Xcalibur, Eos diffractometer
Detector resolution: 8.0797 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
$T_{min} = 0.920$, $T_{max} = 1.000$
6379 measured reflections
2857 independent reflections
2363 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
$h = -16 \rightarrow 16$
$k = -8 \rightarrow 9$
$l = -19 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.097$
$S = 1.06$
2857 reflections
227 parameters
7 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.6283P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.24$ e Å^{-3} $\Delta\rho_{min} = -0.32$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.000000	0.500000	0.500000	0.01832 (16)
O2	0.07337 (15)	0.5517 (3)	0.63317 (12)	0.0295 (5)
O1	−0.00268 (15)	0.2362 (2)	0.53062 (14)	0.0279 (4)
O6	0.06975 (17)	0.3317 (3)	0.75578 (14)	0.0403 (5)
N1	0.15498 (16)	0.4896 (2)	0.48932 (14)	0.0218 (5)
C1	0.23952 (19)	0.4220 (3)	0.55153 (18)	0.0243 (6)
H1	0.231285	0.368884	0.600701	0.029*
C3	0.3528 (2)	0.5005 (3)	0.47719 (17)	0.0235 (6)
C2	0.3375 (2)	0.4249 (3)	0.54841 (18)	0.0269 (6)
H2	0.394535	0.375488	0.594749	0.032*
C4	0.2643 (2)	0.5672 (3)	0.41120 (17)	0.0256 (6)
H4	0.269716	0.617840	0.360394	0.031*
C6	0.4539 (2)	0.5179 (3)	0.46934 (18)	0.0251 (6)
H6	0.453831	0.558952	0.414775	0.030*
C5	0.1695 (2)	0.5594 (3)	0.41982 (17)	0.0246 (6)
H5	0.110758	0.606167	0.374029	0.029*
C14	0.0849 (3)	0.3932 (4)	0.8412 (2)	0.0470 (8)
H14A	0.159070	0.415178	0.873617	0.071*
H14B	0.060297	0.306700	0.872498	0.071*
H14C	0.045634	0.500216	0.836491	0.071*
S1	0.22227 (5)	0.97890 (8)	0.66335 (4)	0.02490 (18)
O3	0.14978 (14)	0.9925 (2)	0.57179 (12)	0.0310 (5)
O5	0.21658 (15)	0.8109 (2)	0.70032 (13)	0.0336 (5)
O4	0.21348 (15)	1.1211 (2)	0.71723 (13)	0.0362 (5)
C7	0.3476 (2)	0.9925 (3)	0.65937 (17)	0.0225 (6)
C8	0.4272 (2)	1.0780 (3)	0.72377 (17)	0.0283 (6)
H8	0.413993	1.136967	0.769296	0.034*
C11	0.4661 (2)	0.9110 (3)	0.59080 (19)	0.0312 (7)
H11	0.478876	0.854123	0.544533	0.037*
C9	0.5267 (2)	1.0775 (3)	0.72171 (18)	0.0309 (7)
H9	0.581277	1.136606	0.766118	0.037*
C12	0.3668 (2)	0.9108 (3)	0.59167 (18)	0.0298 (6)
H12	0.311753	0.855117	0.546108	0.036*
C10	0.5476 (2)	0.9924 (3)	0.65615 (19)	0.0292 (6)
C13	0.6567 (2)	0.9835 (4)	0.6563 (2)	0.0413 (8)
H13A	0.653625	0.983917	0.595625	0.062*
H13B	0.690467	0.877556	0.685580	0.062*
H13C	0.696653	1.083302	0.687642	0.062*

H2A	0.078 (3)	0.485 (3)	0.6748 (17)	0.061 (12)*
H2B	0.113 (2)	0.633 (3)	0.6576 (18)	0.042 (9)*
H1A	−0.0508 (17)	0.176 (3)	0.4972 (17)	0.043 (10)*
H1B	0.0490 (17)	0.171 (3)	0.5494 (19)	0.043 (9)*
H6A	0.120 (2)	0.256 (4)	0.756 (2)	0.061 (11)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0129 (3)	0.0212 (3)	0.0211 (3)	−0.0002 (2)	0.0065 (2)	0.0006 (2)
O2	0.0277 (11)	0.0355 (11)	0.0217 (11)	−0.0106 (9)	0.0052 (9)	−0.0011 (9)
O1	0.0181 (10)	0.0212 (10)	0.0383 (12)	0.0007 (8)	0.0035 (9)	0.0010 (9)
O6	0.0434 (13)	0.0432 (12)	0.0396 (13)	0.0106 (10)	0.0215 (11)	0.0085 (10)
N1	0.0183 (11)	0.0229 (11)	0.0252 (12)	−0.0008 (9)	0.0092 (10)	0.0004 (9)
C1	0.0196 (14)	0.0281 (14)	0.0271 (14)	0.0022 (11)	0.0108 (12)	0.0068 (11)
C3	0.0218 (14)	0.0230 (13)	0.0281 (15)	−0.0009 (11)	0.0119 (12)	−0.0046 (11)
C2	0.0170 (13)	0.0324 (14)	0.0296 (16)	0.0036 (11)	0.0068 (12)	0.0071 (12)
C4	0.0247 (14)	0.0309 (14)	0.0246 (14)	−0.0020 (11)	0.0130 (12)	−0.0002 (11)
C6	0.0231 (13)	0.0281 (14)	0.0296 (15)	−0.0007 (11)	0.0161 (12)	−0.0003 (12)
C5	0.0176 (13)	0.0307 (14)	0.0248 (15)	0.0017 (11)	0.0071 (12)	0.0025 (12)
C14	0.051 (2)	0.052 (2)	0.047 (2)	−0.0027 (17)	0.0281 (18)	0.0034 (16)
S1	0.0210 (4)	0.0225 (3)	0.0289 (4)	0.0001 (3)	0.0066 (3)	−0.0020 (3)
O3	0.0209 (10)	0.0340 (10)	0.0309 (11)	0.0040 (8)	0.0014 (9)	0.0018 (9)
O5	0.0293 (11)	0.0295 (10)	0.0376 (12)	−0.0057 (9)	0.0074 (9)	0.0040 (9)
O4	0.0340 (11)	0.0359 (11)	0.0415 (12)	0.0006 (9)	0.0173 (10)	−0.0112 (9)
C7	0.0233 (14)	0.0162 (12)	0.0241 (14)	0.0016 (10)	0.0043 (11)	0.0009 (10)
C8	0.0286 (15)	0.0254 (14)	0.0272 (15)	−0.0014 (11)	0.0062 (13)	−0.0059 (12)
C11	0.0314 (16)	0.0286 (14)	0.0364 (17)	0.0003 (12)	0.0158 (14)	−0.0047 (12)
C9	0.0227 (15)	0.0274 (14)	0.0328 (16)	−0.0051 (11)	−0.0011 (13)	−0.0023 (12)
C12	0.0238 (15)	0.0287 (14)	0.0320 (16)	−0.0025 (12)	0.0048 (13)	−0.0089 (12)
C10	0.0263 (15)	0.0227 (13)	0.0351 (16)	0.0013 (11)	0.0073 (13)	0.0046 (12)
C13	0.0247 (16)	0.0435 (18)	0.053 (2)	−0.0018 (13)	0.0116 (15)	0.0061 (15)

Geometric parameters (Å, º)

Fe1—O1	2.1135 (18)	C6—H6	0.9500
Fe1—O1^{i}	2.1135 (18)	C5—H5	0.9500
Fe1—O2	2.0773 (19)	C14—H14A	0.9800
Fe1—O2^{i}	2.0773 (19)	C14—H14B	0.9800
Fe1—N1^{i}	2.218 (2)	C14—H14C	0.9800
Fe1—N1	2.218 (2)	S1—O3	1.4673 (19)
O2—H2A	0.839 (17)	S1—O5	1.4535 (19)
O2—H2B	0.839 (17)	S1—O4	1.4482 (19)
O1—H1A	0.832 (17)	S1—C7	1.764 (3)
O1—H1B	0.837 (17)	C7—C8	1.380 (4)
O6—C14	1.421 (4)	C7—C12	1.387 (4)
O6—H6A	0.910 (18)	C8—H8	0.9500
N1—C1	1.341 (3)	C8—C9	1.391 (4)

N1—C5	1.344 (3)	C11—H11	0.9500
C1—H1	0.9500	C11—C12	1.380 (4)
C1—C2	1.376 (3)	C11—C10	1.386 (4)
C3—C2	1.393 (4)	C9—H9	0.9500
C3—C4	1.398 (4)	C9—C10	1.382 (4)
C3—C6	1.459 (4)	C12—H12	0.9500
C2—H2	0.9500	C10—C13	1.511 (4)
C4—H4	0.9500	C13—H13A	0.9800
C4—C5	1.372 (3)	C13—H13B	0.9800
C6—C6^{ii}	1.327 (5)	C13—H13C	0.9800

O2—Fe1—O2^{i}	180.00 (11)	N1—C5—C4	123.8 (2)
O2^{i}—Fe1—O1^{i}	88.98 (8)	N1—C5—H5	118.1
O2^{i}—Fe1—O1	91.02 (8)	C4—C5—H5	118.1
O2—Fe1—O1^{i}	91.01 (8)	O6—C14—H14A	109.5
O2—Fe1—O1	88.98 (8)	O6—C14—H14B	109.5
O2^{i}—Fe1—N1	91.06 (8)	O6—C14—H14C	109.5
O2^{i}—Fe1—N1^{i}	88.94 (8)	H14A—C14—H14B	109.5
O2—Fe1—N1^{i}	91.06 (8)	H14A—C14—H14C	109.5
O2—Fe1—N1	88.94 (8)	H14B—C14—H14C	109.5
O1^{i}—Fe1—O1	180.0	O3—S1—C7	105.38 (12)
O1—Fe1—N1	94.96 (7)	O5—S1—O3	111.68 (11)
O1—Fe1—N1^{i}	85.04 (7)	O5—S1—C7	106.02 (11)
O1^{i}—Fe1—N1^{i}	94.96 (7)	O4—S1—O3	112.92 (11)
O1^{i}—Fe1—N1	85.04 (7)	O4—S1—O5	113.58 (12)
N1—Fe1—N1^{i}	180.0	O4—S1—C7	106.52 (12)
Fe1—O2—H2A	127 (2)	C8—C7—S1	121.1 (2)
Fe1—O2—H2B	129 (2)	C8—C7—C12	119.8 (3)
H2A—O2—H2B	104 (3)	C12—C7—S1	119.1 (2)
Fe1—O1—H1A	118 (2)	C7—C8—H8	120.2
Fe1—O1—H1B	126 (2)	C7—C8—C9	119.7 (3)
H1A—O1—H1B	105 (3)	C9—C8—H8	120.2
C14—O6—H6A	113 (2)	C12—C11—H11	119.4
C1—N1—Fe1	123.36 (17)	C12—C11—C10	121.3 (3)
C1—N1—C5	116.1 (2)	C10—C11—H11	119.4
C5—N1—Fe1	120.44 (17)	C8—C9—H9	119.5
N1—C1—H1	118.0	C10—C9—C8	121.1 (3)
N1—C1—C2	123.9 (2)	C10—C9—H9	119.5
C2—C1—H1	118.0	C7—C12—H12	120.1
C2—C3—C4	116.3 (2)	C11—C12—C7	119.7 (3)
C2—C3—C6	124.3 (2)	C11—C12—H12	120.1
C4—C3—C6	119.4 (2)	C11—C10—C13	120.3 (3)
C1—C2—C3	119.9 (2)	C9—C10—C11	118.3 (3)
C1—C2—H2	120.1	C9—C10—C13	121.3 (3)
C3—C2—H2	120.1	C10—C13—H13A	109.5
C3—C4—H4	120.0	C10—C13—H13B	109.5
C5—C4—C3	120.0 (2)	C10—C13—H13C	109.5
C5—C4—H4	120.0	H13A—C13—H13B	109.5

C3—C6—H6	116.7	H13A—C13—H13C	109.5
C6^{ii}—C6—C3	126.6 (3)	H13B—C13—H13C	109.5
C6^{ii}—C6—H6	116.7		

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O3^{i}	0.83 (2)	1.93 (2)	2.753 (3)	172 (3)
O1—H1*B*···O3^{iii}	0.84 (2)	1.90 (2)	2.726 (2)	168 (3)
O2—H2*A*···O6	0.84 (2)	1.82 (2)	2.654 (3)	172 (3)
O2—H2*B*···O5	0.84 (2)	1.92 (2)	2.752 (3)	170 (3)
O6—H6*A*···O4^{iii}	0.91 (2)	1.95 (2)	2.823 (3)	161 (3)
C4—H4···O5^{iv}	0.95	2.51	3.406 (3)	157
C13—H13*B*···O4^{v}	0.98	2.59	3.562 (4)	172
C13—H13*C*···O5^{vi}	0.98	2.51	3.465 (4)	165

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) *x*, −*y*+3/2, *z*−1/2; (v) −*x*+1, *y*−1/2, −*z*+3/2; (vi) −*x*+1, *y*+1/2, −*z*+3/2.