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Crystal structure of tetraaqua[2-(pyridin-2-yl)-1*H*-imidazole-κ^2N^2,N^3]iron(II) sulfate

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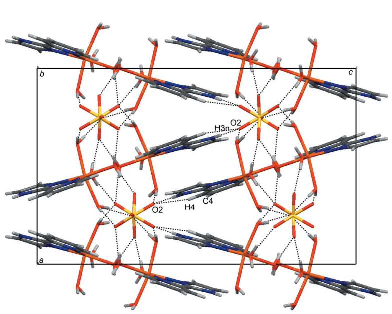
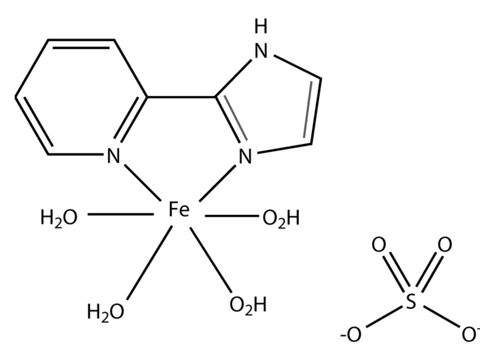
In the title compound, $[Fe(C_8H_7N_3)(H_2O)_4]SO_4$, the central Fe^{II} ion is octahedrally coordinated by two N atoms from the bidentate 2-(pyridin-2-yl)-1*H*-imidazole ligand and by four O atoms of the aqua ligands. The largest deviation from the ideal octahedral geometry is reflected by the small N—Fe—N bite angle of 76.0 (1)°. The Fe—N coordination bonds have markedly different lengths [2.1361 (17) and 2.243 (2) Å], with the shorter one to the pyrimidine N atom. The four Fe—O coordination bond lengths vary from 2.1191 (18) to 2.1340 (17) Å. In the crystal, the cations and anions are arranged by means of medium-strength O—H⋯O hydrogen bonds into layers parallel to the *ab* plane. Neighbouring layers further interconnect by N—H⋯O hydrogen bonds involving the imidazole fragment as donor group to one sulfate O atom as an acceptor. The resulting three-dimensional network is consolidated by C—H⋯O, C—H⋯π and π–π interactions.



1. Chemical context

Polynitrile anions have recently received considerable attention in the fields of coordination chemistry and molecular materials (Benmansour *et al.*, 2010). These organic anions are of interest due to their ability to act towards metal atoms with various coordination modes and for their high degree of electronic delocalization (Miyazaki *et al.*, 2003; Atmani *et al.*, 2008; Benmansour *et al.*, 2008, 2012; Setifi *et al.*, 2002, 2013, 2014; Addala *et al.*, 2015).



We are interested in using these anionic ligands in combination with other neutral bridging co-ligands to explore their structural features and properties relevant to the field of molecular materials exhibiting the spin crossover (SCO) phenomenon (Dupouy *et al.*, 2008, 2009). In an attempt to prepare such an iron(II) complex using hydrothermal synth-

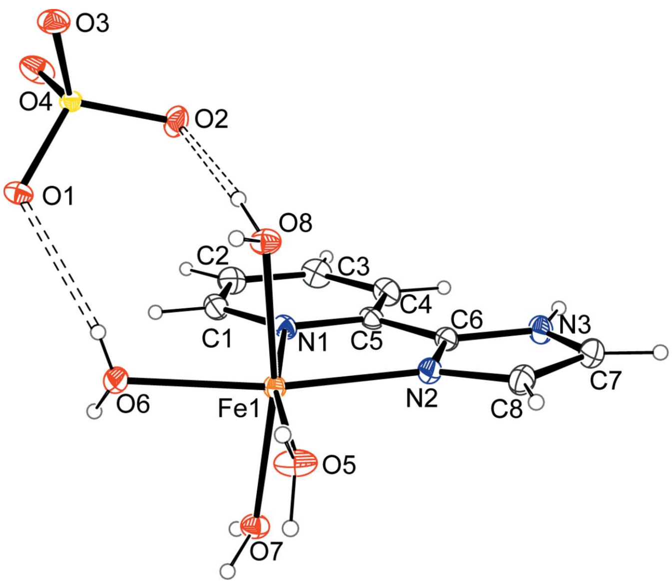


Figure 1
The molecular structure of (I), with atom labels and displacement ellipsoids at the 50% probability level. Hydrogen bonds are shown as double dashed lines.

esis, we obtained instead the title compound [Fe(pyim)(H_2O)$_4$]SO_4, (I), where pyim is 2-(pyridin-2-yl)-1*H*-imidazole.

2. Structural commentary

Fig. 1 shows the asymmetric unit of (I). The main building units in the crystal structure of (I) are octahedral [Fe(pyim)(H_2O)$_4$]$^{2+}$ complex cations and [SO_4]$^{2-}$ anions. The distorted octahedral environment of the central Fe^{II} ion is defined by two N donor atoms of the pyim ligand and by the O atoms of two water molecules in the equatorial plane, while the two remaining water molecules coordinate at the axial sites. The bite angle N1—Fe—N2 of 76.04 (7)° shows the most significant deviation from the ideal octahedral geometry, with the other coordination angles deviating by 0.21 (7) to 11.91 (7)°.

The Fe—N coordination bonds with the chelate ligand have markedly different lengths, Fe—N1 = 2.243 (2) and Fe—N2 = 2.1361 (17) Å, which are also dissimilar to those in the previously reported [Fe(dmbpy)(H_2O)$_4$]SO_4 complex where dmbpy is 5,5′-dimethyl-2,2′-bipyridine (Belamri *et al.*, 2014.) comprising a nearly symmetrical dipyridyl ligand [Fe—N = 2.176 (3) Å on average]. The torsion angles within the approximately planar five-membered chelate ring of (I) vary from 0.6 (3) to −5.2 (2)° and reflect a more pronounced deviation from planarity in comparison with the dmbpy Fe^{II} complex that exhibits a maximal torsion angle of 2.0 (3)°. The dihedral angle of 5.5 (1) ° between the aromatic rings of the pyim ligand is within the range of the values reported for the eight independent molecules in the crystal structure of the non-coordinating ligand [1(1) to 17 (1)°; Tinant *et al.*, 2010]. In the present complex, all four Fe—O bond lengths, ranging from 2.1191 (18) to 2.1340 (17) Å, are longer than the corresponding ones in the [Fe(dmbpy)(H_2O)$_4$]SO_4 complex, which range from 2.079 (2) to 2.110 (2) Å.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1*O*5···O3^{i}	0.78 (3)	2.00 (3)	2.785 (3)	175 (3)
O5—H2*O*5···O1^{ii}	0.85 (4)	2.00 (3)	2.845 (3)	172 (4)
O6—H1*O*6···O1	0.71 (3)	2.15 (3)	2.857 (3)	170 (3)
O6—H2*O*6···O3^{iii}	0.89 (3)	1.85 (3)	2.736 (3)	175 (3)
O7—H1*O*7···O1^{iii}	0.64 (4)	2.17 (3)	2.809 (3)	173 (4)
O7—H2*O*7···O4^{ii}	0.90 (4)	1.83 (3)	2.720 (3)	168 (4)
O8—H1*O*8···O4^{i}	0.76 (3)	1.96 (3)	2.722 (3)	178 (4)
O8—H2*O*8···O2	0.84 (3)	1.90 (3)	2.737 (3)	175 (3)
N3—H3*N*···O2^{iv}	0.93 (3)	1.93 (3)	2.858 (3)	178 (3)
C4—H4···O2^{iv}	0.93	2.40	3.287 (3)	160

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

3. Supramolecular features

The crystal packing of (I) is stabilized by a complex hydrogen-bonding network involving the coordinating water molecules and the imidazole fragment as donors to the O acceptors atoms of the sulfate anion. Each cationic [Fe(pyim)(H_2O)$_4$]$^{2+}$ unit is surrounded by five [SO_4]$^{2-}$ anions. Similarly to the crystal structure of [Fe(dmbpy)(H_2O)$_4$]SO_4, pairs of axially and equatorially coordinating water molecules bind to pairs of O acceptor atoms from the same [SO_4]$^{2-}$ group, forming eight medium-strength interactions (Table 1). These hydrogen bonds arrange the complex molecules into layers parallel to

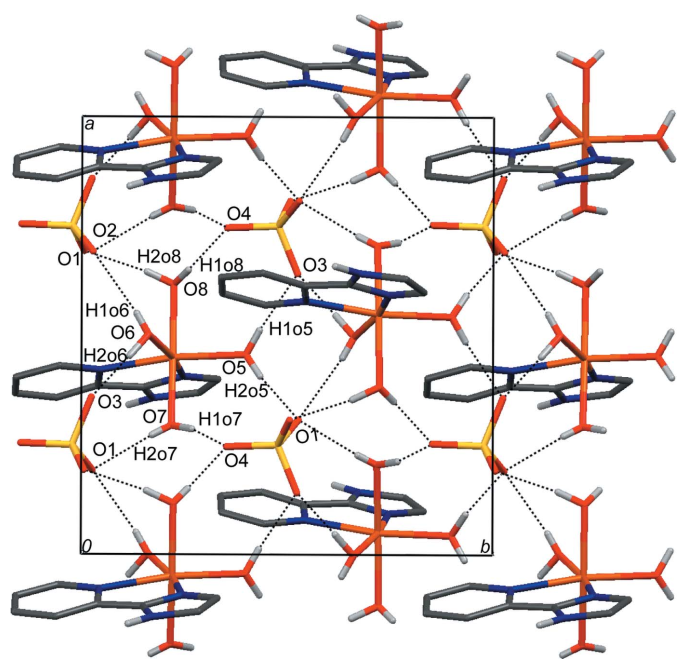


Figure 2
O—H···O interactions (dashed lines) connect cationic and anionic units into layers parallel to the *ab* plane (view of a single layer down the *c* axis). H atoms not involved in hydrogen bonding have been omitted for the sake of clarity.

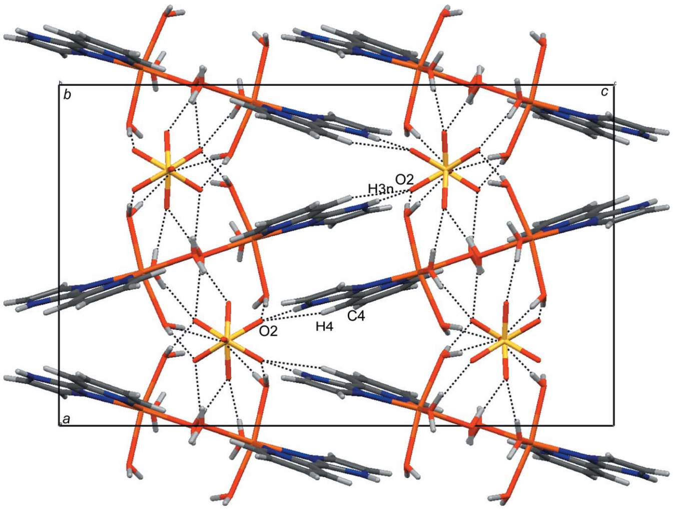


Figure 3
The three-dimensional packing of (I) viewed down the *b* axis.

the *ab* plane (Fig. 2). Additional N—H···O and C—H···O hydrogen bonds involving the donors from the aromatic ligand interconnect adjacent layers into a three-dimensional arrangement (Fig. 3). The vicinity of aromatic rings in the inter-layer region gives rise to C—H···π [H3···$Cg1^{i}$ = 3.033 Å; C3—H3···$Cg1^{i}$ = 117°; symmetry code: (i) = $-x + \frac{1}{2}$, $y + \frac{1}{2}$, z; *Cg*1 is the centroid of the imidazole ring] and weak π–π interactions [$Cg1\cdots Cg2^{ii}$ = 3.821 Å, the shortest interatomic distance N3···$C2^{ii}$ = 3.325 (1) Å; symmetry code: (ii) = $-x + 1$, $-y + 1$, $-z + 1$; *Cg*1 and *Cg*2 are the centroids of the imidazole and pyridine rings, respectively]. C—H···O interactions are also observed (Table 1).

4. Synthesis and crystallization

The title compound was obtained under hydrothermal conditions from a mixture of iron(II) sulfate heptahydrate (28 mg, 0.1 mmol), 2-(pyridin-2-yl)-1*H*-imidazole (15 mg, 0.1 mmol) and potassium tricyanomethanide $KC(CN)_3$ (26 mg, 0.2 mmol) in water-ethanol (4:1 *v/v*, 20 ml). The mixture was transferred to a Teflon-lined autoclave and heated at 423 K for 48 h. The autoclave was then allowed to cool to ambient temperature. Block-like yellow crystals of (I) were collected by filtration, washed with water and dried in air (yield 58%).

5. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to C atoms were placed at geometrically calculated positions and refined using a riding model. C—H distances were fixed to 0.93 Å for aromatic C atoms, with $U_{iso}(H)$ = $1.2U_{eq}(C)$. The H atoms attached to O and N atoms were located in a difference Fourier map and were refined isotropically.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_8H_7N_3)(H_2O)_4]SO_4$
M_r	369.14
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	293
a, *b*, *c* (Å)	12.476 (5), 11.741 (5), 20.313 (7)
V ($Å^3$)	2975.5 (19)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	1.19
Crystal size (mm)	0.34 × 0.20 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.802, 0.871
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20168, 4417, 3008
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.091, 1.08
No. of reflections	4417
No. of parameters	226
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.47, −0.41

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX*(Farrugia, 2012), *Mercury* (Macrae, 2006) and *PARST* (Nardelli, 1995).

Acknowledgements

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supporting information

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Crystal structure of tetraaqua[2-(pyridin-2-yl)-1*H*-imidazole-κ^2N^2,N^3]iron(II) sulfate

Zouaoui Setifi, Fatima Setifi, Bojana M. Francuski, Sladjana B. Novaković and Hocine Merazig

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PARST* (Nardelli, 1995).

Tetraaqua[2-(pyridin-2-yl)-1*H*-imidazole-κ^2N^2,N^3]iron(II) sulfate

Crystal data

$[Fe(C_8H_7N_3)(H_2O)_4]SO_4$
M_r = 369.14
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 12.476 (5) Å
b = 11.741 (5) Å
c = 20.313 (7) Å
V = 2975.5 (19) Å^3
Z = 8
$F(000)$ = 1520
D_x = 1.648 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9606 reflections
θ = 2.5–30.0°
μ = 1.19 mm^{-1}
T = 293 K
Block, yellow
0.34 × 0.20 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ & ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.802, T_{max} = 0.871
20168 measured reflections
4417 independent reflections
3008 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 30.5°, θ_{min} = 2.6°
$h = -17 \rightarrow 17$
$k = -14 \rightarrow 16$
$l = -28 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.091
S = 1.08
4417 reflections
226 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.45016 (2)	0.72203 (3)	0.35060 (2)	0.02305 (9)
S1	0.74974 (4)	0.47721 (5)	0.30259 (2)	0.02198 (11)
O1	0.69197 (10)	0.52744 (13)	0.24568 (6)	0.0295 (3)
O2	0.69268 (12)	0.50603 (15)	0.36361 (7)	0.0378 (4)
O3	0.85850 (11)	0.52416 (15)	0.30581 (7)	0.0368 (4)
O4	0.75368 (13)	0.35340 (15)	0.29605 (7)	0.0441 (4)
O5	0.45617 (15)	0.89924 (16)	0.33077 (10)	0.0416 (4)
O6	0.50247 (15)	0.66267 (16)	0.25674 (7)	0.0336 (4)
O7	0.29469 (14)	0.71843 (19)	0.30864 (8)	0.0322 (4)
O8	0.61694 (12)	0.72412 (17)	0.37388 (8)	0.0314 (4)
N1	0.42117 (13)	0.54515 (16)	0.38829 (7)	0.0274 (4)
N2	0.40687 (14)	0.74690 (16)	0.45132 (8)	0.0294 (4)
N3	0.35709 (14)	0.6734 (2)	0.54639 (8)	0.0353 (5)
C1	0.42985 (17)	0.4458 (2)	0.35520 (10)	0.0357 (5)
H1	0.4548	0.4477	0.3121	0.043*
C2	0.40365 (18)	0.3420 (2)	0.38200 (11)	0.0405 (6)
H2	0.4107	0.2753	0.3577	0.049*
C3	0.36666 (19)	0.3396 (2)	0.44581 (12)	0.0438 (6)
H3	0.3484	0.2707	0.4654	0.053*
C4	0.35690 (17)	0.4400 (2)	0.48053 (11)	0.0387 (6)
H4	0.3314	0.4397	0.5235	0.046*
C5	0.38537 (15)	0.5406 (2)	0.45065 (9)	0.0279 (5)
C6	0.38177 (14)	0.6510 (2)	0.48286 (9)	0.0283 (5)
C7	0.36954 (17)	0.7871 (2)	0.55631 (11)	0.0398 (6)
H7	0.3593	0.8266	0.5955	0.048*
C8	0.40013 (17)	0.8319 (2)	0.49715 (10)	0.0362 (5)
H8	0.4142	0.9085	0.4893	0.043*
H1O5	0.510 (2)	0.932 (2)	0.3248 (13)	0.049 (8)*
H2O5	0.408 (3)	0.933 (3)	0.3090 (15)	0.084 (12)*
H1O6	0.5519 (19)	0.632 (2)	0.2580 (12)	0.036 (8)*
H2O6	0.453 (2)	0.617 (3)	0.2387 (13)	0.062 (9)*
H1O7	0.273 (2)	0.672 (3)	0.2986 (13)	0.045 (11)*
H2O7	0.286 (2)	0.770 (3)	0.2761 (16)	0.066 (10)*
H1O8	0.652 (2)	0.760 (2)	0.3515 (11)	0.038 (8)*
H2O8	0.644 (2)	0.658 (3)	0.3708 (13)	0.050 (9)*
H3N	0.3399 (19)	0.615 (2)	0.5753 (13)	0.054 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.02282 (15)	0.02469 (18)	0.02163 (14)	−0.00077 (12)	0.00178 (10)	0.00238 (11)
S1	0.0206 (2)	0.0222 (3)	0.0231 (2)	0.00159 (19)	−0.00054 (17)	0.00183 (18)
O1	0.0279 (7)	0.0296 (9)	0.0309 (7)	0.0009 (6)	−0.0064 (5)	0.0067 (6)
O2	0.0427 (9)	0.0408 (11)	0.0300 (7)	0.0072 (8)	0.0144 (6)	0.0084 (7)
O3	0.0214 (7)	0.0493 (12)	0.0397 (8)	−0.0045 (7)	−0.0021 (6)	0.0095 (7)
O4	0.0598 (10)	0.0226 (10)	0.0500 (9)	0.0088 (8)	−0.0224 (8)	−0.0042 (7)
O5	0.0300 (9)	0.0299 (11)	0.0649 (11)	−0.0052 (8)	−0.0073 (8)	0.0177 (8)
O6	0.0263 (8)	0.0449 (12)	0.0296 (8)	0.0023 (9)	0.0008 (6)	−0.0053 (7)
O7	0.0292 (8)	0.0304 (11)	0.0370 (9)	−0.0006 (8)	−0.0061 (6)	−0.0014 (8)
O8	0.0250 (8)	0.0322 (11)	0.0372 (8)	−0.0020 (8)	−0.0001 (6)	0.0057 (8)
N1	0.0290 (9)	0.0306 (11)	0.0226 (8)	−0.0024 (8)	−0.0005 (6)	0.0035 (7)
N2	0.0272 (9)	0.0343 (12)	0.0267 (9)	0.0011 (8)	0.0019 (7)	−0.0027 (7)
N3	0.0344 (10)	0.0474 (14)	0.0241 (9)	−0.0006 (9)	0.0072 (7)	0.0031 (8)
C1	0.0399 (12)	0.0366 (15)	0.0305 (11)	0.0023 (11)	−0.0040 (9)	−0.0014 (9)
C2	0.0422 (13)	0.0323 (15)	0.0470 (13)	−0.0037 (12)	−0.0076 (10)	−0.0068 (11)
C3	0.0430 (14)	0.0397 (17)	0.0486 (14)	−0.0108 (12)	−0.0005 (10)	0.0068 (11)
C4	0.0341 (12)	0.0483 (17)	0.0338 (11)	−0.0112 (11)	0.0032 (9)	0.0090 (10)
C5	0.0209 (9)	0.0370 (14)	0.0257 (9)	−0.0040 (9)	−0.0015 (7)	0.0048 (8)
C6	0.0211 (9)	0.0413 (15)	0.0227 (9)	−0.0017 (9)	0.0033 (7)	0.0050 (8)
C7	0.0352 (12)	0.0516 (18)	0.0326 (11)	0.0047 (11)	0.0045 (9)	−0.0049 (10)
C8	0.0353 (12)	0.0340 (15)	0.0395 (12)	0.0010 (11)	0.0022 (9)	−0.0073 (10)

Geometric parameters (Å, º)

Fe1—O7	2.1191 (18)	N1—C1	1.351 (3)
Fe1—O5	2.121 (2)	N2—C6	1.333 (3)
Fe1—O6	2.1323 (15)	N2—C8	1.368 (3)
Fe1—O8	2.1340 (17)	N3—C6	1.353 (2)
Fe1—N2	2.1361 (17)	N3—C7	1.359 (3)
Fe1—N1	2.243 (2)	N3—H3N	0.93 (3)
S1—O4	1.4605 (19)	C1—C2	1.373 (4)
S1—O3	1.4661 (16)	C1—H1	0.9300
S1—O2	1.4688 (14)	C2—C3	1.376 (3)
S1—O1	1.4844 (14)	C2—H2	0.9300
O5—H1O5	0.78 (3)	C3—C4	1.379 (4)
O5—H2O5	0.85 (3)	C3—H3	0.9300
O6—H1O6	0.71 (2)	C4—C5	1.374 (3)
O6—H2O6	0.89 (3)	C4—H4	0.9300
O7—H1O7	0.64 (3)	C5—C6	1.453 (3)
O7—H2O7	0.90 (3)	C7—C8	1.366 (3)
O8—H1O8	0.76 (3)	C7—H7	0.9300
O8—H2O8	0.84 (3)	C8—H8	0.9300
N1—C5	1.344 (2)		
O7—Fe1—O5	88.60 (8)	C5—N1—C1	117.44 (19)

O7—Fe1—O6	85.07 (7)	C5—N1—Fe1	114.36 (15)
O5—Fe1—O6	98.06 (8)	C1—N1—Fe1	128.10 (14)
O7—Fe1—O8	169.08 (6)	C6—N2—C8	105.96 (18)
O5—Fe1—O8	89.79 (7)	C6—N2—Fe1	113.84 (14)
O6—Fe1—O8	84.46 (7)	C8—N2—Fe1	140.12 (17)
O7—Fe1—N2	99.00 (7)	C6—N3—C7	107.85 (19)
O5—Fe1—N2	93.25 (8)	C6—N3—H3N	120.6 (17)
O6—Fe1—N2	168.09 (7)	C7—N3—H3N	131.4 (17)
O8—Fe1—N2	91.87 (7)	N1—C1—C2	123.3 (2)
O7—Fe1—N1	88.35 (7)	N1—C1—H1	118.3
O5—Fe1—N1	168.26 (7)	C2—C1—H1	118.3
O6—Fe1—N1	92.97 (7)	C1—C2—C3	118.2 (2)
O8—Fe1—N1	95.29 (7)	C1—C2—H2	120.9
N2—Fe1—N1	76.04 (7)	C3—C2—H2	120.9
O4—S1—O3	110.31 (10)	C2—C3—C4	119.5 (2)
O4—S1—O2	108.80 (10)	C2—C3—H3	120.2
O3—S1—O2	108.93 (9)	C4—C3—H3	120.2
O4—S1—O1	109.93 (9)	C5—C4—C3	119.1 (2)
O3—S1—O1	109.55 (9)	C5—C4—H4	120.5
O2—S1—O1	109.29 (9)	C3—C4—H4	120.5
Fe1—O5—H1O5	123 (2)	N1—C5—C4	122.4 (2)
Fe1—O5—H2O5	122 (2)	N1—C5—C6	113.50 (18)
H1O5—O5—H2O5	108 (3)	C4—C5—C6	124.04 (19)
Fe1—O6—H1O6	113.3 (19)	N2—C6—N3	110.3 (2)
Fe1—O6—H2O6	110.5 (17)	N2—C6—C5	122.02 (17)
H1O6—O6—H2O6	108 (3)	N3—C6—C5	127.6 (2)
Fe1—O7—H1O7	122 (3)	N3—C7—C8	106.2 (2)
Fe1—O7—H2O7	113.1 (18)	N3—C7—H7	126.9
H1O7—O7—H2O7	106 (3)	C8—C7—H7	126.9
Fe1—O8—H1O8	115.5 (19)	C7—C8—N2	109.6 (2)
Fe1—O8—H2O8	111.1 (18)	C7—C8—H8	125.2
H1O8—O8—H2O8	104 (3)	N2—C8—H8	125.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1*O*5···O3^{i}	0.78 (3)	2.00 (3)	2.785 (3)	175 (3)
O5—H2*O*5···O1^{ii}	0.85 (4)	2.00 (3)	2.845 (3)	172 (4)
O6—H1*O*6···O1	0.71 (3)	2.15 (3)	2.857 (3)	170 (3)
O6—H2*O*6···O3^{iii}	0.89 (3)	1.85 (3)	2.736 (3)	175 (3)
O7—H1*O*7···O1^{iii}	0.64 (4)	2.17 (3)	2.809 (3)	173 (4)
O7—H2*O*7···O4^{ii}	0.90 (4)	1.83 (3)	2.720 (3)	168 (4)
O8—H1*O*8···O4^{i}	0.76 (3)	1.96 (3)	2.722 (3)	178 (4)
O8—H2*O*8···O2	0.84 (3)	1.90 (3)	2.737 (3)	175 (3)
N3—H3*N*···O2^{iv}	0.93 (3)	1.93 (3)	2.858 (3)	178 (3)
C4—H4···O2^{iv}	0.93	2.40	3.287 (3)	160

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