

Crystal structure of tetraaqua(5,5'-dimethyl-2,2'-bipyridyl- κ^2N,N')iron(II) sulfateYamine Belamri,^a Fatima Setifi,^{a*} Bojana M. Francuski,^b Sladjana B. Novaković^b and Setifi Zouaoui^{c,d}Received 31 October 2014
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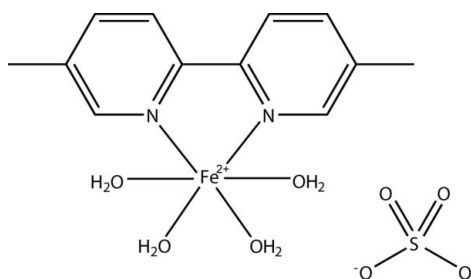
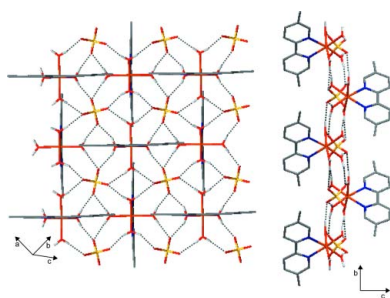
Keywords: crystal structure; 5,5'-dimethyl-2,2'-dipyridyl; tetraaqua(iron(II) complex; sulfate; bipyridine ligand; hydrogen bonding; π - π interactions**CCDC reference:** 1034106**Supporting information:** this article has supporting information at journals.iucr.org/e

^aLaboratoire de Chimie, Ingénierie Moléculaire et Nanostructures (LCIMN), Université Ferhat Abbas Sétif 1, Sétif 19000, Algeria, ^bVinča Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, PO Box 522, University of Belgrade, 11001 Belgrade, Serbia, ^cDépartement de Technologie, Faculté de Technologie, Université 20 Août 1955-Skikda, BP 26, Route d'El-Hadaiek, Skikda 21000, Algeria, and ^dUnité de Recherche de Chimie de l'Environnement et Moléculaire Structurale (CHEMS), Université Constantine 1, Constantine 25000, Algeria.
*Correspondence e-mail: setifi_zouaoui@yahoo.fr

In the title compound, $[\text{Fe}(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})_4]\text{SO}_4$, the central Fe^{II} ion is coordinated by two N atoms from the 5,5'-dimethyl-2,2'-bipyridine ligand and four water O atoms in a distorted octahedral geometry. The Fe—O coordination bond lengths vary from 2.080 (3) to 2.110 (3) Å, while the two Fe—N coordination bonds have practically identical lengths [2.175 (3) and 2.177 (3) Å]. The chelating N—Fe—N angle of 75.6 (1)° shows the largest deviation from an ideal octahedral geometry; the other coordination angles deviate from ideal values by 0.1 (1) to 9.1 (1)°. O—H...O hydrogen bonding between the four aqua ligands of the cationic complex and four O-atom acceptors of the anion leads to the formation of layers parallel to the *ab* plane. Neighbouring layers further interact by means of C—H...O and π - π interactions involving the laterally positioned bipyridine rings. The perpendicular distance between π - π interacting rings is 3.365 (2) Å, with a centroid-centroid distance of 3.702 (3) Å.

1. Chemical context

Coordination compounds containing polynitrile anions as ligands are of current interest for their magnetic properties and their rich architectures and topologies (Setifi *et al.*, 2003; Gaamoune *et al.*, 2010; Váhovská & Potočník, 2012; Setifi, Setifi *et al.*, 2013; Setifi, Domasevitsch *et al.*, 2013; Potočník *et al.*, 2014). Given the crucial role of these anionic ligands, we are interested in using them in combination with other chelating or bridging neutral co-ligands to explore their structural and electronic characteristics in the large field of molecular materials exhibiting the spin crossover (SCO) phenomenon. In an attempt to prepare such a complex, we obtained the title compound, $[\text{Fe}(\text{dmbpy})(\text{H}_2\text{O})_4]\text{SO}_4$ (I), where dmbpy is 5,5'-dimethyl-2,2'-bipyridyl.



The crystal structures of several complexes with general formula $[\text{M}(\text{bpy})(\text{H}_2\text{O})_4]^{2+}$ comprising bipyridine derivatives

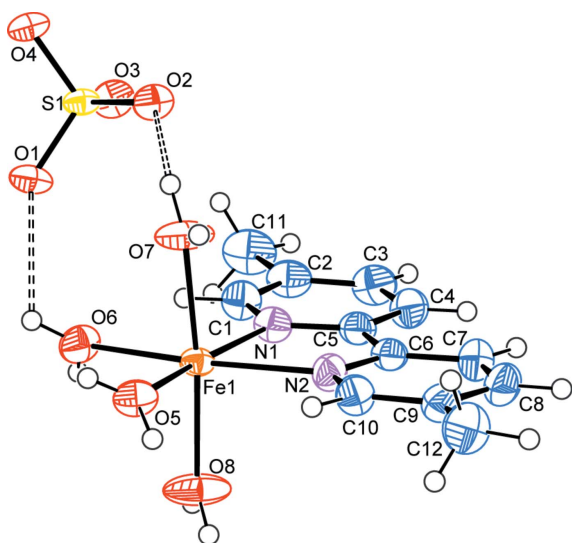


Figure 1
The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. Hydrogen bonds are indicated by dashed lines.

as ligands have been reported previously (Boonlue *et al.*, 2012; Harvey *et al.*, 1999; Kwak *et al.*, 2007; Suarez *et al.*, 2013; Xiao *et al.*, 2003; Yang, 2009; Yu *et al.*, 2007; Zhang *et al.*, 2008; Zhao & Bai, 2009). This is the first complex of this type with Fe^{II} as the central ion.

2. Structural commentary

A molecular view of complex (I), together with the atom-numbering scheme is given in Fig. 1. The crystal structure of (I) consists of the cationic complex [Fe(dmbpy)(H₂O)₄]²⁺ and a free [SO₄]²⁻ counter-ion. The Fe^{II} atom is in a distorted octahedral coordination environment and the equatorial plane

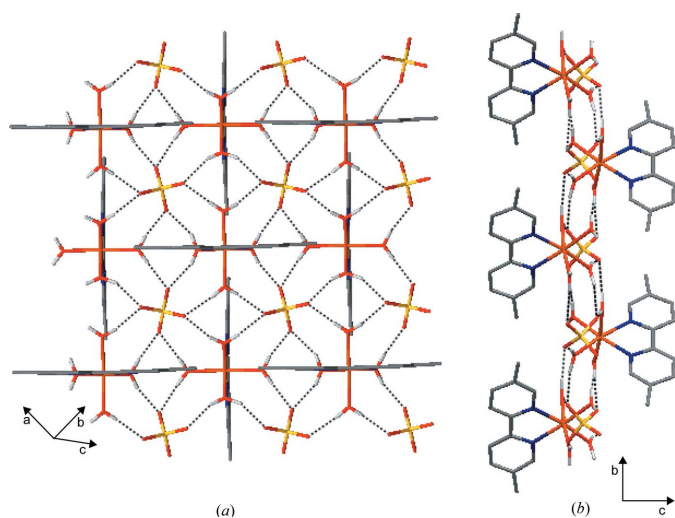


Figure 2
(a) O—H...O interactions (dashed lines) connect the cations and anions into layers parallel to the *ab* plane. (b) View of a single layer down the *a* axis.

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H1O5...O4 ⁱ	0.83	1.92	2.734 (4)	165
O5—H2O5...O2 ⁱⁱ	0.96	1.94	2.794 (4)	147
O6—H1O6...O1	0.94	1.90	2.820 (4)	167
O6—H2O6...O3 ⁱⁱⁱ	0.83	1.95	2.765 (4)	165
O7—H1O7...O4 ⁱⁱ	0.83	1.89	2.722 (4)	175
O7—H2O7...O2	0.82	1.89	2.697 (4)	167
O8—H1O8...O1 ⁱⁱⁱ	0.77	1.95	2.719 (4)	175
O8—H2O8...O3 ⁱ	0.89	1.91	2.792 (5)	174
C4—H4...O4 ^{iv}	0.93	2.54	3.232 (5)	132

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

of the octahedron is formed by a pair of nitrogen donors from the 5,5'-dimethyl-2,2'-bipyridyl ligand and two molecules of water, while the axial sites are occupied by two other water molecules. The equatorial donor atoms are nearly coplanar (r.m.s. deviation = 0.0062 Å), while the deviation of the Fe atom from the least-squares plane is somewhat larger [0.021 (2) Å]. The bipyridine chelating angle N1—Fe—N2 of 75.6 (1)° shows the most significant deviation from an ideal octahedral geometry. The other angular distortions from an ideal octahedral geometry are in the range 0.1 (1) to 9.1 (1)°. The S—O bond lengths [1.466 (3)–1.480 (3) Å] and O—S—O angles [108.8 (2)–109.9 (2)°] indicate a nearly ideal tetrahedral geometry for the anion.

3. Supramolecular features

Within the crystal packing, the charged components are connected by an extensive hydrogen-bonding network (Table 1). Each of the [Fe(dmbpy)(H₂O)₄]²⁺ cations engages all four coordinating water molecules in hydrogen bonding to four [SO₄]²⁻ anions (Fig. 2*a*). The anions surrounding the cationic unit are positioned at similar Fe...S distance of ≈4.9 Å. On the other hand, each of the [SO₄]²⁻ anions appears surrounded with four cationic units, where its four O atoms engage as acceptors in bifurcated O—H...O hydrogen bonds towards neighbouring cations (Fig. 2*a*). Such a mutual

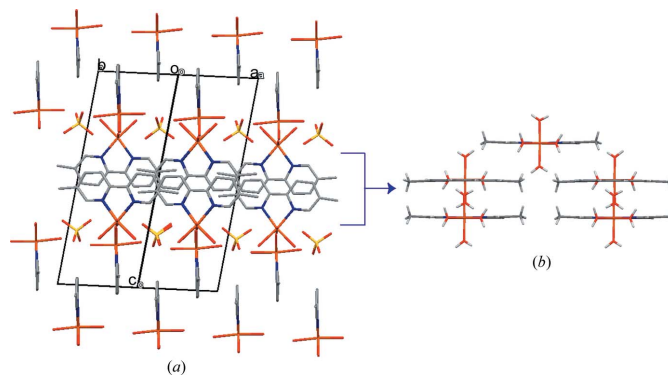


Figure 3
(a) The bipyridine rings from neighbouring layers interact *via* C—H...O and π — π interactions. (b) Orthogonal projection of the central fragment.

arrangement leads to the formation of a two-dimensional hydrogen-bonded network parallel to the *ab* plane (Fig. 2*b*). Laterally arranged aromatic rings of the 5,5'-dimethyl-2,2'-bipyridine ligand in neighbouring layers interact by means of weak C—H···O and π – π interactions, forming the three-dimensional crystal packing (Table 1 and Fig. 3). The centroid–centroid distance for the latter interaction is 3.702 (3) Å.

4. Synthesis and crystallization

The title compound, (I), was synthesized hydrothermally from a mixture of iron(II) sulfate heptahydrate (28 mg, 0.1 mmol), 5,5'-dimethyl-2,2'-bipyridyl (18 mg, 0.1 mmol) and potassium tricyanomethanide $\text{KC}(\text{CN})_3$ (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 410 K for 3 d. The autoclave was then allowed to cool to ambient temperature. Red crystals of (I) were collected by filtration, washed with water and dried in air (yield 35%).

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 at 0.93 and 0.96 Å from aromatic and methyl C atoms, respectively. The $U_{\text{iso}}(\text{H})$ values were equal to 1.2 and 1.5 times U_{eq} of the corresponding $\text{C}(sp^2)$ and $\text{C}(sp^3)$ atoms. The H atoms of the four water molecules were initially located in a difference Fourier map. During the refinement, these H atoms were allowed to ride on their parent O atoms and also to rotate about the corresponding Fe—O bonds. The $U_{\text{iso}}(\text{H})$ values were set equal to 1.2 times U_{eq} of the parent O atom. The reflections (100) and (002) were excluded from the refinement because they were nearly completely obscured by the beamstop.

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$[\text{Fe}(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})_4]\text{SO}_4$
M_r	408.21
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	9.5790 (7), 9.6190 (9), 18.5500 (12)
β (°)	101.527 (5)
V (Å ³)	1674.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ^{−1})	1.07
Crystal size (mm)	0.28 × 0.14 × 0.09
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2009)
T_{min} , T_{max}	0.792, 0.881
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14477, 4868, 3305
R_{int}	0.117
$(\sin \theta/\lambda)_{\text{max}}$ (Å ^{−1})	0.706
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.196, 1.08
No. of reflections	4867
No. of parameters	223
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ^{−3})	0.84, −1.33

Computer programs: *APEX2* and *SAINTE* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006).

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supporting information

Acta Cryst. (2014). E70, 544-546 [doi:10.1107/S1600536814024982]

Crystal structure of tetraaqua(5,5'-dimethyl-2,2'-bipyridyl- κ^2N,N')iron(II) sulfate

Yamine Belamri, Fatima Setifi, Bojana M. Francuski, Sladjana B. Novaković and Setifi Zouaoui

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *CALC-OH* (Nardelli, 1999).

Tetraaqua(5,5'-dimethyl-2,2'-bipyridyl- κ^2N,N')iron(II) sulfate

Crystal data

[Fe(C₁₂H₁₂N₂)(H₂O)₄]₂SO₄

M_r = 408.21

Monoclinic, *P2₁/c*

Hall symbol: -P 2ybc

a = 9.5790 (7) Å

b = 9.6190 (9) Å

c = 18.5500 (12) Å

β = 101.527 (5)°

V = 1674.7 (2) Å³

Z = 4

F(000) = 848

D_x = 1.619 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 4857 reflections

θ = 2.2–29.9°

μ = 1.07 mm⁻¹

T = 293 K

Block, red

0.28 × 0.14 × 0.09 mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω -2 θ scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

T_{min} = 0.792, *T_{max}* = 0.881

14477 measured reflections

4868 independent reflections

3305 reflections with *I* > 2 σ (*I*)

R_{int} = 0.117

θ_{\max} = 30.1°, θ_{\min} = 2.2°

h = -13→13

k = -13→13

l = -26→26

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2 σ (*F*²)] = 0.065

wR(*F*²) = 0.196

S = 1.08

4867 reflections

223 parameters

H-atom parameters constrained

w = 1/[$\sigma^2(F_o^2) + (0.0821P)^2 + 2.0315P$]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.002

$\Delta\rho_{\max}$ = 0.84 e Å⁻³

$\Delta\rho_{\min}$ = -1.33 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.77171 (5)	0.13308 (6)	0.80535 (3)	0.02534 (17)
S1	0.75114 (9)	-0.36313 (10)	0.75262 (5)	0.0251 (2)
O3	0.6693 (3)	-0.4269 (3)	0.80282 (17)	0.0376 (7)
O1	0.6620 (3)	-0.2600 (3)	0.70522 (17)	0.0364 (7)
O2	0.8783 (3)	-0.2931 (3)	0.79546 (16)	0.0338 (6)
O4	0.7980 (3)	-0.4722 (3)	0.70641 (16)	0.0347 (6)
O5	0.8418 (3)	0.2477 (3)	0.72229 (16)	0.0361 (7)
H1O5	0.8129	0.3296	0.7171	0.043*
H2O5	0.9194	0.2065	0.7043	0.043*
O6	0.6213 (3)	0.0261 (3)	0.72705 (17)	0.0399 (7)
H1O6	0.6389	-0.0652	0.7130	0.048*
H2O6	0.5378	0.0556	0.7195	0.048*
O7	0.9191 (3)	-0.0166 (3)	0.7871 (2)	0.0489 (9)
H1O7	1.0046	-0.0016	0.7863	0.059*
H2O7	0.8929	-0.0981	0.7879	0.059*
O8	0.6224 (3)	0.2876 (4)	0.8109 (2)	0.0619 (11)
H1O8	0.5422	0.2701	0.8053	0.074*
H2O8	0.6333	0.3793	0.8107	0.074*
N1	0.7224 (4)	0.0244 (4)	0.90015 (19)	0.0340 (8)
N2	0.9173 (4)	0.2218 (4)	0.89908 (19)	0.0337 (8)
C1	0.6251 (5)	-0.0763 (5)	0.8969 (3)	0.0390 (10)
H1	0.5747	-0.1028	0.8508	0.047*
C2	0.5945 (5)	-0.1437 (5)	0.9581 (3)	0.0424 (10)
C3	0.6691 (6)	-0.0975 (5)	1.0262 (3)	0.0452 (11)
H3	0.6497	-0.1362	1.0691	0.054*
C4	0.7709 (5)	0.0043 (5)	1.0307 (2)	0.0412 (10)
H4	0.8219	0.0327	1.0763	0.049*
C5	0.7973 (4)	0.0650 (5)	0.9666 (2)	0.0341 (9)
C6	0.9054 (4)	0.1741 (4)	0.9658 (2)	0.0316 (8)
C7	0.9931 (5)	0.2257 (5)	1.0288 (2)	0.0440 (11)
H7	0.9845	0.1926	1.0748	0.053*
C8	1.0931 (5)	0.3265 (5)	1.0230 (3)	0.0436 (11)
H8	1.1512	0.3617	1.0653	0.052*
C9	1.1071 (5)	0.3750 (5)	0.9549 (3)	0.0411 (10)
C10	1.0156 (5)	0.3184 (5)	0.8947 (2)	0.0381 (9)
H10	1.0231	0.3496	0.8482	0.046*
C11	0.4852 (6)	-0.2566 (6)	0.9492 (3)	0.0594 (14)
H11A	0.3987	-0.2243	0.9184	0.089*
H11B	0.4670	-0.2817	0.9966	0.089*

H11C	0.5198	-0.3363	0.9270	0.089*
C12	1.2165 (5)	0.4814 (6)	0.9444 (3)	0.0553 (13)
H12A	1.2919	0.4366	0.9261	0.083*
H12B	1.2548	0.5249	0.9907	0.083*
H12C	1.1726	0.5504	0.9099	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0228 (3)	0.0200 (3)	0.0332 (3)	0.0001 (2)	0.00542 (19)	0.0011 (2)
S1	0.0219 (4)	0.0171 (4)	0.0374 (5)	0.0005 (3)	0.0084 (3)	0.0000 (4)
O3	0.0387 (16)	0.0309 (16)	0.0461 (17)	-0.0077 (13)	0.0152 (13)	0.0018 (13)
O1	0.0323 (15)	0.0262 (15)	0.0500 (17)	0.0075 (12)	0.0067 (12)	0.0064 (13)
O2	0.0223 (12)	0.0289 (16)	0.0499 (17)	-0.0067 (11)	0.0065 (11)	-0.0046 (13)
O4	0.0371 (15)	0.0236 (14)	0.0455 (16)	0.0052 (12)	0.0135 (12)	-0.0051 (12)
O5	0.0361 (15)	0.0212 (14)	0.0536 (18)	-0.0039 (12)	0.0151 (13)	0.0065 (13)
O6	0.0266 (14)	0.0299 (16)	0.0601 (19)	-0.0038 (12)	0.0013 (13)	-0.0091 (15)
O7	0.0286 (15)	0.0234 (15)	0.098 (3)	0.0025 (12)	0.0207 (17)	0.0004 (17)
O8	0.0270 (16)	0.0275 (17)	0.134 (4)	0.0013 (13)	0.022 (2)	0.000 (2)
N1	0.0345 (17)	0.0336 (19)	0.0351 (18)	0.0003 (15)	0.0102 (14)	0.0042 (15)
N2	0.0352 (18)	0.0307 (18)	0.0336 (17)	-0.0043 (14)	0.0033 (14)	-0.0016 (14)
C1	0.039 (2)	0.036 (2)	0.042 (2)	-0.0060 (19)	0.0111 (18)	0.0020 (19)
C2	0.045 (2)	0.035 (2)	0.051 (3)	0.001 (2)	0.017 (2)	0.009 (2)
C3	0.059 (3)	0.042 (3)	0.040 (2)	0.002 (2)	0.024 (2)	0.012 (2)
C4	0.050 (3)	0.043 (3)	0.033 (2)	0.003 (2)	0.0133 (19)	0.0032 (19)
C5	0.037 (2)	0.032 (2)	0.034 (2)	0.0064 (17)	0.0093 (16)	0.0015 (17)
C6	0.0318 (19)	0.030 (2)	0.034 (2)	0.0048 (16)	0.0078 (16)	0.0014 (16)
C7	0.049 (3)	0.047 (3)	0.034 (2)	0.002 (2)	0.0034 (19)	-0.003 (2)
C8	0.044 (2)	0.040 (3)	0.044 (3)	-0.005 (2)	0.0012 (19)	-0.012 (2)
C9	0.040 (2)	0.035 (2)	0.047 (3)	-0.0016 (19)	0.0050 (18)	-0.005 (2)
C10	0.040 (2)	0.036 (2)	0.038 (2)	-0.0048 (19)	0.0059 (17)	0.0020 (19)
C11	0.061 (3)	0.050 (3)	0.073 (4)	-0.006 (3)	0.028 (3)	0.014 (3)
C12	0.042 (3)	0.051 (3)	0.069 (3)	-0.017 (2)	0.003 (2)	-0.007 (3)

Geometric parameters (Å, °)

Fe1—O8	2.080 (3)	C1—H1	0.9300
Fe1—O7	2.091 (3)	C2—C3	1.394 (7)
Fe1—O6	2.099 (3)	C2—C11	1.494 (7)
Fe1—O5	2.110 (3)	C3—C4	1.373 (7)
Fe1—N2	2.175 (3)	C3—H3	0.9300
Fe1—N1	2.177 (3)	C4—C5	1.392 (6)
S1—O3	1.466 (3)	C4—H4	0.9300
S1—O2	1.477 (3)	C5—C6	1.477 (6)
S1—O1	1.479 (3)	C6—C7	1.388 (6)
S1—O4	1.480 (3)	C7—C8	1.382 (7)
O5—H1O5	0.8346	C7—H7	0.9300
O5—H2O5	0.9588	C8—C9	1.379 (7)

O6—H1O6	0.9409	C8—H8	0.9300
O6—H2O6	0.8339	C9—C10	1.385 (6)
O7—H1O7	0.8346	C9—C12	1.504 (7)
O7—H2O7	0.8248	C10—H10	0.9300
O8—H1O8	0.7727	C11—H11A	0.9600
O8—H2O8	0.8889	C11—H11B	0.9600
N1—C1	1.337 (6)	C11—H11C	0.9600
N1—C5	1.354 (5)	C12—H12A	0.9600
N2—C10	1.336 (5)	C12—H12B	0.9600
N2—C6	1.345 (5)	C12—H12C	0.9600
C1—C2	1.389 (6)		
O8—Fe1—O7	173.50 (16)	C2—C1—H1	117.9
O8—Fe1—O6	90.06 (14)	C1—C2—C3	116.0 (4)
O7—Fe1—O6	86.71 (13)	C1—C2—C11	120.5 (5)
O8—Fe1—O5	89.18 (14)	C3—C2—C11	123.6 (4)
O7—Fe1—O5	85.26 (13)	C4—C3—C2	120.7 (4)
O6—Fe1—O5	91.46 (12)	C4—C3—H3	119.6
O8—Fe1—N2	90.98 (15)	C2—C3—H3	119.6
O7—Fe1—N2	93.10 (14)	C3—C4—C5	119.7 (4)
O6—Fe1—N2	170.92 (13)	C3—C4—H4	120.1
O5—Fe1—N2	97.58 (13)	C5—C4—H4	120.1
O8—Fe1—N1	92.32 (15)	N1—C5—C4	120.2 (4)
O7—Fe1—N1	93.60 (14)	N1—C5—C6	116.1 (4)
O6—Fe1—N1	95.39 (13)	C4—C5—C6	123.7 (4)
O5—Fe1—N1	172.99 (13)	N2—C6—C7	120.3 (4)
N2—Fe1—N1	75.55 (14)	N2—C6—C5	116.1 (4)
O3—S1—O2	109.72 (18)	C7—C6—C5	123.6 (4)
O3—S1—O1	109.88 (18)	C8—C7—C6	119.8 (4)
O2—S1—O1	109.25 (18)	C8—C7—H7	120.1
O3—S1—O4	109.51 (18)	C6—C7—H7	120.1
O2—S1—O4	108.76 (17)	C9—C8—C7	120.3 (4)
O1—S1—O4	109.70 (18)	C9—C8—H8	119.8
Fe1—O5—H1O5	115.4	C7—C8—H8	119.8
Fe1—O5—H2O5	114.8	C8—C9—C10	116.3 (4)
H1O5—O5—H2O5	127.9	C8—C9—C12	123.1 (4)
Fe1—O6—H1O6	120.9	C10—C9—C12	120.6 (4)
Fe1—O6—H2O6	116.9	N2—C10—C9	124.4 (4)
H1O6—O6—H2O6	119.3	N2—C10—H10	117.8
Fe1—O7—H1O7	125.5	C9—C10—H10	117.8
Fe1—O7—H2O7	115.7	C2—C11—H11A	109.5
H1O7—O7—H2O7	118.0	C2—C11—H11B	109.5
Fe1—O8—H1O8	120.9	H11A—C11—H11B	109.5
Fe1—O8—H2O8	128.8	C2—C11—H11C	109.5
H1O8—O8—H2O8	109.3	H11A—C11—H11C	109.5
C1—N1—C5	119.2 (4)	H11B—C11—H11C	109.5
C1—N1—Fe1	125.0 (3)	C9—C12—H12A	109.5
C5—N1—Fe1	115.8 (3)	C9—C12—H12B	109.5

C10—N2—C6	118.9 (4)	H12A—C12—H12B	109.5
C10—N2—Fe1	124.9 (3)	C9—C12—H12C	109.5
C6—N2—Fe1	116.3 (3)	H12A—C12—H12C	109.5
N1—C1—C2	124.1 (4)	H12B—C12—H12C	109.5
N1—C1—H1	117.9		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O5—H1O5 \cdots O4 ⁱ	0.83	1.92	2.734 (4)	165
O5—H2O5 \cdots O2 ⁱⁱ	0.96	1.94	2.794 (4)	147
O6—H1O6 \cdots O1	0.94	1.90	2.820 (4)	167
O6—H2O6 \cdots O3 ⁱⁱⁱ	0.83	1.95	2.765 (4)	165
O7—H1O7 \cdots O4 ⁱⁱ	0.83	1.89	2.722 (4)	175
O7—H2O7 \cdots O2	0.82	1.89	2.697 (4)	167
O8—H1O8 \cdots O1 ⁱⁱⁱ	0.77	1.95	2.719 (4)	175
O8—H2O8 \cdots O3 ⁱ	0.89	1.91	2.792 (5)	174
C4—H4 \cdots O4 ^{iv}	0.93	2.54	3.232 (5)	132

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