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Crystal structure of high-spin tetraaquabis(2-chloropyrazine- κN^4)iron(II) bis(4-methylbenzene-sulfonate)

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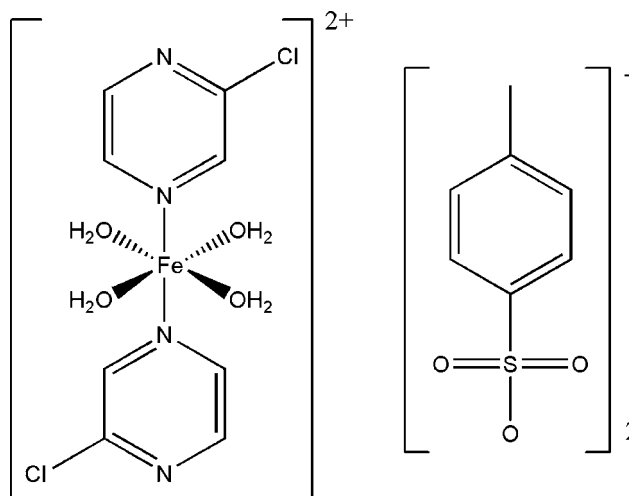
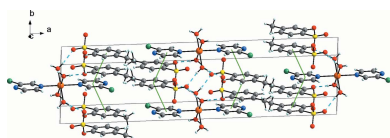
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The title salt, $[\text{Fe}^{\text{II}}(\text{C}_4\text{H}_3\text{ClN}_2)_2(\text{H}_2\text{O})_4](\text{C}_7\text{H}_7\text{O}_3\text{S})_2$, contains a complex cation with point group symmetry $2/m$. The high-spin Fe^{II} cation is hexacoordinated by four symmetry-related water and two N -bound 2-chloropyrazine molecules in a *trans* arrangement, forming a distorted FeN_2O_4 octahedron. The three-dimensional supramolecular structure is supported by intermolecular $\text{O} \cdots \text{H}$ hydrogen bonds between the complex cations and tosylate anions, and additional π - π interactions between benzene and pyrazine rings. The methyl H atoms of the tosylate anion are equally disordered over two positions.

1. Chemical context

Transition metal complexes containing pyrazine or substituted pyrazines as ligands are of current interest due to their supramolecular arrangements and the probability of being spin-crossover compounds. Spin crossover, 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 *via* influence of external stimuli such as temperature, pressure, light irradiation, magnetic field or guest effects (Gütlich & Goodwin, 2004). As a result of the appearance of such features as thermochromic effects, magnetic susceptibility changes, changes of cell volume, *etc.* that accompany the molecular switching between high-spin and low-spin states, they can be applied in the development of micro-thermometers and photonic devices (Gural'skiy *et al.*, 2012).



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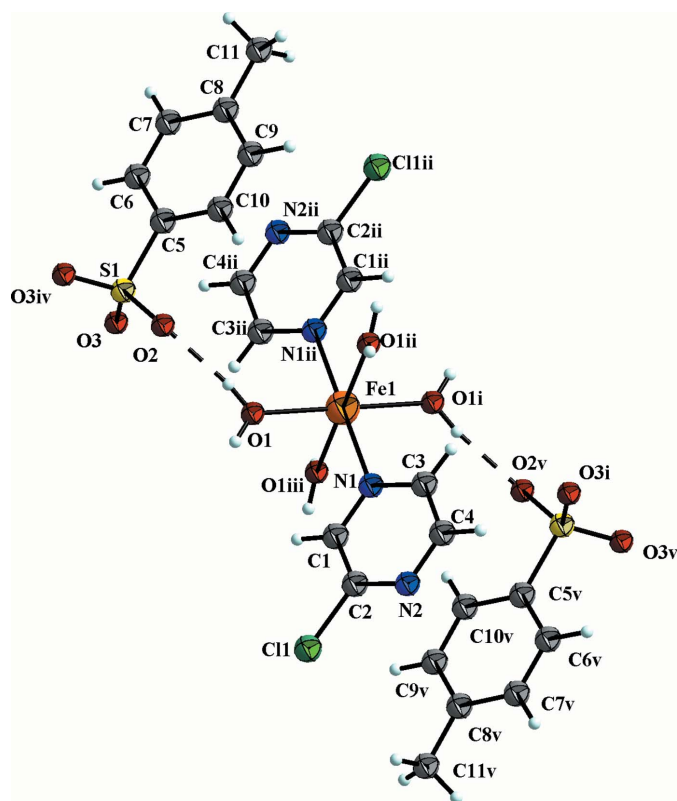


Figure 1

The structure of the cationic and anionic components in the title salt. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are indicated by dashed lines. [Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $1-x, y, 1-z$; (iii) $x, -y, z$; (iv) $x, 1-y, z$; (v) $1-x, -1+y, 1-z$.]

Aromatic ligands bearing two or more N atoms are known for their ability to form different coordination polymers and molecular complexes. Thus, a number of mononuclear high-spin Fe^{II} complexes with substituted pyrazines have been reported recently (Shylin *et al.*, 2015). These heterocyclic ligands are also known for their ability to create three-dimensional metal-organic framework structures, so called analogues of Hofmann clathrates with general formula

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1A\cdots O2$	0.82 (2)	1.91 (2)	2.7238 (19)	171 (4)
$O1-H1B\cdots O3^i$	0.81 (2)	1.95 (2)	2.7624 (19)	177 (3)

Symmetry code: (i) $-x+1, y, -z+2$.

Table 2

Geometric parameters of $\pi-\pi$ stacking (\AA , $^\circ$).

centroid (2-chloropyrazine)—centroid (tosylate anion)	3.7098 (1)
centroid (2-chloropyrazine)—centroid (tosylate anion)—centroid (2-chloropyrazine)	130.283 (1)

$[\text{Fe}(L)_x[M_y(\text{CN})_z]]_\infty$ where $M = \text{Ni, Pd, Pt, etc.}$. Series of thiocyanato coordination polymers $[M(\text{NCS})_2L_2]_\infty$ (with $M = \text{Mn, Fe, Co, Ni, and } L = \text{pyrazine}$) in which the small-sized thiocyanate anions are terminally N-bound and therefore not involved in any magnetic exchange interactions are also known (Wriedt & Näther, 2011). Although 2-chloropyrazine could possess a N,N' -manner of coordination, it is frequently found to act as a monodentate ligand due to the bulky chlorine atom being in direct proximity to one of the nitrogen atoms (Wöhlert & Näther, 2013).

In this paper, we report on the crystal structure of $[\text{Fe}^{\text{II}}(\text{C}_4\text{H}_3\text{ClN}_2)_2(\text{H}_2\text{O})_4](\text{C}_7\text{H}_7\text{O}_3\text{S})_2$ containing a cationic iron(II) complex with 2-chloropyrazine and aqua ligands, and tosylate as an anion.

2. Structural commentary

The structure of the title compound consists of a complex cation $[\text{Fe}(\text{2-chloropyrazine})_2(\text{H}_2\text{O})_4]^{2+}$ and two tosylate anions. The Fe^{II} atom, located on a special position with site symmetry $2/m$, is sixfold coordinated by two N atoms of two symmetry-related 2-chloropyrazine ligands occupying the axial positions and four O atoms of four H_2O molecules forming the equatorial plane (Fig. 1). The distances between

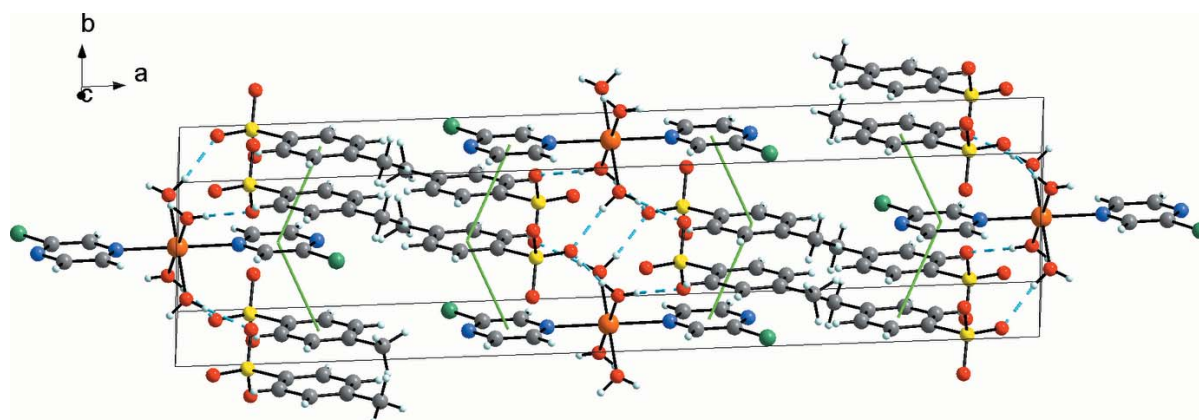


Figure 2

The crystal structure of the title compound, showing hydrogen bonds as dashed cyan lines and $\pi-\pi$ contacts as green lines. Colour key: orange Fe, yellow S, blue N, grey C, green Cl, red O and white H.

Table 3
Experimental details.

Crystal data	
Chemical formula	[Fe(C ₄ H ₃ ClN ₂) ₂ (H ₂ O) ₄] (C ₇ H ₇ O ₃ S) ₂
<i>M</i> _r	699.35
Crystal system, space group	Monoclinic, <i>C2/m</i>
Temperature (K)	133
<i>a</i> , <i>b</i> , <i>c</i> (Å)	30.691 (3), 6.7321 (3), 6.9435 (6)
β (°)	99.811 (7)
<i>V</i> (Å ³)	1413.63 (19)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ^{−1})	0.93
Crystal size (mm)	0.26 × 0.14 × 0.06
Data collection	
Diffractometer	Stoe IPDS II
Absorption correction	Numerical (<i>X-RED</i> ; Stoe & Cie, 2002)
<i>T</i> _{min} , <i>T</i> _{max}	0.697, 0.925
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	9102, 1630, 1380
<i>R</i> _{int}	0.066
(sin θ/λ) _{max} (Å ^{−1})	0.633
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.028, 0.067, 1.00
No. of reflections	1630
No. of parameters	126
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.38, −0.36

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Fe^{II} and the O atoms [2.1004 (14) Å] of the H₂O molecules are significantly shorter than those between Fe^{II} and N [2.200 (2) Å] atoms of the two 2-chloropyrazine ligands, hence the resulting FeO₄N₂ octahedron is distorted. The metal-to-ligand distances clearly signalize the high-spin nature of the complex described in here (Shylin *et al.*, 2015). Similar structural features have been reported for other related compounds (Shylin *et al.*, 2013). The angles between the coordinating O atoms [O1ⁱ–Fe1–O1ⁱⁱⁱ = 90.83 (11)°; for symmetry codes see caption to Fig. 1], and coordinating N and O atoms [O1ⁱⁱ–Fe1–N1 = 90.68 (5)°] indicate only a small angular distortion.

3. Supramolecular features

In the title compound, the crystal packing is stabilized by O1–H1A···O2 and O1–H1B···O3ⁱ hydrogen bonds (Table 1) between the complex cations and the counter-anions (Figs. 1 and 2). Only two O atoms of the tosylate anion are involved in hydrogen bonding. Additional π–π stacking interactions (for numerical details, see: Table 2) between the pyrazine and benzene rings of the tosylate anion contribute to the

stabilization (Fritsky *et al.*, 2004) of the three-dimensional network (Fig. 2).

4. Synthesis and crystallization

Crystals of the title compound were obtained by adding 2-chloropyrazine (0.046 g, 0.4 mmol) to Fe(OTs)₂·6H₂O (0.096 g, 0.2 mmol) (OTs = *p*-toluenesulfonate) and ascorbic acid (0.001 g) in water (5 ml). After seven days this yielded colourless blocks of the title compound that were collected, washed with water and dried in air. Yield 0.090 g (64%).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All non-water H atoms were positioned geometrically and allowed to ride on their parent atoms, with *d*(C–H) = 0.95 Å for aromatic and 0.98 Å for CH₃ hydrogen atoms. Because of the symmetry of the complete complex cation, methyl H atoms were modelled as equally disordered over two sets of sites. The H atoms of the water molecule were located from a difference Fourier map and were modelled with a common isotropic displacement parameter fixed at 0.08 Å². The O–H bonds lengths were constrained to 0.82 Å. The *U*_{iso} values were constrained to be 1.5*U*_{eq} of the carrier atom for methyl H atoms and 1.2*U*_{eq} for the remaining H atoms.

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Crystal structure of high-spin tetraaquabis(2-chloropyrazine- κN^4)iron(II) bis(4-methylbenzenesulfonate)

Bohdan O. Golub, Sergii I. Shylin, Sebastian Dechert, Maria L. Malysheva and Il'ya A. Gural'skiy

Computing details

Data collection: *X-Area* (Stoe & Cie, 2002); cell refinement: *X-Area* (Stoe & Cie, 2002); data reduction: *X-Red* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *Olex2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Tetraaquabis(2-chloropyrazine- κN^4)iron(II) bis(4-methylbenzenesulfonate)

Crystal data

$[\text{Fe}(\text{C}_4\text{H}_3\text{ClN}_2)_2(\text{H}_2\text{O})_4](\text{C}_7\text{H}_7\text{O}_3\text{S})_2$
 $M_r = 699.35$
 Monoclinic, $C2/m$
 $a = 30.691(3) \text{ \AA}$
 $b = 6.7321(3) \text{ \AA}$
 $c = 6.9435(6) \text{ \AA}$
 $\beta = 99.811(7)^\circ$
 $V = 1413.63(19) \text{ \AA}^3$
 $Z = 2$

$F(000) = 720$
 $D_x = 1.643 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 9102 reflections
 $\theta = 1.4\text{--}26.7^\circ$
 $\mu = 0.93 \text{ mm}^{-1}$
 $T = 133 \text{ K}$
 Block, colourless
 $0.26 \times 0.14 \times 0.06 \text{ mm}$

Data collection

Stoe IPDS II
 diffractometer
 φ scans and ω scans with κ offset
 Absorption correction: numerical
 (*X-Red*; Stoe & Cie, 2002)
 $T_{\min} = 0.697$, $T_{\max} = 0.925$
 9102 measured reflections

1630 independent reflections
 1380 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$
 $\theta_{\max} = 26.7^\circ$, $\theta_{\min} = 1.4^\circ$
 $h = -38 \rightarrow 38$
 $k = -8 \rightarrow 6$
 $l = -8 \rightarrow 8$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.067$
 $S = 1.00$
 1630 reflections
 126 parameters
 2 restraints

Primary atom site location: structure-invariant
 direct methods
 Hydrogen site location: mixed
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0395P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.38 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$$

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Fe1	0.5000	0.0000	0.5000	0.01386 (13)	
Cl1	0.68495 (2)	0.0000	0.84806 (9)	0.02791 (16)	
O1	0.51119 (5)	0.2190 (3)	0.7183 (2)	0.0399 (4)	
N1	0.57111 (7)	0.0000	0.4870 (3)	0.0161 (4)	
N2	0.66150 (7)	0.0000	0.4683 (3)	0.0206 (4)	
C1	0.60191 (8)	0.0000	0.6491 (3)	0.0171 (5)	
H1	0.5932	0.0000	0.7741	0.021*	
C2	0.64619 (8)	0.0000	0.6350 (3)	0.0184 (5)	
C3	0.58590 (8)	0.0000	0.3161 (3)	0.0192 (5)	
H3	0.5652	0.0000	0.1977	0.023*	
C4	0.63061 (8)	0.0000	0.3081 (3)	0.0211 (5)	
H4	0.6396	0.0000	0.1839	0.025*	
S1	0.41620 (2)	0.5000	0.91435 (8)	0.01630 (14)	
O2	0.45581 (6)	0.5000	0.8231 (2)	0.0206 (4)	
O3	0.41275 (4)	0.32011 (19)	1.02718 (16)	0.0237 (3)	
C5	0.37118 (8)	0.5000	0.7189 (3)	0.0165 (5)	
C6	0.32788 (8)	0.5000	0.7567 (3)	0.0223 (5)	
H6	0.3226	0.5000	0.8876	0.027*	
C7	0.29303 (8)	0.5000	0.6040 (4)	0.0239 (5)	
H7	0.2637	0.5000	0.6308	0.029*	
C8	0.29970 (8)	0.5000	0.4102 (3)	0.0205 (5)	
C9	0.34283 (8)	0.5000	0.3749 (3)	0.0211 (5)	
H9	0.3480	0.5000	0.2438	0.025*	
C10	0.37849 (8)	0.5000	0.5263 (3)	0.0188 (5)	
H10	0.4078	0.5000	0.4993	0.023*	
C11	0.26090 (9)	0.5000	0.2452 (4)	0.0283 (6)	
H11A	0.2351	0.4424	0.2904	0.042*	0.5
H11B	0.2681	0.4209	0.1364	0.042*	0.5
H11C	0.2542	0.6367	0.2013	0.042*	0.5
H1A	0.4925 (10)	0.299 (5)	0.740 (5)	0.080*	
H1B	0.5338 (8)	0.251 (5)	0.791 (4)	0.080*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0130 (2)	0.0152 (2)	0.0129 (2)	0.000	0.00075 (16)	0.000
Cl1	0.0162 (3)	0.0456 (4)	0.0203 (3)	0.000	−0.0017 (2)	0.000
O1	0.0192 (7)	0.0481 (10)	0.0481 (9)	0.0068 (7)	−0.0063 (6)	−0.0343 (7)

N1	0.0165 (10)	0.0157 (10)	0.0159 (9)	0.000	0.0021 (7)	0.000
N2	0.0182 (10)	0.0241 (11)	0.0202 (9)	0.000	0.0051 (8)	0.000
C1	0.0183 (12)	0.0194 (12)	0.0139 (10)	0.000	0.0033 (9)	0.000
C2	0.0178 (12)	0.0194 (12)	0.0168 (10)	0.000	−0.0002 (9)	0.000
C3	0.0212 (13)	0.0210 (12)	0.0155 (10)	0.000	0.0032 (9)	0.000
C4	0.0216 (13)	0.0255 (13)	0.0170 (11)	0.000	0.0054 (9)	0.000
S1	0.0149 (3)	0.0189 (3)	0.0142 (3)	0.000	−0.0001 (2)	0.000
O2	0.0143 (8)	0.0235 (9)	0.0240 (8)	0.000	0.0030 (7)	0.000
O3	0.0224 (7)	0.0263 (7)	0.0203 (6)	−0.0031 (5)	−0.0025 (5)	0.0066 (5)
C5	0.0163 (12)	0.0173 (11)	0.0155 (10)	0.000	0.0014 (9)	0.000
C6	0.0190 (13)	0.0338 (15)	0.0139 (10)	0.000	0.0025 (9)	0.000
C7	0.0138 (12)	0.0354 (15)	0.0229 (12)	0.000	0.0040 (9)	0.000
C8	0.0183 (12)	0.0234 (13)	0.0181 (11)	0.000	−0.0018 (9)	0.000
C9	0.0211 (13)	0.0268 (13)	0.0153 (11)	0.000	0.0028 (9)	0.000
C10	0.0176 (12)	0.0223 (12)	0.0171 (10)	0.000	0.0046 (9)	0.000
C11	0.0217 (13)	0.0391 (16)	0.0216 (12)	0.000	−0.0030 (10)	0.000

Geometric parameters (Å, °)

Fe1—O1 ⁱ	2.1004 (14)	S1—O2	1.4632 (17)
Fe1—O1 ⁱⁱ	2.1004 (14)	S1—O3 ^{iv}	1.4560 (12)
Fe1—O1 ⁱⁱⁱ	2.1004 (14)	S1—O3	1.4560 (12)
Fe1—O1	2.1004 (14)	S1—C5	1.764 (2)
Fe1—N1 ⁱ	2.200 (2)	C5—C6	1.398 (3)
Fe1—N1	2.200 (2)	C5—C10	1.393 (3)
C11—C2	1.733 (2)	C6—H6	0.9500
O1—H1A	0.820 (18)	C6—C7	1.372 (3)
O1—H1B	0.814 (18)	C7—H7	0.9500
N1—C1	1.341 (3)	C7—C8	1.395 (3)
N1—C3	1.341 (3)	C8—C9	1.387 (3)
N2—C2	1.321 (3)	C8—C11	1.506 (3)
N2—C4	1.333 (3)	C9—H9	0.9500
C1—H1	0.9500	C9—C10	1.383 (3)
C1—C2	1.379 (3)	C10—H10	0.9500
C3—H3	0.9500	C11—H11A	0.9800
C3—C4	1.383 (4)	C11—H11B	0.9800
C4—H4	0.9500	C11—H11C	0.9800
O1 ⁱ —Fe1—O1 ⁱⁱⁱ	90.83 (11)	N2—C4—H4	118.8
O1 ⁱ —Fe1—O1	180.0	C3—C4—H4	118.8
O1 ⁱⁱⁱ —Fe1—O1	89.17 (11)	O2—S1—C5	105.44 (10)
O1 ⁱⁱⁱ —Fe1—O1 ⁱⁱ	180.0	O3 ^{iv} —S1—O2	112.02 (6)
O1 ⁱ —Fe1—O1 ⁱⁱ	89.17 (11)	O3—S1—O2	112.02 (6)
O1 ⁱⁱ —Fe1—O1	90.83 (11)	O3—S1—O3 ^{iv}	112.56 (10)
O1 ⁱⁱⁱ —Fe1—N1	89.32 (5)	O3—S1—C5	107.14 (7)
O1 ⁱⁱ —Fe1—N1 ⁱ	89.32 (5)	O3 ^{iv} —S1—C5	107.14 (7)
O1 ⁱ —Fe1—N1 ⁱ	89.32 (5)	C6—C5—S1	120.03 (17)
O1 ⁱⁱ —Fe1—N1	90.68 (5)	C10—C5—S1	120.37 (18)

O1—Fe1—N1	89.32 (5)	C10—C5—C6	119.6 (2)
O1 ⁱ —Fe1—N1	90.68 (5)	C5—C6—H6	120.1
O1 ⁱⁱⁱ —Fe1—N1 ⁱ	90.68 (5)	C7—C6—C5	119.7 (2)
O1—Fe1—N1 ⁱ	90.68 (5)	C7—C6—H6	120.1
N1 ⁱ —Fe1—N1	180.0	C6—C7—H7	119.3
Fe1—O1—H1A	124 (3)	C6—C7—C8	121.5 (2)
Fe1—O1—H1B	131 (2)	C8—C7—H7	119.3
H1A—O1—H1B	105 (3)	C7—C8—C11	120.5 (2)
C1—N1—Fe1	121.88 (15)	C9—C8—C7	118.2 (2)
C1—N1—C3	116.5 (2)	C9—C8—C11	121.4 (2)
C3—N1—Fe1	121.60 (16)	C8—C9—H9	119.3
C2—N2—C4	115.0 (2)	C10—C9—C8	121.4 (2)
N1—C1—H1	119.9	C10—C9—H9	119.3
N1—C1—C2	120.2 (2)	C5—C10—H10	120.2
C2—C1—H1	119.9	C9—C10—C5	119.6 (2)
N2—C2—Cl1	116.93 (19)	C9—C10—H10	120.2
N2—C2—C1	124.4 (2)	C8—C11—H11A	109.5
C1—C2—Cl1	118.71 (18)	C8—C11—H11B	109.5
N1—C3—H3	119.2	C8—C11—H11C	109.5
N1—C3—C4	121.6 (2)	H11A—C11—H11B	109.5
C4—C3—H3	119.2	H11A—C11—H11C	109.5
N2—C4—C3	122.4 (2)	H11B—C11—H11C	109.5
Fe1—N1—C1—C2	180.000 (1)	O2—S1—C5—C10	0.000 (1)
Fe1—N1—C3—C4	180.000 (1)	O3 ^{iv} —S1—C5—C6	−60.51 (6)
N1—C1—C2—Cl1	180.000 (1)	O3—S1—C5—C6	60.51 (6)
N1—C1—C2—N2	0.000 (1)	O3 ^{iv} —S1—C5—C10	119.49 (6)
N1—C3—C4—N2	0.000 (1)	O3—S1—C5—C10	−119.49 (6)
C1—N1—C3—C4	0.000 (1)	C5—C6—C7—C8	0.000 (1)
C2—N2—C4—C3	0.000 (1)	C6—C5—C10—C9	0.000 (1)
C3—N1—C1—C2	0.000 (1)	C6—C7—C8—C9	0.000 (1)
C4—N2—C2—Cl1	180.000 (1)	C6—C7—C8—C11	180.000 (1)
C4—N2—C2—C1	0.000 (1)	C7—C8—C9—C10	0.000 (1)
S1—C5—C6—C7	180.000 (1)	C8—C9—C10—C5	0.000 (1)
S1—C5—C10—C9	180.000 (1)	C10—C5—C6—C7	0.000 (1)
O2—S1—C5—C6	180.000 (1)	C11—C8—C9—C10	180.000 (1)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O2	0.82 (2)	1.91 (2)	2.7238 (19)	171 (4)
O1—H1B \cdots O3 ^v	0.81 (2)	1.95 (2)	2.7624 (19)	177 (3)

Symmetry code: (v) $-x+1, y, -z+2$.