

Crystal structure of diaquabis(4-cyanopyridine- κN)bis(thiocyanato- κN)iron(II) 4-cyanopyridine disolvate

Aleksej Jochim,* Inke Jess and Christian Näther

Institut für Anorganische Chemie, Christian-Albrechts-Universität Kiel, Max-Eyth Strasse 2, D-24118 Kiel, Germany.

*Correspondence e-mail: ajochim@ac.uni-kiel.de

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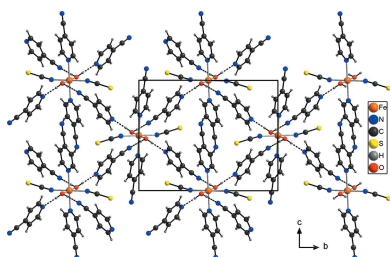
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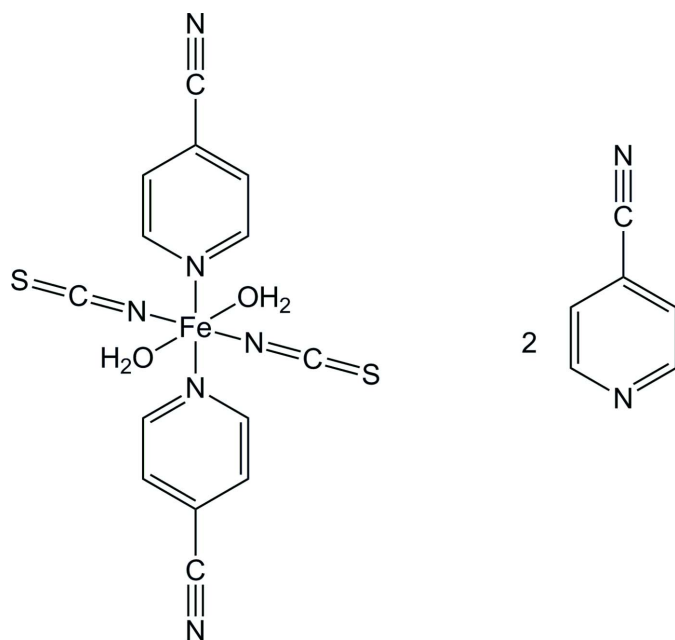
Edited by M. Weil, Vienna University of
Technology, Austria**Keywords:** crystal structure; hydrogen bonding;
4-cyanopyridine; iron; thiocyanate.**CCDC reference:** 1534965**Supporting information:** this article has
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The asymmetric unit of the title compound, $[\text{Fe}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{C}_6\text{H}_4\text{N}_2$, comprises one Fe^{II} cation occupying an inversion centre as well as one thiocyanate anion, one water molecule and two 4-cyanopyridine molecules in general positions. The iron cations are coordinated by two N-bonded thiocyanate anions, two (pyridine)N-bonded 4-cyanopyridine ligands and two water molecules into discrete complexes. The resulting coordination polyhedron can be described as a slightly distorted octahedron. The discrete complexes are connected through centrosymmetric pairs of (pyridine)C—H \cdots N(cyano) hydrogen bonds into chains that are further linked into a three-dimensional network through intermolecular O—H \cdots N hydrogen bonds involving the 4-cyanopyridine solvent molecules.

1. Chemical context

Thiocyanate anions are versatile ligands that can coordinate in different modes to metal cations. In most cases the anionic ligands are terminally N-bonded to the metal cation but there are also several examples for a $\mu_{-1,3}$ bridging mode (Werner *et al.*, 2015; Boeckmann & Näther, 2012; Palion-Gazda *et al.*, 2015). The latter coordination is of special interest if the compounds contain paramagnetic metal cations because then cooperative magnetic properties can be expected (Palion-Gazda *et al.*, 2015). In this context, we have reported on several compounds with one- or two-dimensional structures based on Mn, Fe, Co or Ni as metals, thiocyanate ligands and different N-donor co-ligands that show different magnetic properties (Suckert *et al.*, 2016; Rams *et al.*, 2017; Boeckmann *et al.*, 2012). Whereas compounds with a terminal coordination of the anionic ligands can usually be synthesized straightforwardly, compounds with bridging ligands are sometimes difficult to obtain from solution. Therefore, we have developed an alternative procedure which is based on thermal decomposition of precursors with a terminal NCS coordination that frequently transform into the desired polymeric compounds on heating. In the course of our investigations on the synthesis of coordination polymers with iron as metal, thiocyanate ligands and 4-cyanopyridine as co-ligands, we obtained the title compound which was identified by single crystal X-ray diffraction. Unfortunately, all samples were always contaminated with a second unknown crystalline phase, preventing any further investigations.





2. Structural commentary

The asymmetric unit of $[\text{Fe}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{C}_6\text{H}_4\text{N}_2$ contains one Fe^{II} cation that is located on an inversion centre, one thiocyanate anion, one water molecule and two 4-cyanopyridine molecules (Fig. 1). Discrete centrosymmetric $[\text{Fe}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2]$ complexes are formed, in which the Fe^{II} cations are octahedrally coordinated by two N-bonded thiocyanate anions, two (pyridine)N-bonded 4-cyanopyridine ligands and two water molecules, each of them in a *trans*-position (Fig. 1). The disparate bond lengths are similar to those in related thiocyanate compounds. The

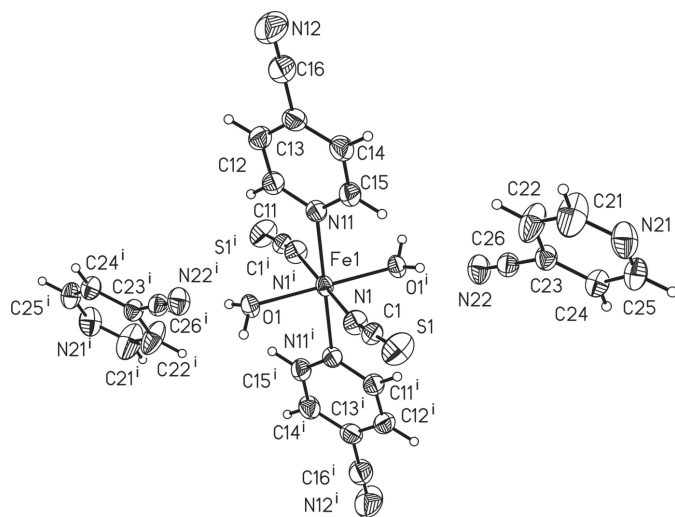


Figure 1
The discrete complex and the solvent molecule of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $1 - x, 1 - y, 2 - z$.]

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{C12}-\text{H12} \cdots \text{N12}^{\text{i}}$	0.95	2.52	3.437 (3)	162
$\text{C14}-\text{H14} \cdots \text{S1}^{\text{iii}}$	0.95	3.01	3.960 (2)	177
$\text{O1}-\text{H1} \cdots \text{N22}^{\text{iii}}$	0.84	2.00	2.8380 (19)	177
$\text{O1}-\text{H2} \cdots \text{N21}^{\text{iv}}$	0.84	1.89	2.7159 (19)	168

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

distortion of the octahedron is also reflected by the deviation of the bond angles from ideal values. The structure contains additional 4-cyanopyridine solvate molecules that are located in the cavities of the structure.

3. Supramolecular features

The discrete complexes are linked into chains parallel to $[101]$ by centrosymmetric pairs of intermolecular $\text{C}-\text{H} \cdots \text{N}$ hydrogen bonds between the cyano group of the coordinating 4-cyanopyridine ligand and one of the pyridine H atoms (Fig. 2, Table 1). These chains are further linked by the 4-cyanopyridine solvate molecules through intermolecular $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonding. One water H atom is hydrogen-bonded to the N atom of the cyano group and the other H atom to the pyridine N atom of another 4-cyanopyridine solvate molecule. Since all water H atoms are involved in hydrogen bonding, each of the complexes is surrounded by four 4-cyanopyridine ligands, of which two are hydrogen-bonded *via* the cyano group, whereas the other two are hydrogen-bonded *via* the pyridine N atom (Fig. 3, Table 1). This arrangement leads to a three-dimensional network structure. It is noted that there are additional short contacts between the thiocyanate anions and the pyridine H atoms of the coordinating 4-cyanopyridine ligand of a neighbouring complex, which is indicative of weak $\text{C}-\text{H} \cdots \text{S}$ hydrogen bonding (Table 1).

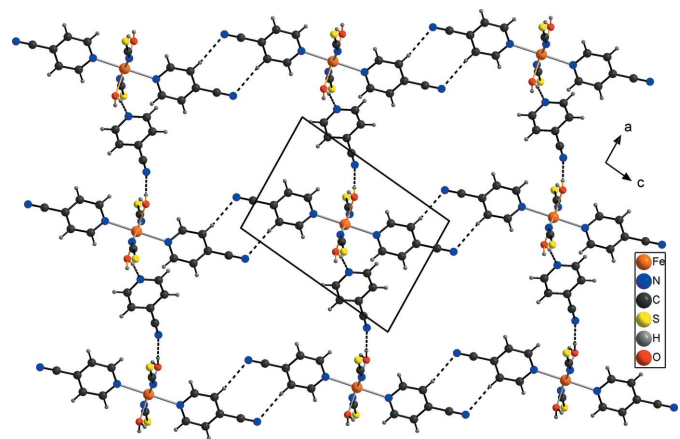


Figure 2
Part of the crystal structure of the title compound in a view along the b axis with emphasis on the connection of discrete complexes and solvent molecules by intermolecular hydrogen bonding (dashed lines).

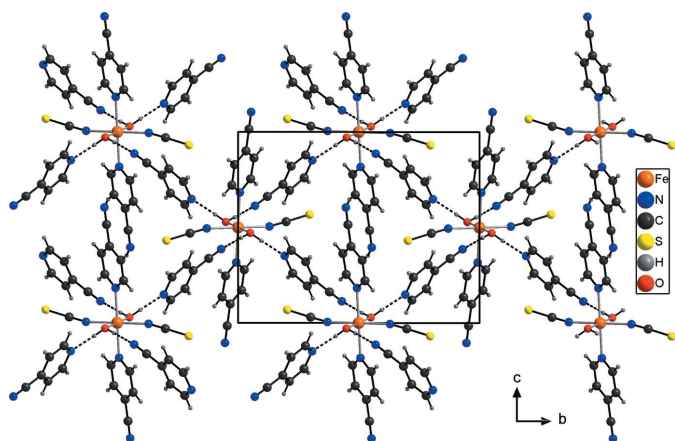


Figure 3
The crystal structure of the title compound in a view along the *a* axis. Intermolecular hydrogen bonding is shown as dashed lines.

4. Database survey

In the Cambridge Structure Database (Version 5.38, last update 2016; Groom *et al.*, 2016), five structures of coordination polymers with 4-cyanopyridine and thiocyanate as ligands are reported, in which the metal cations are solely connected through $\mu_{-1,3}$ bridging thiocyanate anions. Two of these compounds contain copper, two cadmium and one is a bimetallic compound in which copper and mercury are present. The two copper-containing compounds are built up of chains, in which the cations are either tetrahedrally (Lin *et al.*, 2004) or octahedrally (Machura *et al.*, 2013a) coordinated. In the bimetallic compound the cations are linked into a three-dimensional structure (Machura *et al.*, 2013b), whereas the two cadmium-containing compounds exhibit either one-dimensional or three-dimensional coordination networks (Chen *et al.*, 2002).

5. Synthesis and crystallization

Iron(II) chloride tetrahydrate, potassium thiocyanate and 4-cyanopyridine were obtained from Alfa Aesar and used without further purification.

29.8 mg iron(II) chloride tetrahydrate (0.15 mmol) and 29.2 mg KSCN (0.30 mmol) were reacted with 62.5 mg 4-cyanopyridine (0.60 mmol) in 1.5 ml water at room temperature. After two days, single crystals suitable for structure analysis were obtained. The batch contained a small amount of an additional crystalline phase that could not be identified.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms of the water molecule were located from a difference map, and C-bound hydrogen atoms were refined in calculated positions [$C-H = 0.95 \text{ \AA}$ and $O-H = 0.84 \text{ \AA}$] with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ [1.5 for $U_{\text{eq}}(O)$] using a riding model (O–H hydrogen atoms were allowed to rotate but not to tip).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[\text{Fe}(\text{NCS})_2(\text{C}_6\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{C}_6\text{H}_4\text{N}_2$
M_r	624.49
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	200
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.5376 (4), 15.220 (1), 12.1214 (6)
β (°)	96.195 (6)
<i>V</i> (Å ³)	1565.88 (15)
<i>Z</i>	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.66
Crystal size (mm)	0.13 × 0.10 × 0.06
Data collection	
Diffractometer	Stoe IPDS1
Absorption correction	Numerical (<i>X-RED</i> and <i>X-SHAPE</i> ; Stoe & Cie, 2008)
T_{min} , T_{max}	0.884, 0.953
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18486, 3743, 2960
R_{int}	0.047
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.663
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.037, 0.094, 1.03
No. of reflections	3743
No. of parameters	188
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.26, -0.46

Computer programs: *X-AREA* (Stoe & Cie, 2008), *SHELXS97* and *XP* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2014) and *publCIF* (Westrip, 2010).

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Crystal structure of diaquabis(4-cyanopyridine- κ N)bis(thiocyanato- κ N)iron(II) 4-cyanopyridine disolvate

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2008); cell refinement: *X-AREA* (Stoe & Cie, 2008); data reduction: *X-AREA* (Stoe & Cie, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *XP* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2014); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Diaquabis(4-cyanopyridine- κ N)bis(thiocyanato- κ N)iron(II) 4-cyanopyridine disolvate

Crystal data

[Fe(NCS)₂(C₆H₄N₂)₂(H₂O)₂] \cdot 2C₆H₄N₂
 M_r = 624.49
 Monoclinic, $P2_1/c$
 a = 8.5376 (4) Å
 b = 15.220 (1) Å
 c = 12.1214 (6) Å
 β = 96.195 (6)°
 V = 1565.88 (15) Å³
 Z = 2

$F(000)$ = 640
 D_x = 1.324 Mg m⁻³
 Mo $K\alpha$ radiation, λ = 0.71073 Å
 Cell parameters from 18864 reflections
 θ = 3.8–56.3°
 μ = 0.66 mm⁻¹
 T = 200 K
 Block, yellow
 0.13 \times 0.10 \times 0.06 mm

Data collection

Stoe IPDS-1
 diffractometer
 Phi scans
 Absorption correction: numerical
 (*X-RED* and *X-SHAPE*; Stoe & Cie, 2008)
 T_{\min} = 0.884, T_{\max} = 0.953
 18486 measured reflections

3743 independent reflections
 2960 reflections with $I > 2\sigma(I)$
 R_{int} = 0.047
 θ_{max} = 28.1°, θ_{min} = 2.7°
 h = -11 \rightarrow 10
 k = -20 \rightarrow 20
 l = -16 \rightarrow 16

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)]$ = 0.037
 $wR(F^2)$ = 0.094
 S = 1.03
 3743 reflections
 188 parameters
 0 restraints
 Hydrogen site location: mixed
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.1102P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}}$ = 0.001
 $\Delta\rho_{\text{max}}$ = 0.26 e Å⁻³
 $\Delta\rho_{\text{min}}$ = -0.46 e Å⁻³
 Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.019 (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	0.5000	0.5000	1.0000	0.02513 (11)
N1	0.58788 (18)	0.62971 (9)	0.99472 (12)	0.0358 (3)
C1	0.62673 (19)	0.69914 (10)	0.96961 (13)	0.0305 (3)
S1	0.68128 (7)	0.79604 (3)	0.93149 (5)	0.05165 (16)
N11	0.42359 (17)	0.50738 (9)	0.81712 (11)	0.0317 (3)
C11	0.2830 (2)	0.47429 (11)	0.77885 (14)	0.0351 (4)
H11	0.2267	0.4414	0.8283	0.042*
C12	0.2158 (2)	0.48550 (11)	0.67119 (15)	0.0390 (4)
H12	0.1150	0.4617	0.6472	0.047*
C13	0.2990 (2)	0.53234 (13)	0.59914 (14)	0.0399 (4)
C14	0.4458 (2)	0.56588 (13)	0.63609 (15)	0.0425 (4)
H14	0.5055	0.5976	0.5877	0.051*
C15	0.5029 (2)	0.55172 (12)	0.74578 (14)	0.0381 (4)
H15	0.6036	0.5747	0.7718	0.046*
C16	0.2332 (3)	0.54478 (18)	0.48511 (18)	0.0570 (6)
N12	0.1795 (3)	0.5537 (2)	0.39540 (17)	0.0837 (8)
O1	0.28045 (13)	0.55033 (7)	1.02877 (9)	0.0320 (2)
H1	0.2201	0.5134	1.0535	0.048*
H2	0.2728	0.5951	1.0684	0.048*
N21	1.2086 (2)	0.80713 (12)	0.64837 (15)	0.0523 (4)
C21	1.0626 (3)	0.7796 (2)	0.6202 (2)	0.0774 (9)
H21	1.0072	0.8031	0.5546	0.093*
C22	0.9863 (3)	0.71950 (19)	0.67912 (19)	0.0685 (8)
H22	0.8813	0.7018	0.6554	0.082*
C23	1.0672 (2)	0.68573 (11)	0.77413 (14)	0.0347 (4)
C24	1.2197 (2)	0.71283 (11)	0.80597 (15)	0.0378 (4)
H24	1.2775	0.6904	0.8713	0.045*
C25	1.2856 (2)	0.77362 (13)	0.73992 (17)	0.0445 (4)
H25	1.3907	0.7923	0.7609	0.053*
C26	0.9913 (2)	0.62137 (12)	0.83758 (14)	0.0361 (4)
N22	0.9307 (2)	0.56987 (11)	0.88643 (14)	0.0460 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.02351 (17)	0.02120 (16)	0.03167 (17)	-0.00047 (11)	0.00745 (11)	0.00057 (11)
N1	0.0402 (9)	0.0231 (6)	0.0448 (8)	-0.0057 (5)	0.0075 (6)	0.0016 (5)
C1	0.0277 (8)	0.0303 (8)	0.0329 (8)	-0.0006 (6)	0.0004 (6)	-0.0007 (6)
S1	0.0599 (3)	0.0304 (2)	0.0628 (3)	-0.0137 (2)	-0.0017 (2)	0.0132 (2)

N11	0.0305 (7)	0.0324 (7)	0.0328 (7)	0.0002 (5)	0.0053 (5)	-0.0015 (5)
C11	0.0343 (9)	0.0308 (8)	0.0408 (9)	-0.0028 (6)	0.0061 (7)	-0.0035 (6)
C12	0.0341 (9)	0.0375 (9)	0.0446 (9)	0.0010 (7)	0.0001 (7)	-0.0080 (7)
C13	0.0397 (10)	0.0458 (10)	0.0338 (8)	0.0094 (8)	0.0022 (7)	-0.0055 (7)
C14	0.0393 (10)	0.0550 (11)	0.0342 (8)	0.0011 (8)	0.0086 (7)	0.0046 (8)
C15	0.0325 (9)	0.0472 (10)	0.0353 (8)	-0.0032 (7)	0.0071 (7)	0.0014 (7)
C16	0.0451 (12)	0.0819 (16)	0.0433 (11)	0.0035 (11)	0.0015 (9)	-0.0003 (10)
N12	0.0618 (14)	0.140 (2)	0.0460 (11)	-0.0095 (14)	-0.0079 (9)	0.0126 (13)
O1	0.0272 (6)	0.0284 (5)	0.0422 (6)	-0.0004 (4)	0.0117 (5)	-0.0031 (4)
N21	0.0464 (10)	0.0518 (10)	0.0607 (10)	-0.0051 (8)	0.0144 (8)	0.0215 (8)
C21	0.0541 (15)	0.111 (2)	0.0643 (15)	-0.0162 (14)	-0.0084 (11)	0.0537 (15)
C22	0.0417 (12)	0.105 (2)	0.0554 (13)	-0.0231 (12)	-0.0112 (10)	0.0401 (13)
C23	0.0313 (9)	0.0379 (9)	0.0351 (8)	-0.0039 (7)	0.0048 (6)	0.0051 (6)
C24	0.0338 (10)	0.0367 (9)	0.0421 (9)	-0.0014 (7)	0.0005 (7)	0.0066 (7)
C25	0.0341 (10)	0.0406 (10)	0.0593 (11)	-0.0058 (7)	0.0068 (8)	0.0074 (8)
C26	0.0315 (9)	0.0419 (9)	0.0351 (8)	-0.0026 (7)	0.0039 (6)	0.0020 (7)
N22	0.0397 (9)	0.0490 (9)	0.0508 (9)	-0.0068 (7)	0.0122 (7)	0.0104 (7)

Geometric parameters (Å, °)

Fe1—O1 ⁱ	2.0888 (11)	C14—H14	0.9500
Fe1—O1	2.0888 (11)	C15—H15	0.9500
Fe1—N1	2.1153 (13)	C16—N12	1.141 (3)
Fe1—N1 ⁱ	2.1153 (13)	O1—H1	0.8400
Fe1—N11 ⁱ	2.2451 (14)	O1—H2	0.8400
Fe1—N11	2.2451 (14)	N21—C21	1.325 (3)
N1—C1	1.158 (2)	N21—C25	1.329 (3)
C1—S1	1.6286 (16)	C21—C22	1.368 (3)
N11—C15	1.337 (2)	C21—H21	0.9500
N11—C11	1.338 (2)	C22—C23	1.377 (3)
C11—C12	1.378 (3)	C22—H22	0.9500
C11—H11	0.9500	C23—C24	1.380 (3)
C12—C13	1.382 (3)	C23—C26	1.442 (2)
C12—H12	0.9500	C24—C25	1.382 (3)
C13—C14	1.382 (3)	C24—H24	0.9500
C13—C16	1.447 (3)	C25—H25	0.9500
C14—C15	1.383 (3)	C26—N22	1.140 (2)
O1 ⁱ —Fe1—O1	180.0	C14—C13—C16	120.42 (19)
O1 ⁱ —Fe1—N1	90.55 (5)	C13—C14—C15	117.86 (17)
O1—Fe1—N1	89.45 (5)	C13—C14—H14	121.1
O1 ⁱ —Fe1—N1 ⁱ	89.45 (5)	C15—C14—H14	121.1
O1—Fe1—N1 ⁱ	90.55 (5)	N11—C15—C14	123.35 (17)
N1—Fe1—N1 ⁱ	180.0	N11—C15—H15	118.3
O1 ⁱ —Fe1—N11 ⁱ	88.63 (5)	C14—C15—H15	118.3
O1—Fe1—N11 ⁱ	91.37 (5)	N12—C16—C13	179.0 (3)
N1—Fe1—N11 ⁱ	90.59 (5)	Fe1—O1—H1	114.2
N1 ⁱ —Fe1—N11 ⁱ	89.41 (5)	Fe1—O1—H2	121.3

O1 ⁱ —Fe1—N11	91.37 (5)	H1—O1—H2	104.5
O1—Fe1—N11	88.63 (5)	C21—N21—C25	117.42 (17)
N1—Fe1—N11	89.41 (5)	N21—C21—C22	124.4 (2)
N1 ⁱ —Fe1—N11	90.59 (5)	N21—C21—H21	117.8
N11 ⁱ —Fe1—N11	180.0	C22—C21—H21	117.8
C1—N1—Fe1	166.44 (14)	C21—C22—C23	117.5 (2)
N1—C1—S1	178.74 (15)	C21—C22—H22	121.2
C15—N11—C11	117.64 (15)	C23—C22—H22	121.2
C15—N11—Fe1	123.39 (12)	C22—C23—C24	119.69 (17)
C11—N11—Fe1	118.54 (11)	C22—C23—C26	119.08 (17)
N11—C11—C12	123.23 (17)	C24—C23—C26	121.22 (15)
N11—C11—H11	118.4	C23—C24—C25	117.94 (17)
C12—C11—H11	118.4	C23—C24—H24	121.0
C11—C12—C13	118.18 (17)	C25—C24—H24	121.0
C11—C12—H12	120.9	N21—C25—C24	123.03 (18)
C13—C12—H12	120.9	N21—C25—H25	118.5
C12—C13—C14	119.72 (17)	C24—C25—H25	118.5
C12—C13—C16	119.85 (19)	N22—C26—C23	179.1 (2)

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

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

<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>
C12—H12 \cdots N12 ⁱⁱ	0.95	2.52	3.437 (3)	162
C14—H14 \cdots S1 ⁱⁱⁱ	0.95	3.01	3.960 (2)	177
O1—H1 \cdots N22 ⁱ	0.84	2.00	2.8380 (19)	177
O1—H2 \cdots N21 ^{iv}	0.84	1.89	2.7159 (19)	168

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