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Pyridinium bis(pyridine-κN)tetrakis(thiocyanato-κN)ferrate(III)

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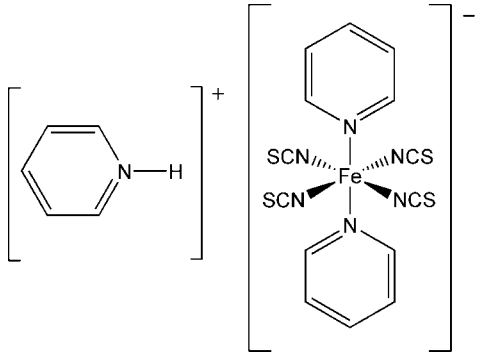
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.035; wR factor = 0.065; data-to-parameter ratio = 16.9.

In the title compound, $(C_5H_6N)[Fe(NCS)_4(C_5H_5N)_2]$, the Fe^{III} ion is coordinated by four thiocyanate N atoms and two pyridine N atoms in a *trans* arrangement, forming an FeN_6 polyhedron with a slightly distorted octahedral geometry. Charge balance is achieved by one pyridinium cation bound to the complex anion *via* N—H···S hydrogen bonding. The asymmetric unit consists of one Fe^{III} cation, four thiocyanate anions, two coordinated pyridine molecules and one pyridinium cation. The structure exhibits π–π interactions between pyridine rings [centroid–centroid distances = 3.7267 (2), 3.7811 (2) and 3.8924 (2) Å]. The N atom and a neighboring C atom of the pyridinium cation are statistically disordered with an occupancy ratio of 0.58 (2):0.42 (2).

Related literature

For the use of materials with molecular assemblies comprising cationic and anionic modules, see: Fritsky *et al.* (1998, 2004); Strotmeyer *et al.* (2003); Kanderal *et al.* (2005). For Fe^{II}–thiocyanate complexes with aromatic *N*-donor ligands indicating spin crossover, see: Gamez *et al.* (2009). For related structures, see: Petrusenko *et al.* (1997); Moroz *et al.* (2010); Penkova *et al.* (2010); Shylin *et al.* (2013).



Experimental

Crystal data

$(C_5H_6N)[Fe(NCS)_4(C_5H_5N)_2]$
M_r = 526.48
Monoclinic, $P2_1/n$
a = 10.7650 (7) Å
b = 14.0424 (8) Å
c = 15.7266 (9) Å
β = 103.244 (3)°
V = 2314.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 120 K
0.21 × 0.14 × 0.07 mm

Data collection

Bruker Kappa APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.814, T_{max} = 0.929
17377 measured reflections
4739 independent reflections
3027 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.065
S = 0.92
4739 reflections
281 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected bond lengths (Å).

Fe1—N1	2.1591 (18)	Fe1—N4	2.026 (2)
Fe1—N2	2.1727 (19)	Fe1—N5	2.049 (2)
Fe1—N3	2.012 (2)	Fe1—N6	2.034 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7A···S3^{i}	0.88	2.82	3.532 (2)	139
N7—H7A···S2	0.88	2.86	3.462 (2)	127
N7A—H7AA···S4^{ii}	0.88	2.81	3.558 (2)	144
N7A—H7AA···S2	0.88	2.94	3.504 (2)	124

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5698).

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supporting information

Acta Cryst. (2013). E**69**, m298–m299 [doi:10.1107/S1600536813011628]

Pyridinium bis(pyridine-*κN*)tetrakis(thiocyanato-*κN*)ferrate(III)

Sergii I. Shylin, Il'ya A. Gural'skiy, Matti Haukka, Anatoliy A. Kapshuk and Elena V. Prisyazhnaya

S1. Comment

Molecular assemblies consisting of cationic and anionic modules are of great interest for crystal engineering and molecular magnetism (Strotmeyer *et al.*, 2003; Fritsky *et al.*, 2004). Target properties of such compounds can be tuned by different types of intermolecular interactions, such as coordination and hydrogen bonds, π–π and lone pair – π contacts, *etc*. (Fritsky *et al.*, 1998; Kanderal *et al.*, 2005). In certain cases, even the existence of spin crossover in these complexes can be observed. Therefore, Fe^{II} isothiocyanate complexes with aromatic N-donor ligands attract much attention considering the possible metal ion spin state modulation by variation of a ligand (Gamez *et al.*, 2009). Herein, we attempted to synthesize Fe^{II} thiocyanate complex with 1,5-naphthyridine, however, the reaction of it and $[Fe^{II}(NCS)_2(py)_4]$ (py = pyridine) in $CHCl_3$ in air led to the oxidation of Fe^{II} and to the formation of the title compound.

The compound consists of complex anion $[Fe(NCS)_4(py)_2]^-$ and pyridinium cation the N7 atom of which is disordered over two alternative sites with the occupancy ratio of 0.58 (2): 0.42 (2). The Fe^{III} ion is sixfold coordinated by four N atoms of thiocyanate anions forming the equatorial plane and two N atoms of two pyridine ligands occupying axial positions (Fig. 1). The distances between Fe^{III} ion and N atoms of the thiocyanate anions are shorter than those between Fe^{III} and N atoms of the pyridine ligands (Table 1), hence FeN_6 octahedron is slightly distorted. A similar distortion of the coordination polyhedron was reported for the related compound $(Hpy)[Fe(NCS)_4(py)_2].4(cnpz).(py)$, where cnpz = pyrazine-2-carbonitrile (Shylin *et al.*, 2013). The thiocyanate ligands are only bound through N atoms and are quasi-linear, while the Fe–NCS linkages are bent [Fe1—N3—C11 = 162.43 (19)°, Fe1—N4—C12 = 161.67 (19)°, Fe1—N5—C13 = 165.7 (2)°, Fe1—N6—C14 = 158.7 (2)°]. These structural features are typical for the complexes where the NCS group is N-bound (Petrusenko *et al.*, 1997). The C—N and C—C bond lengths in the coordinated pyridine ligands are normal and close to the values observed in the related structures (Moroz *et al.*, 2010; Penkova *et al.*, 2010).

In the title compound pyridine ligands and pyridinium cations interact with one another *via* π–π stacking, with distances between the centroids of 3.7267 (2), 3.7811 (2) and 3.8924 (2) Å (Fig. 2). Pyridinium cations are also bound to the anionic complex through a number of N—H···S hydrogen bonds (Table 2).

S2. Experimental

Crystals of the title compound were obtained by adding 1,5-naphthyridine (26 mg, 0.2 mmol) to tetrakis(pyridine)bis(iso-thiocyanato)iron(II) $[Fe(NCS)_2(py)_4]$ (48.8 mg, 0.1 mmol) in $CHCl_3$ (5 ml). The solution was left to evaporate in air. In one day this yielded red crystals that were collected, washed with water and dried in air. Yield is 16 mg (30% relative to Fe).

S3. Refinement

The N atom of the pyridinium cation was disordered over two alternative sites with the occupancy ratio of 0.58/0.42. Hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.95 and N—

H = 0.88 Å, and U_{iso} = 1.2 U_{eq}(C, N).

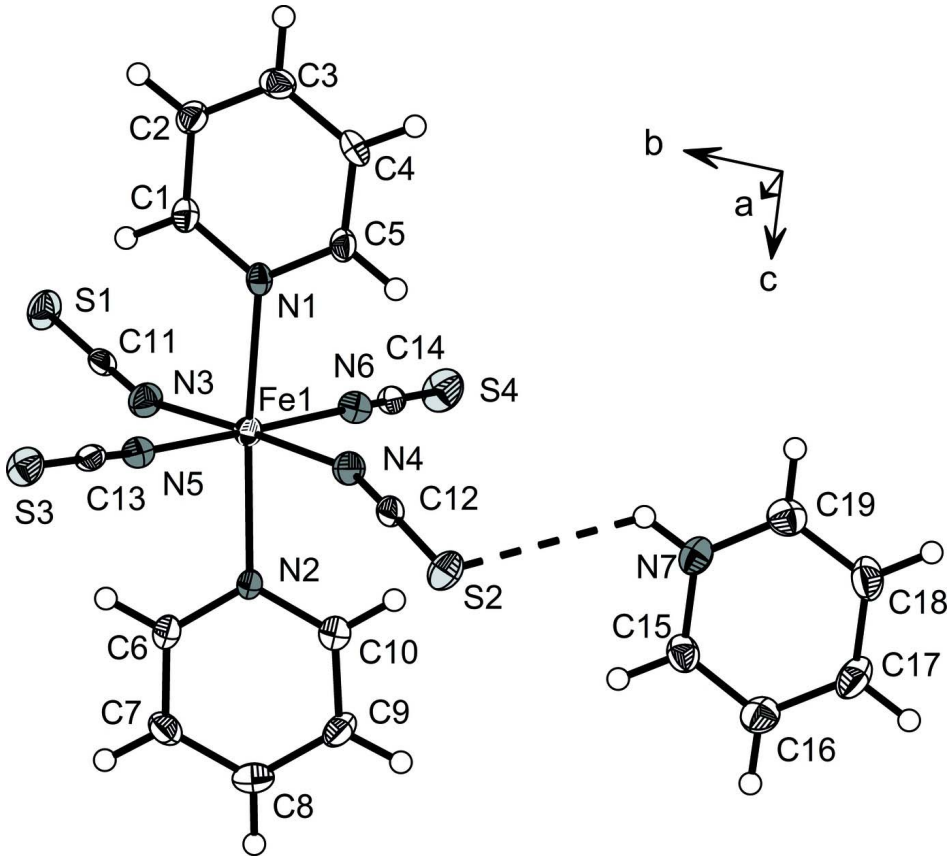

Figure 1

Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level.

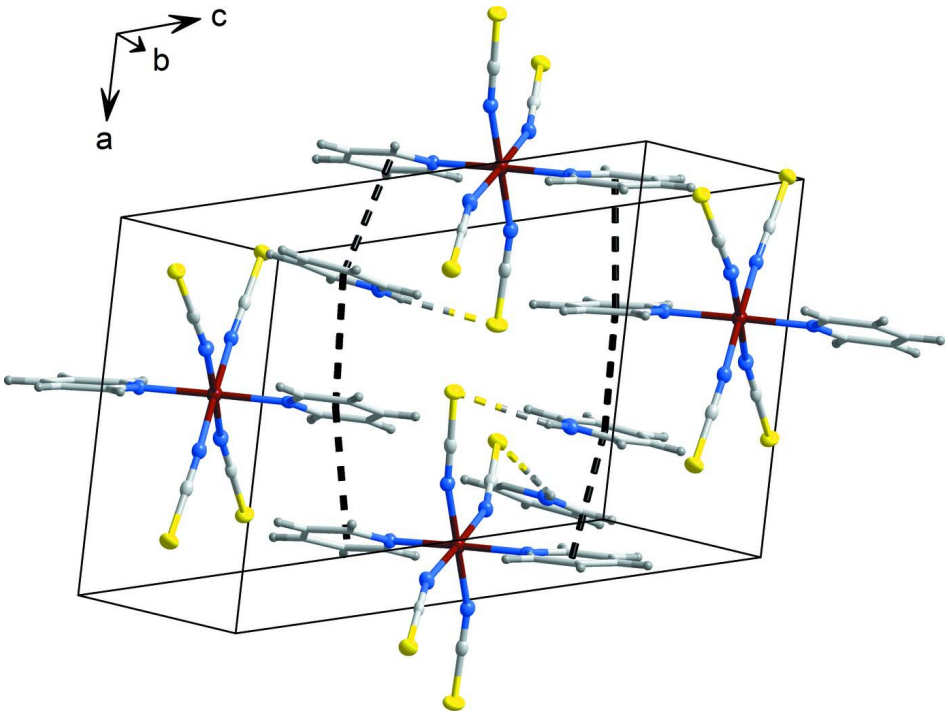

Figure 2

Crystal structure of the title compound showing hydrogen bonds and π–π contacts as dashed lines (carmine = Fe, yellow = S, blue = N, light-grey = C, grey = H).

Pyridinium bis(pyridine-κN)tetrakis(thiocyanato-κN)ferrate(III)

Crystal data

$(C_5H_6N)[Fe(NCS)_4(C_5H_5N)_2]$
M_r = 526.48
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.7650 (7) Å
b = 14.0424 (8) Å
c = 15.7266 (9) Å
β = 103.244 (3)°
V = 2314.1 (2) Å^3
Z = 4
$F(000)$ = 1076
D_x = 1.511 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3249 reflections
θ = 2.5–26.9°
μ = 1.03 mm^{-1}
T = 120 K
Block, red
0.21 × 0.14 × 0.07 mm

Data collection

Bruker Kappa APEXII DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Curved graphite crystal monochromator
Detector resolution: 16 pixels mm^{-1}
φ scans and ω scans with κ offset
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.814, T_{max} = 0.929
17377 measured reflections
4739 independent reflections
3027 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 26.4°, θ_{min} = 2.0°
$h = -13 \rightarrow 13$
$k = -17 \rightarrow 17$
$l = -19 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.065$
$S = 0.92$
4739 reflections
281 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.024P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.02757 (4)	0.74386 (2)	0.35673 (2)	0.01575 (10)	
S1	−0.26742 (7)	0.99542 (5)	0.35060 (4)	0.02555 (18)	
S2	0.33249 (7)	0.49516 (5)	0.37979 (4)	0.02563 (18)	
S3	0.41585 (7)	0.90657 (5)	0.34609 (4)	0.02646 (18)	
S4	−0.37170 (7)	0.61072 (5)	0.37071 (5)	0.03125 (19)	
N1	−0.02004 (18)	0.75765 (14)	0.21626 (11)	0.0158 (5)	
N2	0.0714 (2)	0.71819 (13)	0.49668 (12)	0.0160 (5)	
N3	−0.0733 (2)	0.86076 (15)	0.37176 (13)	0.0227 (5)	
N4	0.1344 (2)	0.62743 (14)	0.34665 (13)	0.0212 (5)	
N5	0.1848 (2)	0.82818 (14)	0.36327 (12)	0.0204 (5)	
N6	−0.1316 (2)	0.66311 (14)	0.34861 (13)	0.0224 (5)	
N7	0.2005 (2)	0.26981 (16)	0.34397 (14)	0.0236 (7)	0.58 (2)
H7A	0.1943	0.3257	0.3180	0.028*	0.58 (2)
N7A	0.2499 (2)	0.26424 (16)	0.43092 (15)	0.0236 (7)	0.42 (2)
H7AA	0.2757	0.3165	0.4606	0.028*	0.42 (2)
C12	0.2170 (3)	0.57121 (17)	0.36058 (15)	0.0181 (6)	
C14	−0.2322 (3)	0.64138 (17)	0.35776 (15)	0.0185 (6)	
C11	−0.1543 (3)	0.91796 (17)	0.36277 (14)	0.0171 (6)	
C13	0.2810 (3)	0.86161 (17)	0.35567 (15)	0.0183 (6)	
C5	−0.0212 (2)	0.68043 (17)	0.16522 (15)	0.0185 (6)	
H5	0.0013	0.6204	0.1923	0.022*	
C1	−0.0523 (2)	0.84165 (17)	0.17635 (15)	0.0192 (6)	
H1	−0.0526	0.8967	0.2114	0.023*	
C15	0.2499 (2)	0.26424 (16)	0.43092 (15)	0.0236 (7)	0.58 (2)
H15	0.2777	0.3207	0.4630	0.028*	0.58 (2)

C15A	0.2005 (2)	0.26981 (16)	0.34397 (14)	0.0236 (7)	0.42 (2)
H15A	0.1938	0.3301	0.3159	0.028*	0.42 (2)
C6	0.1024 (2)	0.78922 (17)	0.55371 (15)	0.0187 (6)	
H6	0.1088	0.8517	0.5320	0.022*	
C10	0.0651 (3)	0.63017 (18)	0.52842 (16)	0.0220 (6)	
H10	0.0438	0.5788	0.4884	0.026*	
C4	−0.0536 (2)	0.68502 (18)	0.07530 (15)	0.0207 (6)	
H4	−0.0546	0.6290	0.0413	0.025*	
C3	−0.0846 (2)	0.77183 (18)	0.03525 (16)	0.0232 (6)	
H3	−0.1053	0.7768	−0.0266	0.028*	
C8	0.1183 (3)	0.68517 (18)	0.67526 (16)	0.0246 (6)	
H8	0.1336	0.6740	0.7364	0.030*	
C7	0.1258 (3)	0.77584 (17)	0.64337 (15)	0.0227 (6)	
H7	0.1466	0.8283	0.6821	0.027*	
C2	−0.0849 (2)	0.85126 (18)	0.08662 (15)	0.0208 (6)	
H2	−0.1073	0.9118	0.0607	0.025*	
C16	0.2603 (3)	0.18020 (18)	0.47284 (17)	0.0272 (7)	
H16	0.2947	0.1771	0.5341	0.033*	
C19	0.1606 (3)	0.19118 (18)	0.29654 (17)	0.0268 (7)	
H19	0.1259	0.1959	0.2355	0.032*	
C9	0.0882 (3)	0.61079 (18)	0.61679 (16)	0.0245 (7)	
H9	0.0834	0.5474	0.6369	0.029*	
C17	0.2203 (3)	0.09859 (19)	0.42586 (17)	0.0303 (7)	
H17	0.2271	0.0387	0.4546	0.036*	
C18	0.1707 (3)	0.10391 (18)	0.33741 (17)	0.0301 (7)	
H18	0.1436	0.0478	0.3047	0.036*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01694 (19)	0.01441 (19)	0.01572 (17)	0.00150 (16)	0.00334 (13)	−0.00003 (15)
S1	0.0250 (4)	0.0179 (4)	0.0332 (4)	0.0067 (3)	0.0055 (3)	0.0014 (3)
S2	0.0244 (4)	0.0204 (4)	0.0326 (4)	0.0075 (3)	0.0075 (3)	0.0044 (3)
S3	0.0224 (4)	0.0271 (4)	0.0307 (4)	−0.0042 (3)	0.0077 (3)	0.0048 (3)
S4	0.0240 (4)	0.0326 (4)	0.0386 (4)	−0.0042 (3)	0.0104 (3)	0.0080 (3)
N1	0.0135 (12)	0.0135 (11)	0.0204 (11)	−0.0022 (9)	0.0042 (8)	−0.0012 (9)
N2	0.0197 (13)	0.0120 (11)	0.0163 (10)	−0.0010 (9)	0.0039 (9)	0.0003 (9)
N3	0.0276 (14)	0.0194 (12)	0.0216 (12)	0.0044 (11)	0.0071 (10)	0.0003 (10)
N6	0.0251 (15)	0.0219 (12)	0.0192 (12)	−0.0014 (11)	0.0030 (10)	0.0001 (10)
N5	0.0216 (14)	0.0203 (12)	0.0187 (11)	−0.0004 (10)	0.0033 (9)	0.0013 (9)
N4	0.0239 (14)	0.0186 (12)	0.0209 (12)	0.0031 (11)	0.0048 (10)	−0.0014 (10)
C12	0.0216 (16)	0.0162 (14)	0.0165 (13)	−0.0051 (12)	0.0044 (11)	−0.0002 (11)
C14	0.0257 (18)	0.0139 (14)	0.0145 (13)	0.0025 (12)	0.0014 (12)	−0.0010 (11)
C11	0.0233 (16)	0.0172 (14)	0.0105 (12)	−0.0051 (12)	0.0033 (11)	−0.0020 (10)
C13	0.0258 (17)	0.0151 (13)	0.0133 (13)	0.0056 (13)	0.0026 (11)	0.0011 (11)
C5	0.0186 (15)	0.0141 (13)	0.0223 (14)	−0.0044 (12)	0.0037 (11)	−0.0004 (11)
C1	0.0206 (16)	0.0148 (14)	0.0223 (14)	−0.0033 (12)	0.0055 (11)	−0.0003 (11)
C15	0.0283 (16)	0.0215 (15)	0.0229 (14)	−0.0032 (12)	0.0100 (11)	−0.0042 (11)

N7	0.0261 (15)	0.0195 (14)	0.0273 (15)	0.0031 (11)	0.0102 (11)	0.0026 (11)
N7A	0.0283 (16)	0.0215 (15)	0.0229 (14)	−0.0032 (12)	0.0100 (11)	−0.0042 (11)
C15A	0.0261 (15)	0.0195 (14)	0.0273 (15)	0.0031 (11)	0.0102 (11)	0.0026 (11)
C6	0.0186 (15)	0.0144 (13)	0.0233 (14)	−0.0005 (11)	0.0051 (11)	0.0013 (11)
C10	0.0243 (16)	0.0194 (14)	0.0220 (14)	−0.0008 (12)	0.0047 (12)	0.0002 (12)
C4	0.0211 (16)	0.0198 (15)	0.0209 (14)	−0.0049 (12)	0.0041 (11)	−0.0082 (12)
C3	0.0217 (16)	0.0288 (16)	0.0177 (13)	−0.0087 (12)	0.0014 (11)	0.0024 (12)
C8	0.0242 (17)	0.0326 (16)	0.0171 (13)	0.0022 (13)	0.0047 (12)	0.0040 (13)
C7	0.0249 (16)	0.0229 (15)	0.0189 (14)	−0.0007 (12)	0.0023 (12)	−0.0060 (12)
C2	0.0207 (16)	0.0189 (14)	0.0223 (14)	−0.0019 (12)	0.0036 (12)	0.0037 (12)
C16	0.0354 (19)	0.0279 (16)	0.0213 (14)	0.0020 (14)	0.0125 (13)	0.0014 (13)
C19	0.0294 (18)	0.0295 (16)	0.0231 (14)	0.0027 (14)	0.0094 (12)	−0.0024 (13)
C9	0.0303 (17)	0.0186 (15)	0.0248 (15)	0.0010 (13)	0.0065 (12)	0.0079 (12)
C17	0.044 (2)	0.0209 (16)	0.0305 (16)	0.0029 (14)	0.0187 (14)	0.0070 (13)
C18	0.041 (2)	0.0208 (16)	0.0314 (16)	−0.0046 (14)	0.0131 (14)	−0.0068 (13)

Geometric parameters (Å, º)

Fe1—N1	2.1591 (18)	C15—H15	0.9500
Fe1—N2	2.1727 (19)	N7—C19	1.346 (3)
Fe1—N3	2.012 (2)	N7—H7A	0.8800
Fe1—N4	2.026 (2)	C6—C7	1.387 (3)
Fe1—N5	2.049 (2)	C6—H6	0.9500
Fe1—N6	2.034 (2)	C10—C9	1.382 (3)
S1—C11	1.611 (3)	C10—H10	0.9500
S2—C12	1.614 (3)	C4—C3	1.377 (3)
S3—C13	1.621 (3)	C4—H4	0.9500
S4—C14	1.620 (3)	C3—C2	1.378 (3)
N1—C1	1.344 (3)	C3—H3	0.9500
N1—C5	1.347 (3)	C8—C7	1.378 (3)
N2—C6	1.332 (3)	C8—C9	1.380 (3)
N2—C10	1.341 (3)	C8—H8	0.9500
N3—C11	1.170 (3)	C7—H7	0.9500
N6—C14	1.165 (3)	C2—H2	0.9500
N5—C13	1.168 (3)	C16—C17	1.378 (3)
N4—C12	1.172 (3)	C16—H16	0.9500
C5—C4	1.378 (3)	C19—C18	1.377 (3)
C5—H5	0.9500	C19—H19	0.9500
C1—C2	1.380 (3)	C9—H9	0.9500
C1—H1	0.9500	C17—C18	1.373 (4)
C15—C16	1.344 (3)	C17—H17	0.9500
C15—N7	1.351 (3)	C18—H18	0.9500
N3—Fe1—N4	177.50 (9)	C19—N7—H7A	119.5
N3—Fe1—N6	89.58 (9)	C15—N7—H7A	119.5
N4—Fe1—N6	91.74 (9)	N2—C6—C7	122.8 (2)
N3—Fe1—N5	89.11 (9)	N2—C6—H6	118.6
N4—Fe1—N5	89.60 (9)	C7—C6—H6	118.6

N6—Fe1—N5	178.43 (9)	N2—C10—C9	122.9 (2)
N3—Fe1—N1	92.24 (8)	N2—C10—H10	118.5
N4—Fe1—N1	89.90 (8)	C9—C10—H10	118.5
N6—Fe1—N1	89.24 (8)	C3—C4—C5	119.2 (2)
N5—Fe1—N1	89.96 (8)	C3—C4—H4	120.4
N3—Fe1—N2	90.81 (8)	C5—C4—H4	120.4
N4—Fe1—N2	87.13 (8)	C4—C3—C2	118.8 (2)
N6—Fe1—N2	87.45 (8)	C4—C3—H3	120.6
N5—Fe1—N2	93.43 (8)	C2—C3—H3	120.6
N1—Fe1—N2	175.48 (7)	C7—C8—C9	118.8 (2)
C1—N1—C5	117.51 (19)	C7—C8—H8	120.6
C1—N1—Fe1	122.14 (16)	C9—C8—H8	120.6
C5—N1—Fe1	120.33 (15)	C8—C7—C6	118.9 (2)
C6—N2—C10	117.8 (2)	C8—C7—H7	120.6
C6—N2—Fe1	121.38 (15)	C6—C7—H7	120.6
C10—N2—Fe1	120.83 (15)	C3—C2—C1	119.1 (2)
C11—N3—Fe1	162.43 (19)	C3—C2—H2	120.5
C14—N6—Fe1	158.7 (2)	C1—C2—H2	120.5
C13—N5—Fe1	165.7 (2)	C15—C16—C17	119.1 (2)
C12—N4—Fe1	161.67 (19)	C15—C16—H16	120.4
N4—C12—S2	179.0 (2)	C17—C16—H16	120.4
N6—C14—S4	179.7 (3)	N7—C19—C18	119.4 (2)
N3—C11—S1	179.1 (2)	N7—C19—H19	120.3
N5—C13—S3	179.0 (2)	C18—C19—H19	120.3
N1—C5—C4	122.6 (2)	C8—C9—C10	118.8 (2)
N1—C5—H5	118.7	C8—C9—H9	120.6
C4—C5—H5	118.7	C10—C9—H9	120.6
N1—C1—C2	122.8 (2)	C18—C17—C16	119.9 (2)
N1—C1—H1	118.6	C18—C17—H17	120.0
C2—C1—H1	118.6	C16—C17—H17	120.0
C16—C15—N7	121.1 (2)	C17—C18—C19	119.5 (2)
C16—C15—H15	119.4	C17—C18—H18	120.3
N7—C15—H15	119.4	C19—C18—H18	120.3
C19—N7—C15	121.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7*A*···S3^{i}	0.88	2.82	3.532 (2)	139
N7—H7*A*···S2	0.88	2.86	3.462 (2)	127
N7*A*—H7*AA*···S4^{ii}	0.88	2.81	3.558 (2)	144
N7*A*—H7*AA*···S2	0.88	2.94	3.504 (2)	124

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