Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis(ethanol-*κO*)bis(pyridine-3-carbaldehyde-*κN* thiosemicarbazone)bis(thiocyanato-*κN*)iron(II)–pyridine-3-carbaldehyde thiosemicarbazone (1/2)

Shao-Mei Wang

College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang, Henan 455000, People's Republic of China
Correspondence e-mail: wang_shaomei@yahoo.cn

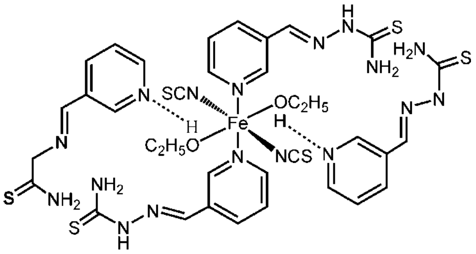
Received 5 June 2009; accepted 23 June 2009

Key indicators: single-crystal X-ray study; *T* = 173 K; mean σ(C–C) = 0.005 Å; *R* factor = 0.042; *wR* factor = 0.134; data-to-parameter ratio = 14.3.

The crystal structure of the title Fe^{II} complex, $[Fe(NCS)_2(C_7H_8N_4S)_2(CH_3CH_2OH)_2]\cdot 2C_7H_8N_4S$, based on the Schiff base ligand pyridine-3-carbaldehyde thiosemicarbazone (pct), results from the cocrystallization of an Fe^{II} coordination compound together with two of the pct ligands. The complex unit is mononuclear, with the central Fe^{II} ion located on a crystallographic centre of inversion and coordinated by four N atoms from two pct ligands and two thiocyanate anions. The slightly distorted octahedral coordination is completed by two O atoms from ethanol molecules. The crystal packing is accomplished intermolecular N—H···S hydrogen bonds.

Related literature

For the structures of metal complexes of Schiff base ligands synthesized by condensation of pyridine-3-carbaldehyde and amino compounds, see: Brook *et al.* (2000); Deng *et al.* (2007); Garbelini *et al.* (2008); Kowol *et al.* (2007); Zhong *et al.* (2007). For the corresponding Mn(II) complex of pyridine-3-carbaldehyde thiosemicarbazone, see: Li *et al.* (2006).



Experimental

Crystal data

$[Fe(NCS)_2(C_7H_8N_4S)_2(C_2H_6O)_2]\cdot 2C_7H_8N_4S$
M_r = 985.08
Triclinic, $P\overline{1}$
a = 8.916 (4) Å
b = 9.556 (5) Å
c = 14.538 (7) Å
α = 87.341 (8)°
β = 88.191 (8)°
γ = 69.604 (8)°
V = 1160 (1) Å^3
Z = 1
Mo *Kα* radiation
μ = 0.65 mm^{-1}
T = 173 K
0.32 × 0.26 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.819, T_{max} = 0.871
8300 measured reflections
4037 independent reflections
2953 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.134
S = 1.01
4037 reflections
282 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N9—H9*B*···S3^{i}	0.88	2.67	3.533 (3)	165
N4—H4*B*···S1^{ii}	0.88	2.52	3.373 (3)	164
N4—H4*A*···S2	0.88	2.80	3.360 (3)	123
N3—H3···S3^{iii}	0.88	2.59	3.414 (3)	156

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2122).

References

Brook, D.-J.-R., Fornell, S., Stevens, J.-E., Noll, B., Koch, T.-H. & Eisfeld, W. (2000). *Inorg. Chem.* **39**, 562–567.
Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Deng, J.-H., Guo, G.-Q. & Zhong, D.-C. (2007). *Acta Cryst.* E**63**, m2696–m2697.
Garbelini, E.-R., Horner, M., Behm, M.-B., Evans, D.-J. & Nunes, F.-S. (2008). *Z. Anorg. Allg. Chem.* **634**, 1801–1806.
Kowol, C.-R., Eichinger, R., Jakupec, M.-A., Galanski, M., Arion, V.-B. & Keppler, B.-K. (2007). *J. Inorg. Biochem.* **101**, 1946–1957.
Li, M.-X., Zhou, J., Wang, J.-P. & Wang, Z.-L. (2006). *Chin. J. Struct. Chem.* **25**, 1275–1279.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhong, D.-C., Guo, G.-Q. & Deng, J.-H. (2007). *Acta Cryst.* E**63**, m1747.

supporting information

Acta Cryst. (2009). E**65**, m847 [doi:10.1107/S1600536809024076]

Bis(ethanol-*κO*)bis(pyridine-3-carbaldehyde-*κN* thiosemicarbazone)bis(thiocyanato-*κN*)iron(II)–pyridine-3-carbaldehyde thiosemicarbazone (1/2)

Shao-Mei Wang

S1. Comment

Several crystal structures of metal complexes based on Schiff base ligands being synthesized by condensation of pyridine-3-carbaldehyde and amino compounds have been previously reported (Brook *et al.*, 2000; Deng *et al.*, 2007; Garbelini *et al.*, 2008; Kowol *et al.*, 2007; Zhong *et al.*, 2007). However, with regard to pyridine-3-carbaldehyde thiosemicarbazone (pct), only the corresponding Mn(II) complex has been documented (Li *et al.*, 2006). Herein, we report the synthesis and crystal crystal structure of its Fe^{II} complex.

The structure of the title compound, (I), consists of discrete [Fe($C_7H_8N_4S$)$_2$(SCN)$_2$(C_2H_5OH)$_2$] neutral units and uncoordinated pct molecules. The two semicarbazone ligands are planar, and each binds to Fe^{II} via the pyridine N atom. Therefore, pct acts as a monodentate ligand with the sulphur and nitrogen atoms of the semicarbazone subunit remaining uncoordinated. In addition to pct, the central Fe^{II} is coordinated by two SCN$^-$ anions and two C_2H_5OH molecules via the N and O atoms, respectively. (Fig. 1)

The molecules are held together by intermolecular hydrogen bonding interactions. The imino nitrogen N3 acts as a hydrogen donor site towards S3 of the uncoordinated pct molecule forming intermolecular N3—H3···S3 hydrogen bonds. S3 also accepts a hydrogen bond from N9 of a neighboring uncoordinated pct to form N9—H9B···S3 hydrogen bonds. In addition, the SCN$^-$ also is involved in the construction of the hydrogen bond network by establishing an interaction between the terminal S atoms accept and the hydrogen atom at N4 to form N4—H4A···S2 and N4—H4B···S1 hydrogen bonds (Table 1, Fig. 2).

S2. Experimental

A mixture of 0.5 mmol $FeCl_2 \times 6 H_2O$, 1.0 mmol of $(NH_4)SCN$ and 10 ml water-ethanol (1:2 *v*/*v*) was stirred for *ca.* 2 hrs at 343 K. Then 1.0 mmol pct in 10 ml water-ethanol mixture (1:2 *v*/*v*) was added. The mixture was further stirred for another 2 h, then filtered. The resultant filtrate was left to stand for slow evaporation at room temperature. Dark green single crystals of (**I**) suitable for X-ray structure analysis were obtained after a period of one week (yield 63%).

S3. Refinement

Hydrogen atoms attached to carbon atoms and nitrogen atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å, N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(C or N). The H atom attached to the hydroxy group of the ethanol ligand was located from difference density maps and was refined with distance restraints of O–H = 0.82 (1) Å.

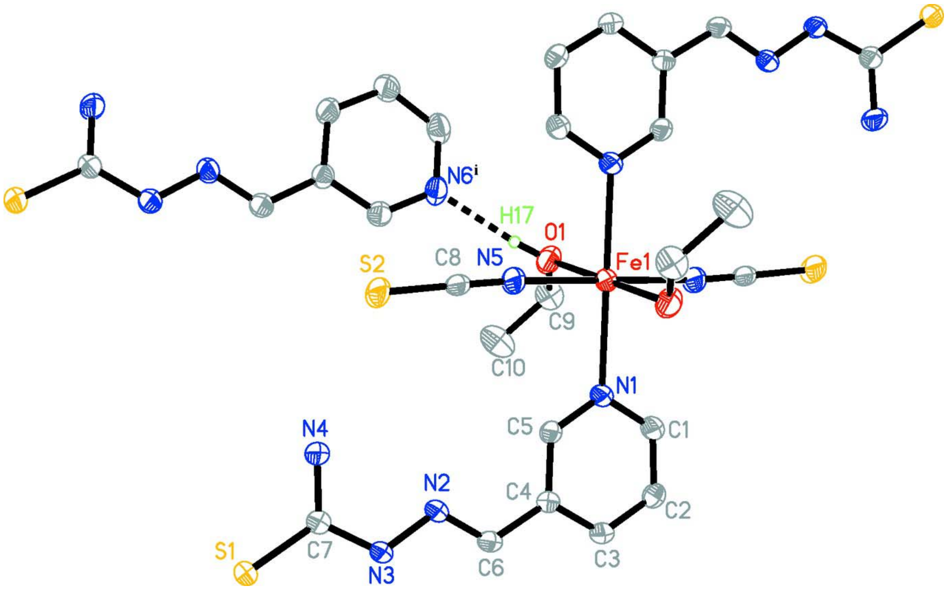


Figure 1

The structure of (**I**) × pct, symmetry code: (i) -*x* + 2, -*y*, -*z* + 1.

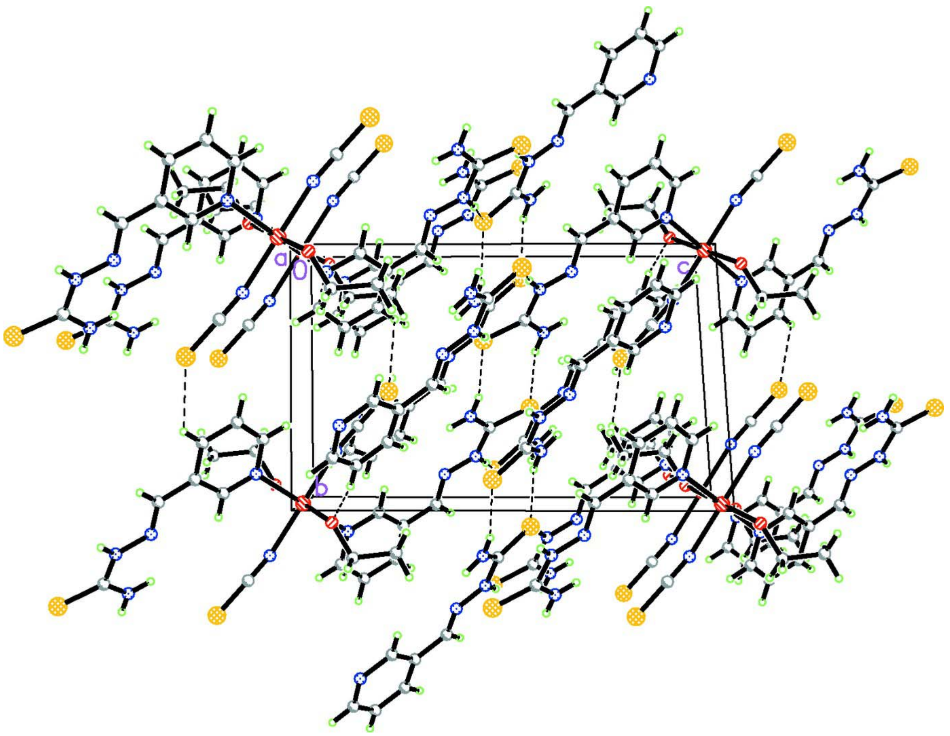


Figure 2

Three-dimensional supramolecular network constructed by hydrogen bonding interactions (dashed lines).

Bis(ethanol-*κO*)bis(pyridine-3-carbaldehyde-*κN* thiosemicarbazone-*κN*)bis(thiocyanato)iron(II)– pyridine-3-carbaldehyde thiosemicarbazone (1/2)

Crystal data

$[Fe(NCS)_2(C_7H_8N_4S)_2(C_2H_6O)_2]\cdot 2C_7H_8N_4S$
$M_r = 985.08$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.916$ (4) Å
$b = 9.556$ (5) Å
$c = 14.538$ (7) Å
$\alpha = 87.341$ (8)°
$\beta = 88.191$ (8)°
$\gamma = 69.604$ (8)°
$V = 1160$ (1) Å^3

$Z = 1$
$F(000) = 512$
$D_x = 1.411$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3773 reflections
$\theta = 2.3$–26.9°
$\mu = 0.65$ mm^{-1}
$T = 173$ K
Block, dark green
0.32 × 0.26 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.819$, $T_{\max} = 0.871$

8300 measured reflections
4037 independent reflections
2953 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.022$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 1.4°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.134$
$S = 1.01$
4037 reflections
282 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 0.3403P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.43$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ 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*	$U_{\text{iso}}*/U_{\text{eq}}$
Fe1	0.5000	0.0000	0.0000	0.0416 (2)

N1	0.2848 (3)	0.1196 (3)	0.09806 (16)	0.0410 (6)
N2	0.1975 (3)	−0.0995 (3)	0.33648 (15)	0.0389 (6)
N3	0.1640 (3)	−0.1698 (3)	0.41443 (16)	0.0413 (6)
H3	0.0676	−0.1382	0.4397	0.050*
N4	0.4186 (3)	−0.3344 (3)	0.40767 (19)	0.0659 (9)
H4A	0.4316	−0.2885	0.3557	0.079*
H4B	0.4981	−0.4112	0.4298	0.079*
N5	0.5606 (3)	−0.2022 (3)	0.08302 (19)	0.0536 (7)
C12	0.7900 (4)	0.3134 (4)	0.8792 (2)	0.0604 (9)
H12	0.6944	0.3331	0.9150	0.072*
N7	0.8316 (3)	0.5754 (3)	0.64455 (16)	0.0424 (6)
N8	0.8582 (3)	0.6617 (3)	0.57213 (17)	0.0453 (6)
H8	0.9546	0.6403	0.5474	0.054*
N9	0.5924 (3)	0.7961 (3)	0.5738 (2)	0.0652 (8)
H9A	0.5814	0.7316	0.6163	0.078*
H9B	0.5080	0.8711	0.5547	0.078*
O1	0.6741 (3)	0.0634 (3)	0.07601 (15)	0.0541 (6)
S1	0.24701 (9)	−0.36692 (9)	0.55347 (5)	0.0500 (2)
S2	0.64184 (10)	−0.43494 (10)	0.21504 (7)	0.0632 (3)
S3	0.76674 (9)	0.89666 (9)	0.45668 (6)	0.0525 (3)
C1	0.1770 (4)	0.2554 (3)	0.0754 (2)	0.0457 (7)
H1	0.1962	0.3076	0.0218	0.055*
C2	0.0403 (4)	0.3210 (3)	0.1271 (2)	0.0471 (7)
H2	−0.0332	0.4165	0.1092	0.057*
C3	0.0117 (3)	0.2462 (3)	0.20499 (19)	0.0416 (7)
H3A	−0.0815	0.2902	0.2418	0.050*
C4	0.1196 (3)	0.1064 (3)	0.22943 (18)	0.0354 (6)
C5	0.2540 (3)	0.0486 (3)	0.17329 (19)	0.0405 (7)
H5	0.3286	−0.0473	0.1895	0.049*
C6	0.0921 (3)	0.0255 (3)	0.3116 (2)	0.0409 (7)
H6	−0.0039	0.0653	0.3468	0.049*
C7	0.2808 (3)	−0.2882 (3)	0.4521 (2)	0.0424 (7)
C8	0.5957 (3)	−0.2995 (3)	0.1376 (2)	0.0409 (7)
C9	0.6438 (4)	0.1960 (4)	0.1234 (2)	0.0602 (9)
H9C	0.5507	0.2751	0.0956	0.072*
H9D	0.7375	0.2286	0.1155	0.072*
C10	0.6107 (5)	0.1792 (5)	0.2242 (3)	0.0809 (13)
H10A	0.5138	0.1535	0.2327	0.121*
H10B	0.5952	0.2735	0.2538	0.121*
H10C	0.7015	0.0997	0.2521	0.121*
C11	0.9244 (4)	0.1953 (4)	0.9025 (2)	0.0577 (9)
H11	0.9201	0.1350	0.9557	0.069*
N6	1.0609 (3)	0.1611 (3)	0.85410 (18)	0.0512 (7)
C13	1.0645 (4)	0.2479 (3)	0.7803 (2)	0.0457 (7)
H13	1.1613	0.2244	0.7453	0.055*
C14	0.9344 (3)	0.3714 (3)	0.7514 (2)	0.0404 (7)
C15	0.7945 (4)	0.4035 (4)	0.8032 (2)	0.0533 (8)
H15	0.7026	0.4867	0.7865	0.064*

C16	0.9506 (3)	0.4637 (3)	0.6721 (2)	0.0419 (7)
H16	1.0508	0.4406	0.6406	0.050*
C17	0.7345 (3)	0.7807 (3)	0.53873 (19)	0.0417 (7)
H17	0.747 (3)	−0.006 (3)	0.099 (2)	0.067 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0384 (3)	0.0424 (4)	0.0381 (4)	−0.0086 (3)	0.0034 (2)	0.0106 (3)
N1	0.0387 (13)	0.0410 (14)	0.0383 (13)	−0.0092 (11)	0.0062 (10)	0.0063 (11)
N2	0.0372 (13)	0.0431 (14)	0.0345 (13)	−0.0130 (11)	0.0060 (10)	0.0047 (11)
N3	0.0344 (13)	0.0445 (14)	0.0391 (13)	−0.0085 (11)	0.0080 (10)	0.0102 (11)
N4	0.0418 (15)	0.073 (2)	0.0584 (18)	0.0057 (14)	0.0150 (13)	0.0275 (15)
N5	0.0464 (16)	0.0499 (16)	0.0545 (16)	−0.0076 (12)	0.0044 (12)	0.0220 (14)
C12	0.0473 (19)	0.075 (2)	0.058 (2)	−0.0233 (18)	0.0052 (16)	0.0173 (18)
N7	0.0404 (14)	0.0469 (15)	0.0407 (14)	−0.0173 (12)	−0.0005 (11)	0.0076 (11)
N8	0.0379 (13)	0.0464 (15)	0.0485 (15)	−0.0129 (11)	0.0044 (11)	0.0104 (12)
N9	0.0362 (15)	0.071 (2)	0.0734 (19)	−0.0046 (13)	0.0092 (13)	0.0306 (16)
O1	0.0492 (14)	0.0503 (14)	0.0551 (14)	−0.0065 (11)	−0.0113 (11)	−0.0028 (11)
S1	0.0399 (4)	0.0577 (5)	0.0429 (5)	−0.0078 (4)	0.0058 (3)	0.0164 (4)
S2	0.0511 (5)	0.0507 (5)	0.0736 (6)	−0.0045 (4)	0.0042 (4)	0.0327 (4)
S3	0.0410 (4)	0.0548 (5)	0.0520 (5)	−0.0077 (4)	0.0059 (4)	0.0184 (4)
C1	0.0456 (17)	0.0447 (17)	0.0418 (17)	−0.0112 (14)	0.0055 (13)	0.0094 (14)
C2	0.0442 (17)	0.0364 (16)	0.0482 (18)	0.0007 (13)	0.0010 (14)	0.0061 (14)
C3	0.0349 (15)	0.0430 (17)	0.0404 (16)	−0.0061 (13)	0.0061 (12)	−0.0018 (13)
C4	0.0319 (14)	0.0388 (15)	0.0347 (15)	−0.0115 (12)	0.0024 (11)	−0.0008 (12)
C5	0.0370 (15)	0.0333 (15)	0.0431 (16)	−0.0036 (12)	0.0037 (12)	0.0090 (13)
C6	0.0350 (15)	0.0429 (17)	0.0403 (16)	−0.0090 (13)	0.0086 (12)	0.0013 (13)
C7	0.0378 (16)	0.0458 (17)	0.0401 (16)	−0.0114 (13)	0.0033 (13)	0.0044 (13)
C8	0.0312 (14)	0.0402 (17)	0.0454 (17)	−0.0063 (12)	0.0083 (12)	0.0018 (14)
C9	0.066 (2)	0.062 (2)	0.059 (2)	−0.0292 (19)	−0.0024 (17)	−0.0029 (18)
C10	0.103 (3)	0.092 (3)	0.063 (3)	−0.054 (3)	0.015 (2)	−0.007 (2)
C11	0.060 (2)	0.064 (2)	0.053 (2)	−0.0279 (18)	−0.0082 (17)	0.0184 (17)
N6	0.0501 (16)	0.0493 (16)	0.0521 (16)	−0.0155 (13)	−0.0111 (13)	0.0132 (13)
C13	0.0415 (17)	0.0480 (18)	0.0475 (18)	−0.0159 (14)	−0.0004 (13)	0.0023 (14)
C14	0.0389 (16)	0.0409 (17)	0.0428 (16)	−0.0161 (13)	−0.0033 (13)	0.0042 (13)
C15	0.0388 (17)	0.056 (2)	0.060 (2)	−0.0117 (15)	−0.0008 (15)	0.0154 (16)
C16	0.0389 (16)	0.0433 (17)	0.0438 (17)	−0.0157 (14)	0.0018 (13)	0.0029 (13)
C17	0.0406 (16)	0.0466 (17)	0.0365 (16)	−0.0139 (13)	0.0010 (13)	0.0025 (13)

Geometric parameters (Å, º)

Fe1—N5^{i}	2.140 (3)	S1—C7	1.690 (3)
Fe1—N5	2.140 (3)	S2—C8	1.623 (3)
Fe1—O1^{i}	2.196 (2)	S3—C17	1.677 (3)
Fe1—O1	2.196 (2)	C1—C2	1.377 (4)
Fe1—N1	2.339 (2)	C1—H1	0.9500
Fe1—N1^{i}	2.339 (2)	C2—C3	1.375 (4)

N1—C5	1.332 (3)	C2—H2	0.9500
N1—C1	1.352 (4)	C3—C4	1.385 (4)
N2—C6	1.280 (4)	C3—H3A	0.9500
N2—N3	1.368 (3)	C4—C5	1.388 (4)
N3—C7	1.350 (4)	C4—C6	1.453 (4)
N3—H3	0.8800	C5—H5	0.9500
N4—C7	1.312 (4)	C6—H6	0.9500
N4—H4A	0.8800	C9—C10	1.498 (5)
N4—H4B	0.8800	C9—H9C	0.9900
N5—C8	1.156 (4)	C9—H9D	0.9900
C12—C11	1.368 (5)	C10—H10A	0.9800
C12—C15	1.377 (4)	C10—H10B	0.9800
C12—H12	0.9500	C10—H10C	0.9800
N7—C16	1.274 (4)	C11—N6	1.332 (4)
N7—N8	1.373 (3)	C11—H11	0.9500
N8—C17	1.361 (4)	N6—C13	1.332 (4)
N8—H8	0.8800	C13—C14	1.395 (4)
N9—C17	1.312 (4)	C13—H13	0.9500
N9—H9A	0.8800	C14—C15	1.383 (4)
N9—H9B	0.8800	C14—C16	1.453 (4)
O1—C9	1.408 (4)	C15—H15	0.9500
O1—H17	0.816 (10)	C16—H16	0.9500

N5^{i}—Fe1—N5	180.00 (14)	C2—C3—H3A	120.2
N5^{i}—Fe1—O1^{i}	88.99 (10)	C4—C3—H3A	120.2
N5—Fe1—O1^{i}	91.01 (10)	C3—C4—C5	117.5 (2)
N5^{i}—Fe1—O1	91.01 (10)	C3—C4—C6	120.6 (2)
N5—Fe1—O1	88.99 (10)	C5—C4—C6	121.9 (3)
O1^{i}—Fe1—O1	180.00 (14)	N1—C5—C4	123.9 (3)
N5^{i}—Fe1—N1	88.53 (9)	N1—C5—H5	118.0
N5—Fe1—N1	91.47 (9)	C4—C5—H5	118.0
O1^{i}—Fe1—N1	85.58 (9)	N2—C6—C4	119.9 (2)
O1—Fe1—N1	94.42 (9)	N2—C6—H6	120.0
N5^{i}—Fe1—N1^{i}	91.47 (9)	C4—C6—H6	120.0
N5—Fe1—N1^{i}	88.53 (9)	N4—C7—N3	116.9 (3)
O1^{i}—Fe1—N1^{i}	94.42 (9)	N4—C7—S1	123.1 (2)
O1—Fe1—N1^{i}	85.58 (9)	N3—C7—S1	119.9 (2)
N1—Fe1—N1^{i}	180.00 (12)	N5—C8—S2	179.0 (3)
C5—N1—C1	117.4 (2)	O1—C9—C10	113.3 (3)
C5—N1—Fe1	120.69 (18)	O1—C9—H9C	108.9
C1—N1—Fe1	121.52 (18)	C10—C9—H9C	108.9
C6—N2—N3	116.9 (2)	O1—C9—H9D	108.9
C7—N3—N2	119.2 (2)	C10—C9—H9D	108.9
C7—N3—H3	120.4	H9C—C9—H9D	107.7
N2—N3—H3	120.4	C9—C10—H10A	109.5
C7—N4—H4A	120.0	C9—C10—H10B	109.5
C7—N4—H4B	120.0	H10A—C10—H10B	109.5
H4A—N4—H4B	120.0	C9—C10—H10C	109.5

C8—N5—Fe1	170.5 (3)	H10A—C10—H10C	109.5
C11—C12—C15	119.4 (3)	H10B—C10—H10C	109.5
C11—C12—H12	120.3	N6—C11—C12	122.9 (3)
C15—C12—H12	120.3	N6—C11—H11	118.5
C16—N7—N8	117.2 (2)	C12—C11—H11	118.5
C17—N8—N7	119.6 (2)	C11—N6—C13	117.4 (3)
C17—N8—H8	120.2	N6—C13—C14	123.9 (3)
N7—N8—H8	120.2	N6—C13—H13	118.1
C17—N9—H9A	120.0	C14—C13—H13	118.1
C17—N9—H9B	120.0	C15—C14—C13	117.1 (3)
H9A—N9—H9B	120.0	C15—C14—C16	122.6 (3)
C9—O1—Fe1	126.7 (2)	C13—C14—C16	120.3 (3)
C9—O1—H17	112 (3)	C12—C15—C14	119.2 (3)
Fe1—O1—H17	115 (3)	C12—C15—H15	120.4
N1—C1—C2	122.6 (3)	C14—C15—H15	120.4
N1—C1—H1	118.7	N7—C16—C14	120.5 (3)
C2—C1—H1	118.7	N7—C16—H16	119.7
C3—C2—C1	119.1 (3)	C14—C16—H16	119.7
C3—C2—H2	120.5	N9—C17—N8	116.1 (3)
C1—C2—H2	120.5	N9—C17—S3	123.4 (2)
C2—C3—C4	119.6 (3)	N8—C17—S3	120.5 (2)

Symmetry code: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N9—H9*B*···S3^{ii}	0.88	2.67	3.533 (3)	165
N4—H4*B*···S1^{iii}	0.88	2.52	3.373 (3)	164
N4—H4*A*···S2	0.88	2.80	3.360 (3)	123
N3—H3···S3^{iv}	0.88	2.59	3.414 (3)	156

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