Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Bis{2-[3-(cyclohexylamino)propyliminomethyl]phenolato-κ^2N,O}bis(thiocyanato-κN)iron(II)

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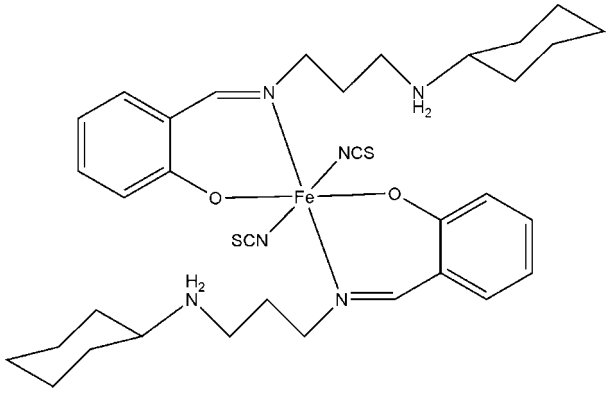
Received 20 May 2007; accepted 25 June 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; R factor = 0.062; wR factor = 0.198; data-to-parameter ratio = 14.5.

The title complex, $[Fe(NCS)_2(C_{32}H_{46}N_4O_2)_2]$, is a mononuclear iron(II) complex with a distorted octahedral coordination geometry and the central Fe^{2+} ion, located on an inversion centre, is coordinated by four N atoms and two O atoms from two Schiff-base ligands and two thiocyanate anions. The Schiff base was obtained by condensation of equimolar amounts of salicylaldehyde and *N*-cyclohexyl-1,3-diaminopropane in acetonitrile. The crystal structure involves intermolecular N—H···O and N—H···S hydrogen bonds.

Related literature

For related literature, see: Liu *et al.* (2004); Nie (2004); You *et al.* (2003, 2004, 2005); Yue *et al.* (2005); You & Zhu (2004); Zhu, Xia *et al.* (2003); Zhu, Zeng *et al.* (2003).



Experimental

Crystal data

$[Fe(NCS)_2(C_{32}H_{46}N_4O_2)_2]$
M_r = 692.75
Monoclinic, $P2_1/c$
a = 10.912 (7) Å
b = 7.797 (5) Å
c = 20.778 (13) Å
β = 96.899 (13)°
V = 1755.1 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.15 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.843, T_{max} = 0.917
7131 measured reflections
2975 independent reflections
1337 reflections with $I > 2\sigma(I)$
R_{int} = 0.101

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.198
S = 0.85
2975 reflections
205 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O1^{i}	0.90	1.79	2.683 (6)	175
N2—H2A···S1^{ii}	0.90	2.44	3.337 (6)	173

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The work was supported by the Analytical Test Fund for Dr Chang-Hong Liu in Nanjing University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2128).

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 doi:10.1107/S1600536807031066

supplementary materials

Acta Cryst. (2007). E**63**, m2033 [**doi:10.1107/S1600536807031066**]

trans-Bis{2-[3-(cyclohexylamino)propyliminomethyl]phenolato-κ^2N,O}bis(thiocyanato-κN)iron(II)

K. Chen, Y.-L. Zhang, M.-Q. Feng and C.-H. Liu

Comment

Because of their interesting physical and biological properties, many iron complexes with amines or imines have structurally been studied (Liu *et al.*, 2004; You & Zhu, 2004, You *et al.*, 2004, 2005; Zhu, Xia *et al.*, 2003). When trying to synthesize iron(II) complexes with a Schiff base, condensed from salicylaldehyde and *N*-cyclohexyl-1,3-diaminopropane, we isolated the title complex.

The title complex is a discrete iron(II) complex, which isisostructural to those of the nickel (Zhu, Zeng *et al.*, 2003), the cobalt (You *et al.*, 2003; Yue *et al.*, 2005), and the copper complexes (Nie, 2004). The central iron(II) atom is six-coordinated by two oxygen atoms and two nitrogen atoms from two Schiff base ligands, and by two nitrogen atoms from two thiocyanate anions. The Schiff base acts as a bidentate ligand with the amine nitrogen atom uncoordinated. The iron(II) atom is in a distorted octahedral coordination geometry and is located on an inversion centre.

In the crystal structure, the intramolecular (N2—H2B···O1^{i}, symmetry code $-x$, $-y+1$, $-z+2$) and intermolecular (N2—H2A···S1^{ii}, symmetry code $-x$, $-y+2$, $-z+2$) hydrogen bonds link the molecules to form one-dimensional chains along *b* axis. As expected, the cyclohexyl groups in the complex are in chair conformations.

Experimental

In a similar procedure to that of Zhu, Zeng *et al.* (2003) the title complex was prepared. Yield 43%.

Refinement

C– and N-bound H atoms were included in the riding model approximation with C—H = 0.93–0.97 Å and N—H = 0.90 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

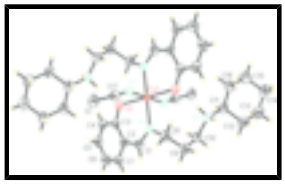


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. [Symmetry code for unlabelled atoms: $-x$, $-y+1$, $-z+2$.]

trans-Bis{2-[3-(cyclohexylamino)propyliminomethyl]phenolato- κ^2N,O}bis(thiocyanato-κN)iron(II)

Crystal data

$[Fe(NCS)_2(C_{32}H_{46}N_4O_2)_2]$	F_{000} = 736
M_r = 692.75	D_x = 1.311 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.912 (7) Å	Cell parameters from 1885 reflections
b = 7.797 (5) Å	θ = 3.4–27.0º
c = 20.778 (13) Å	μ = 0.59 mm^{-1}
β = 96.899 (13)º	T = 293 (2) K
V = 1755.1 (19) Å^3	Prism, red
Z = 2	0.30 × 0.20 × 0.15 mm

Data collection

Bruker APEX area-detector diffractometer	2975 independent reflections
Radiation source: fine-focus sealed tube	1337 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.101
T = 293(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→12
T_{min} = 0.843, T_{max} = 0.917	k = −9→7
7131 measured reflections	l = −12→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.062	H-atom parameters constrained
$wR(F^2)$ = 0.198	$w = 1/[\sigma^2(F_o^2) + (0.0924P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.85	$(\Delta/\sigma)_{max}$ = 0.001
2975 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
205 parameters	$\Delta\rho_{min}$ = −0.56 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Fe1	0.0000	0.5000	1.0000	0.0428 (4)
N1	0.0966 (4)	0.6470 (7)	1.0731 (3)	0.0574 (14)
N2	0.2901 (4)	0.7562 (6)	0.9480 (2)	0.0560 (14)
H2A	0.2919	0.8702	0.9415	0.067*
H2B	0.2109	0.7221	0.9397	0.067*
N3	−0.1560 (5)	0.6574 (7)	1.0106 (3)	0.0685 (16)
O1	−0.0527 (4)	0.3417 (5)	1.0693 (2)	0.0609 (12)
S1	−0.32276 (16)	0.8260 (2)	1.08020 (10)	0.0731 (6)
C1	0.1231 (5)	0.5937 (10)	1.1321 (4)	0.0647 (19)
H1	0.1627	0.6719	1.1614	0.078*
C2	0.0982 (5)	0.4266 (10)	1.1577 (3)	0.0590 (18)
C3	0.0147 (5)	0.3076 (9)	1.1257 (3)	0.0578 (17)
C4	0.0015 (6)	0.1509 (9)	1.1568 (3)	0.0629 (18)
H4	−0.0515	0.0686	1.1366	0.075*
C5	0.0640 (7)	0.1157 (11)	1.2159 (4)	0.073 (2)
H5	0.0534	0.0101	1.2353	0.088*
C6	0.1438 (7)	0.2356 (12)	1.2477 (4)	0.081 (2)
H6	0.1856	0.2120	1.2884	0.097*
C7	0.1591 (6)	0.3859 (11)	1.2186 (3)	0.069 (2)
H7	0.2126	0.4663	1.2398	0.083*
C8	0.1343 (6)	0.8239 (9)	1.0603 (3)	0.0663 (19)
H8A	0.1064	0.8995	1.0927	0.080*
H8B	0.0944	0.8596	1.0182	0.080*
C9	0.2736 (6)	0.8421 (9)	1.0616 (3)	0.073 (2)
H9A	0.2916	0.9589	1.0497	0.087*
H9B	0.3117	0.8241	1.1057	0.087*
C10	0.3333 (6)	0.7209 (9)	1.0174 (3)	0.0674 (19)
H10A	0.4223	0.7337	1.0249	0.081*
H10B	0.3134	0.6035	1.0275	0.081*
C11	0.3644 (5)	0.6695 (8)	0.8995 (3)	0.0569 (17)
H11	0.3747	0.5482	0.9114	0.068*
C12	0.4912 (6)	0.7514 (11)	0.9035 (4)	0.095 (3)
H12A	0.5350	0.7344	0.9464	0.114*
H12B	0.4828	0.8738	0.8958	0.114*
C13	0.5644 (7)	0.6705 (14)	0.8526 (4)	0.111 (3)
H13A	0.6433	0.7284	0.8536	0.134*
H13B	0.5805	0.5510	0.8635	0.134*
C14	0.4981 (7)	0.6816 (11)	0.7869 (4)	0.092 (3)

H14A	0.5451	0.6231	0.7568	0.110*
H14B	0.4902	0.8010	0.7740	0.110*
C15	0.3731 (7)	0.6032 (12)	0.7838 (4)	0.098 (3)
H15A	0.3815	0.4807	0.7912	0.118*
H15B	0.3295	0.6204	0.7408	0.118*
C16	0.2983 (6)	0.6799 (11)	0.8336 (3)	0.083 (2)
H16A	0.2804	0.7990	0.8228	0.099*
H16B	0.2204	0.6193	0.8322	0.099*
C17	−0.2235 (6)	0.7290 (8)	1.0391 (3)	0.0538 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0333 (7)	0.0486 (8)	0.0487 (7)	−0.0031 (5)	0.0143 (5)	−0.0059 (6)
N1	0.045 (3)	0.065 (4)	0.066 (4)	−0.003 (3)	0.021 (3)	−0.013 (3)
N2	0.046 (3)	0.053 (3)	0.070 (4)	−0.006 (2)	0.010 (3)	−0.007 (3)
N3	0.054 (4)	0.068 (4)	0.084 (4)	0.005 (3)	0.012 (3)	−0.011 (3)
O1	0.052 (3)	0.069 (3)	0.063 (3)	−0.014 (2)	0.009 (2)	−0.002 (2)
S1	0.0683 (12)	0.0581 (12)	0.0974 (15)	0.0042 (9)	0.0287 (10)	−0.0034 (11)
C1	0.050 (4)	0.084 (6)	0.061 (5)	−0.001 (4)	0.010 (4)	−0.027 (4)
C2	0.044 (4)	0.070 (5)	0.065 (5)	−0.006 (3)	0.017 (4)	−0.015 (4)
C3	0.037 (4)	0.075 (5)	0.065 (5)	0.008 (3)	0.021 (3)	−0.008 (4)
C4	0.050 (4)	0.063 (5)	0.079 (5)	0.005 (3)	0.019 (4)	0.004 (4)
C5	0.062 (5)	0.086 (6)	0.076 (5)	0.015 (4)	0.022 (4)	0.019 (5)
C6	0.070 (5)	0.100 (7)	0.073 (5)	0.016 (5)	0.014 (4)	0.004 (5)
C7	0.052 (4)	0.094 (6)	0.061 (5)	0.005 (4)	0.005 (4)	−0.011 (4)
C8	0.074 (5)	0.055 (5)	0.073 (5)	−0.004 (3)	0.026 (4)	−0.015 (4)
C9	0.077 (5)	0.067 (5)	0.077 (5)	−0.023 (4)	0.021 (4)	−0.009 (4)
C10	0.053 (4)	0.084 (6)	0.065 (5)	−0.009 (4)	0.006 (3)	−0.001 (4)
C11	0.050 (4)	0.049 (4)	0.075 (5)	0.004 (3)	0.022 (3)	−0.002 (3)
C12	0.045 (4)	0.140 (8)	0.101 (6)	−0.007 (4)	0.020 (4)	−0.031 (6)
C13	0.055 (5)	0.165 (10)	0.119 (8)	−0.012 (5)	0.032 (5)	−0.043 (7)
C14	0.082 (6)	0.086 (6)	0.116 (7)	−0.012 (4)	0.046 (5)	−0.005 (5)
C15	0.072 (6)	0.137 (8)	0.089 (6)	0.007 (5)	0.021 (5)	−0.029 (6)
C16	0.062 (5)	0.118 (7)	0.072 (5)	0.011 (4)	0.021 (4)	−0.013 (5)
C17	0.059 (4)	0.041 (4)	0.061 (4)	−0.001 (3)	0.006 (3)	−0.001 (3)

Geometric parameters (Å, °)

Fe1—O1^{i}	2.031 (4)	C7—H7	0.9300
Fe1—O1	2.031 (4)	C8—C9	1.524 (9)
Fe1—N1^{i}	2.085 (5)	C8—H8A	0.9700
Fe1—N1	2.085 (5)	C8—H8B	0.9700
Fe1—N3	2.132 (6)	C9—C10	1.519 (9)
Fe1—N3^{i}	2.132 (6)	C9—H9A	0.9700
N1—C1	1.294 (8)	C9—H9B	0.9700
N1—C8	1.472 (8)	C10—H10A	0.9700
N2—C10	1.488 (7)	C10—H10B	0.9700

N2—C11	1.524 (7)	C11—C16	1.472 (9)
N2—H2A	0.9000	C11—C12	1.517 (8)
N2—H2B	0.9000	C11—H11	0.9800
N3—C17	1.143 (7)	C12—C13	1.535 (10)
O1—C3	1.333 (7)	C12—H12A	0.9700
S1—C17	1.643 (8)	C12—H12B	0.9700
C1—C2	1.445 (10)	C13—C14	1.468 (11)
C1—H1	0.9300	C13—H13A	0.9700
C2—C7	1.393 (9)	C13—H13B	0.9700
C2—C3	1.410 (9)	C14—C15	1.488 (9)
C3—C4	1.398 (9)	C14—H14A	0.9700
C4—C5	1.359 (9)	C14—H14B	0.9700
C4—H4	0.9300	C15—C16	1.516 (9)
C5—C6	1.389 (10)	C15—H15A	0.9700
C5—H5	0.9300	C15—H15B	0.9700
C6—C7	1.339 (9)	C16—H16A	0.9700
C6—H6	0.9300	C16—H16B	0.9700
$O1^{i}$—Fe1—O1	180.000 (1)	C9—C8—H8B	109.1
$O1^{i}$—Fe1—$N1^{i}$	88.8 (2)	H8A—C8—H8B	107.8
O1—Fe1—$N1^{i}$	91.2 (2)	C10—C9—C8	115.5 (5)
$O1^{i}$—Fe1—N1	91.2 (2)	C10—C9—H9A	108.4
O1—Fe1—N1	88.8 (2)	C8—C9—H9A	108.4
$N1^{i}$—Fe1—N1	180.000 (1)	C10—C9—H9B	108.4
$O1^{i}$—Fe1—N3	91.2 (2)	C8—C9—H9B	108.4
O1—Fe1—N3	88.8 (2)	H9A—C9—H9B	107.5
$N1^{i}$—Fe1—N3	93.0 (2)	N2—C10—C9	111.2 (6)
N1—Fe1—N3	87.0 (2)	N2—C10—H10A	109.4
$O1^{i}$—Fe1—$N3^{i}$	88.8 (2)	C9—C10—H10A	109.4
O1—Fe1—$N3^{i}$	91.2 (2)	N2—C10—H10B	109.4
$N1^{i}$—Fe1—$N3^{i}$	87.0 (2)	C9—C10—H10B	109.4
N1—Fe1—$N3^{i}$	93.0 (2)	H10A—C10—H10B	108.0
N3—Fe1—$N3^{i}$	180.000 (3)	C16—C11—C12	111.6 (6)
C1—N1—C8	115.9 (6)	C16—C11—N2	110.5 (5)
C1—N1—Fe1	123.3 (5)	C12—C11—N2	109.4 (5)
C8—N1—Fe1	120.8 (4)	C16—C11—H11	108.4
C10—N2—C11	115.2 (5)	C12—C11—H11	108.4
C10—N2—H2A	108.5	N2—C11—H11	108.4
C11—N2—H2A	108.5	C11—C12—C13	109.7 (6)
C10—N2—H2B	108.5	C11—C12—H12A	109.7
C11—N2—H2B	108.5	C13—C12—H12A	109.7
H2A—N2—H2B	107.5	C11—C12—H12B	109.7
C17—N3—Fe1	155.0 (5)	C13—C12—H12B	109.7
C3—O1—Fe1	124.8 (4)	H12A—C12—H12B	108.2
N1—C1—C2	127.4 (6)	C14—C13—C12	112.1 (7)
N1—C1—H1	116.3	C14—C13—H13A	109.2
C2—C1—H1	116.3	C12—C13—H13A	109.2

C7—C2—C3	119.3 (7)	C14—C13—H13B	109.2
C7—C2—C1	116.7 (6)	C12—C13—H13B	109.2
C3—C2—C1	124.0 (7)	H13A—C13—H13B	107.9
O1—C3—C4	120.3 (6)	C13—C14—C15	111.3 (7)
O1—C3—C2	122.7 (7)	C13—C14—H14A	109.4
C4—C3—C2	117.0 (7)	C15—C14—H14A	109.4
C5—C4—C3	121.8 (7)	C13—C14—H14B	109.4
C5—C4—H4	119.1	C15—C14—H14B	109.4
C3—C4—H4	119.1	H14A—C14—H14B	108.0
C4—C5—C6	120.7 (8)	C14—C15—C16	112.0 (7)
C4—C5—H5	119.6	C14—C15—H15A	109.2
C6—C5—H5	119.6	C16—C15—H15A	109.2
C7—C6—C5	118.7 (8)	C14—C15—H15B	109.2
C7—C6—H6	120.7	C16—C15—H15B	109.2
C5—C6—H6	120.7	H15A—C15—H15B	107.9
C6—C7—C2	122.5 (7)	C11—C16—C15	111.7 (6)
C6—C7—H7	118.7	C11—C16—H16A	109.3
C2—C7—H7	118.7	C15—C16—H16A	109.3
N1—C8—C9	112.6 (5)	C11—C16—H16B	109.3
N1—C8—H8A	109.1	C15—C16—H16B	109.3
C9—C8—H8A	109.1	H16A—C16—H16B	107.9
N1—C8—H8B	109.1	N3—C17—S1	178.1 (6)
$O1^{i}$—Fe1—N1—C1	−164.6 (5)	C1—C2—C3—O1	−2.5 (9)
O1—Fe1—N1—C1	15.4 (5)	C7—C2—C3—C4	−2.1 (9)
$N1^{i}$—Fe1—N1—C1	−126 (94)	C1—C2—C3—C4	179.7 (5)
N3—Fe1—N1—C1	104.3 (5)	O1—C3—C4—C5	−176.5 (6)
$N3^{i}$—Fe1—N1—C1	−75.7 (5)	C2—C3—C4—C5	1.3 (9)
$O1^{i}$—Fe1—N1—C8	18.1 (4)	C3—C4—C5—C6	0.2 (10)
O1—Fe1—N1—C8	−161.9 (4)	C4—C5—C6—C7	−0.9 (11)
$N1^{i}$—Fe1—N1—C8	57 (93)	C5—C6—C7—C2	0.1 (11)
N3—Fe1—N1—C8	−73.0 (4)	C3—C2—C7—C6	1.5 (10)
$N3^{i}$—Fe1—N1—C8	107.0 (4)	C1—C2—C7—C6	179.8 (6)
$O1^{i}$—Fe1—N3—C17	−136.2 (13)	C1—N1—C8—C9	71.6 (7)
O1—Fe1—N3—C17	43.8 (13)	Fe1—N1—C8—C9	−110.9 (5)
$N1^{i}$—Fe1—N3—C17	135.0 (13)	N1—C8—C9—C10	54.0 (8)
N1—Fe1—N3—C17	−45.0 (13)	C11—N2—C10—C9	167.1 (5)
$N3^{i}$—Fe1—N3—C17	−89 (10)	C8—C9—C10—N2	65.0 (8)
$O1^{i}$—Fe1—O1—C3	−77 (100)	C10—N2—C11—C16	167.1 (6)
$N1^{i}$—Fe1—O1—C3	148.0 (5)	C10—N2—C11—C12	−69.7 (7)
N1—Fe1—O1—C3	−32.0 (5)	C16—C11—C12—C13	−54.8 (9)
N3—Fe1—O1—C3	−119.1 (5)	N2—C11—C12—C13	−177.4 (6)
$N3^{i}$—Fe1—O1—C3	60.9 (5)	C11—C12—C13—C14	55.3 (10)
C8—N1—C1—C2	−179.3 (6)	C12—C13—C14—C15	−55.6 (11)
Fe1—N1—C1—C2	3.3 (9)	C13—C14—C15—C16	54.6 (10)
N1—C1—C2—C7	166.0 (6)	C12—C11—C16—C15	55.0 (9)
N1—C1—C2—C3	−15.8 (10)	N2—C11—C16—C15	176.9 (6)

Fe1—O1—C3—C4	−151.8 (4)	C14—C15—C16—C11	−54.5 (10)
Fe1—O1—C3—C2	30.4 (8)	Fe1—N3—C17—S1	−81 (19)
C7—C2—C3—O1	175.7 (5)		

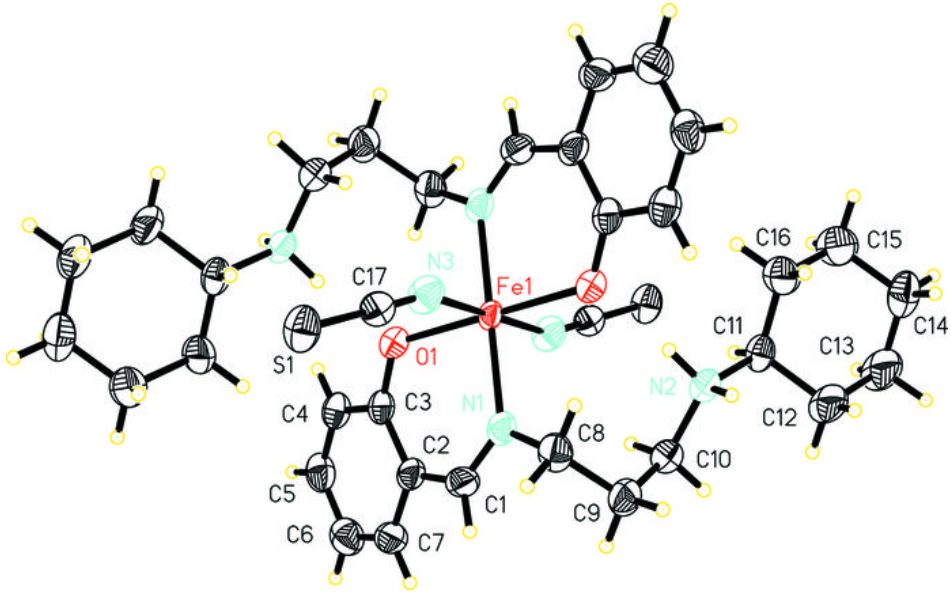
Symmetry codes: (i) −*x*, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···O1^{i}	0.90	1.79	2.683 (6)	175
N2—H2A···S1^{ii}	0.90	2.44	3.337 (6)	173

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

Fig. 1


C16
C15
N3
C17
Fe1
C11
C14
C13
S1
O1
N2
C4
C3
N1
C8
C12
C2
C10
C5
C1
C9
C6
C7