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fac-Tris(dimethyl sulfoxide-κ*O*)tris(thiocyanato-κ*N*)iron(III)

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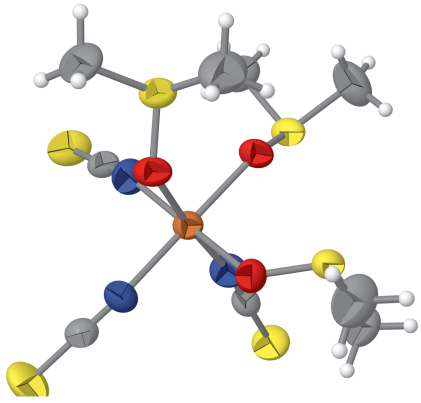
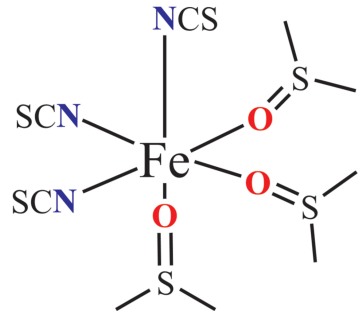
The title complex, $[Fe(SCN)_3(C_2H_6OS)_3]$, was obtained under solvothermal conditions. The asymmetric unit contains one neutral molecule in which the central Fe^{III} atom exhibits a distorted octahedral coordination environment. The three N-bonded thiocyanato ligands and the three O-bonded dimethyl sulfoxide ligands adopt a *fac* configuration. In the crystal, weak C—H···S hydrogen bonds link the complexes into centrosymmetric dimers that are arranged in layers parallel to (001).

3D view



Chemical scheme



Structure description

The reaction that led to the serendipitous crystallization of the title complex, $Fe(NCS)_3(DMSO)_3$ (DMSO is dimethylsulfoxide), (I), was originally designed for the solvothermal synthesis of a heteroleptic iron complex, with acetonitrile serving both as solvent and nitrile substrate for a possible *in situ* azide–nitrile cycloaddition leading to a tetrazole-containing ligand.

The asymmetric unit of (I) contains one neutral complex (Fig. 1). The Fe^{III} atom is in a distorted octahedral environment, coordinated by three N atoms from thiocyanato ligands (N1, N2, N3) and three O atoms from DMSO ligands (O1, O2, O3). The O-bound coordination mode of DMSO is well documented for metal cations classified as 'hard' according to the Pearson (1963) concept, such as Fe^{III}. The Fe—N distances between 1.997 (4) and 2.035 (4) Å and the Fe—O distances between 2.031 (3) and 2.043 (3) Å (Table 1) are consistent with analogous iron(III) isothiocyanate complexes reported by Wang *et al.* (2003). The configuration around the Fe^{III} atom is *fac*, resulting from the three N-bonded thiocyanato ligands and the three O-bonded DMSO ligands occupying opposite triangular faces of the octahedron. The thiocyanato ligands are slightly bent, with Fe—N—C angles between 155.5 (4) and 170.6 (4)° and nearly linear N≡C—S angles between 177.3 (4) and 179.3 (4)°. The methyl groups of each of the three DMSO ligands are in an eclipsed conformation relative to each other.

Table 1
Selected geometric parameters (Å, °).

Fe—O3	2.031 (3)	Fe—O2	2.041 (3)
Fe—N1	2.035 (4)	Fe—N3	2.016 (4)
Fe—O1	2.043 (3)	Fe—N2	1.997 (4)
O3—Fe—N1	174.70 (13)	O2—Fe—O1	88.64 (11)
O3—Fe—O1	87.64 (12)	N3—Fe—O3	90.20 (15)
O3—Fe—O2	85.20 (11)	N3—Fe—O1	177.81 (14)
N1—Fe—O1	89.85 (14)	N2—Fe—O2	175.50 (13)
N1—Fe—O2	90.08 (13)	N2—Fe—N3	92.13 (15)

In the crystal of (I), individual molecules are linked by weak C—H···S hydrogen bonds (Table 2) into centrosymmetric dimers that are arranged in layers parallel to (001) (Fig. 2).

Several crystal structures of iron(III) thiocyanate complexes and related metal complexes containing oxygen-donor co-ligands have been reported over the past decades. The title complex is most closely related to the *fac*-tris-(dimethyl sulfoxide)(thiocyanato)scandium(III) complex crystallizing in the orthorhombic space group $Pna2_1$, $Z = 4$, a = 14.583 (2), b = 14.728 (2), c = 9.849 (2) Å, V = 2115.4 (6) Å^3 (Chenskaya *et al.*, 2000). Both structures comprise mononuclear octahedral complexes featuring three N-bonded thiocyanato ligands and three O-bonded dimethyl sulfoxide ligands with only minor differences in bond lengths reflecting the different nature of the central metal ion. Other related complexes include thiocyanate/DMSO-containing lanthanide compounds (Bu *et al.*, 2002; Li *et al.*, 2004; Miranda *et al.*, 2004; Ilichev *et al.*, 2023). However, to the best of our knowledge, no mononuclear iron(III) complex containing both N-bonded thiocyanato ligands and O-bonded dimethyl sulfoxide ligands has been reported to date.

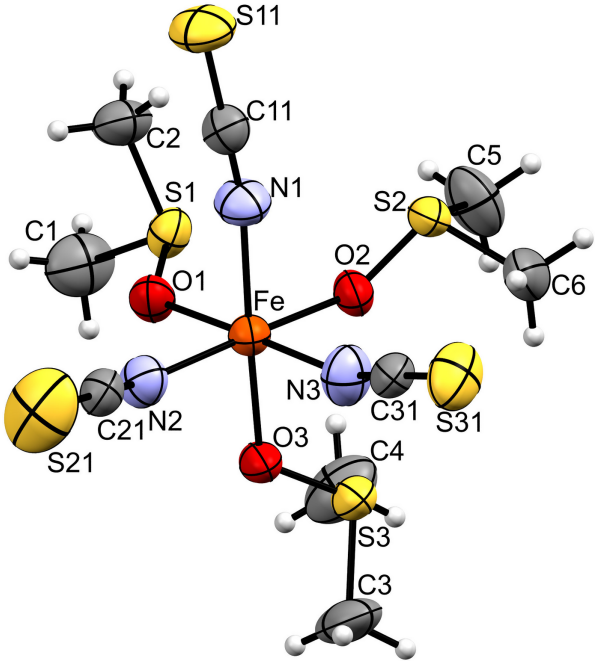


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6A···S31^{i}	0.96	2.84	3.751 (6)	159

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

Synthesis and crystallization

Potassium thiocyanate (2 mmol, 0.199 g) and iron(II) sulfate heptahydrate (1 mmol, 0.278 g) were dissolved in dimethyl sulfoxide (10 ml) in the presence of ascorbic acid as a reducing agent, and the mixture was stirred for 20 min at room temperature. Acetonitrile was present in the reaction medium as the nitrile source. Sodium azide (0.5 mmol, 0.033 g) was dissolved separately in a minimum volume of distilled water and added to the above solution. The reaction mixture was transferred into a 23 ml PTFE-lined stainless-steel autoclave, sealed, and heated at 393 K for 72 h, then allowed to cool slowly to room temperature. Orange prismatic crystals of the title compound were collected by filtration, washed with cold DMSO, and air-dried.

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 3.

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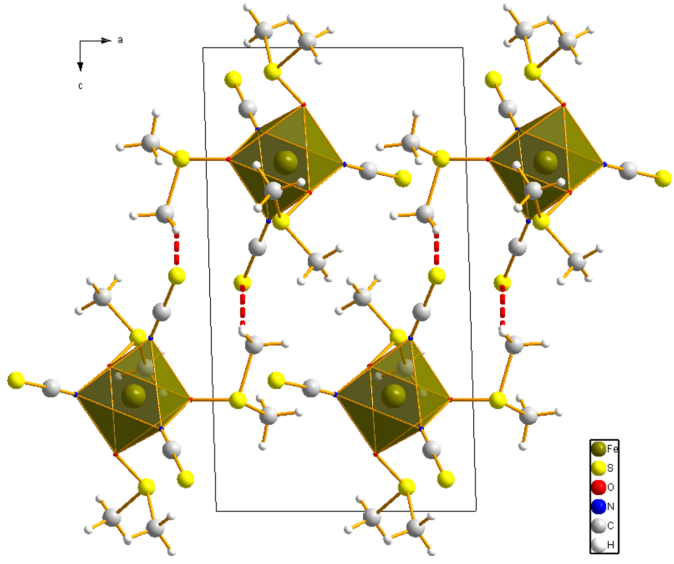

Figure 2
Crystal packing of the title compound in a projection along [010]. The coordination environment around the Fe^{III} atoms is shown in polyhedral representation; red dashed lines indicate weak C—H···S hydrogen bonds.

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[Fe(SCN)_3(C_2H_6OS)_3]$
M_r	464.47
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	7.980 (4), 9.001 (6), 14.340 (7)
α, β, γ (°)	82.233 (18), 87.868 (17), 86.16 (3)
V (Å^3)	1017.8 (9)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.37
Crystal size (mm)	0.20 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.632, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6890, 3801, 2424
R_{int}	0.034
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.115, 0.98
No. of reflections	3801
No. of parameters	205
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.36

Computer programs: *SMART* and, *SAINT* (Bruker, 2009), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *DIAMOND* (Putz & Brandenburg, 2010), *publCIF* (Westrip, 2010).

full crystallographic data

IUCrData (2026). **11**, x260592 [https://doi.org/10.1107/S2414314626005924]

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Crystal data

$[Fe(SCN)_3(C_2H_6OS)_3]$
M_r = 464.47
Triclinic, $P\overline{1}$
a = 7.980 (4) Å
b = 9.001 (6) Å
c = 14.340 (7) Å
α = 82.233 (18)°
β = 87.868 (17)°
γ = 86.16 (3)°
V = 1017.8 (9) Å^3
Z = 2
$F(000)$ = 478
D_x = 1.516 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 295 reflections
θ = 2.9–22.3°
μ = 1.37 mm^{-1}
T = 150 K
Prism, orange
0.20 × 0.15 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.632, T_{max} = 0.746
6890 measured reflections
3801 independent reflections
2424 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.7°, θ_{min} = 3.5°
h = −7→9
k = −10→10
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 0.98
3801 reflections
205 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\s^2(F_o^2) + (0.0546P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Experimental. Single crystals were obtained by solvothermal synthesis at 393 K for 72 h in a PTFE-lined stainless steel autoclave. Reflections 0 0 1, 0 1 0 and 1 1 1 were affected by the beamstop and have been excluded from refinement using OMIT instructions in SHELXL. Data were truncated to 0.82 Ang resolution (SHEL 50 0.82 instruction) to improve data quality and reduce noise at high theta angles.

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.

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 $F^2 > 2\s(F^2)$ 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. Reflections 0 0 1, 0 1 0 and 1 1 1 were excluded from the refinement as they were affected by the beamstop (OMIT instructions in SHELXL). Data were truncated to d_min = 0.82 Ang (SHEL 50 0.82 instruction) to improve data quality and reduce noise at high theta angles.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe	0.30529 (6)	0.47954 (6)	0.24808 (4)	0.03937 (18)
S1	0.26516 (13)	0.69120 (12)	0.05193 (7)	0.0482 (3)
O3	0.3939 (3)	0.6441 (3)	0.31306 (19)	0.0492 (7)
S3	0.28122 (13)	0.73722 (13)	0.37470 (8)	0.0525 (3)
S2	−0.09552 (12)	0.56090 (13)	0.23945 (8)	0.0491 (3)
N1	0.2014 (4)	0.3294 (4)	0.1769 (3)	0.0585 (10)
O1	0.3801 (3)	0.5967 (3)	0.12312 (17)	0.0473 (7)
O2	0.0853 (3)	0.6094 (3)	0.24130 (18)	0.0454 (7)
N3	0.2331 (5)	0.3708 (5)	0.3739 (3)	0.0644 (11)
C1	0.4020 (7)	0.8140 (6)	−0.0133 (3)	0.0829 (17)
H1A	0.4454	0.8779	0.0273	0.124*
H1B	0.3420	0.8744	−0.0631	0.124*
H1C	0.4933	0.7567	−0.0396	0.124*
C2	0.2360 (6)	0.5762 (6)	−0.0361 (3)	0.0653 (13)
H2A	0.3435	0.5402	−0.0593	0.098*
H2B	0.1756	0.6335	−0.0869	0.098*
H2C	0.1732	0.4924	−0.0099	0.098*
C3	0.4139 (7)	0.7773 (7)	0.4617 (3)	0.0900 (19)
H3A	0.4574	0.6850	0.4966	0.135*
H3B	0.3515	0.8364	0.5037	0.135*
H3C	0.5053	0.8322	0.4326	0.135*
C5	−0.2116 (6)	0.7335 (6)	0.2058 (4)	0.0869 (18)
H5A	−0.3296	0.7189	0.2141	0.130*
H5B	−0.1866	0.7684	0.1408	0.130*
H5C	−0.1815	0.8066	0.2441	0.130*
C6	−0.1642 (6)	0.5271 (6)	0.3587 (3)	0.0719 (15)
H6A	−0.1223	0.6008	0.3929	0.108*
H6B	−0.1230	0.4286	0.3856	0.108*
H6C	−0.2848	0.5337	0.3623	0.108*
C31	0.1876 (5)	0.2758 (5)	0.4299 (3)	0.0466 (10)
C11	0.1646 (5)	0.2381 (5)	0.1325 (3)	0.0473 (10)
S11	0.11343 (18)	0.11629 (16)	0.06928 (10)	0.0744 (4)
S31	0.12611 (19)	0.14698 (15)	0.50741 (10)	0.0763 (4)
C4	0.2545 (8)	0.9126 (6)	0.3089 (4)	0.0949 (19)

H4A	0.3624	0.9497	0.2904	0.142*
H4B	0.1938	0.9805	0.3461	0.142*
H4C	0.1925	0.9050	0.2539	0.142*
S21	0.7549 (2)	0.12394 (19)	0.28209 (12)	0.1095 (6)
N2	0.5300 (4)	0.3672 (4)	0.2522 (2)	0.0548 (9)
C21	0.6214 (5)	0.2630 (5)	0.2652 (3)	0.0473 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe	0.0374 (3)	0.0410 (4)	0.0407 (3)	−0.0035 (2)	−0.0001 (2)	−0.0089 (3)
S1	0.0504 (6)	0.0506 (7)	0.0416 (6)	0.0079 (5)	0.0034 (5)	−0.0064 (5)
O3	0.0383 (15)	0.0578 (18)	0.0571 (17)	−0.0050 (13)	0.0010 (12)	−0.0281 (15)
S3	0.0465 (6)	0.0628 (8)	0.0526 (7)	−0.0003 (5)	−0.0010 (5)	−0.0255 (6)
S2	0.0349 (5)	0.0629 (7)	0.0551 (7)	−0.0055 (5)	−0.0023 (5)	−0.0260 (6)
N1	0.062 (2)	0.049 (2)	0.070 (3)	−0.0081 (19)	−0.0061 (19)	−0.021 (2)
O1	0.0420 (15)	0.0564 (18)	0.0419 (16)	−0.0007 (14)	−0.0024 (12)	−0.0017 (13)
O2	0.0329 (14)	0.0505 (17)	0.0543 (17)	−0.0035 (12)	0.0044 (12)	−0.0135 (14)
N3	0.067 (3)	0.068 (3)	0.053 (2)	−0.002 (2)	0.0080 (19)	0.005 (2)
C1	0.113 (5)	0.065 (4)	0.069 (3)	−0.027 (3)	−0.003 (3)	0.010 (3)
C2	0.075 (3)	0.073 (3)	0.051 (3)	−0.010 (3)	−0.013 (2)	−0.015 (2)
C3	0.092 (4)	0.123 (5)	0.066 (3)	0.014 (4)	−0.026 (3)	−0.053 (3)
C5	0.052 (3)	0.090 (4)	0.111 (5)	0.011 (3)	−0.008 (3)	0.005 (4)
C6	0.049 (3)	0.107 (4)	0.063 (3)	−0.021 (3)	0.007 (2)	−0.019 (3)
C31	0.047 (2)	0.052 (3)	0.043 (2)	−0.003 (2)	0.0030 (19)	−0.015 (2)
C11	0.048 (2)	0.042 (3)	0.051 (3)	0.005 (2)	−0.004 (2)	−0.005 (2)
S11	0.0858 (9)	0.0629 (8)	0.0830 (9)	−0.0047 (7)	−0.0180 (7)	−0.0367 (7)
S31	0.0960 (10)	0.0569 (8)	0.0751 (9)	−0.0222 (7)	0.0257 (7)	−0.0044 (7)
C4	0.139 (6)	0.067 (4)	0.078 (4)	0.020 (4)	−0.005 (4)	−0.021 (3)
S21	0.1331 (15)	0.0751 (11)	0.1091 (13)	0.0568 (11)	−0.0088 (11)	−0.0012 (9)
N2	0.053 (2)	0.055 (2)	0.056 (2)	0.011 (2)	−0.0037 (18)	−0.0123 (19)
C21	0.051 (3)	0.048 (3)	0.043 (2)	−0.002 (2)	0.0039 (19)	−0.010 (2)

Geometric parameters (Å, º)

Fe—O3	2.031 (3)	C2—H2A	0.9600
Fe—N1	2.035 (4)	C2—H2B	0.9600
Fe—O1	2.043 (3)	C2—H2C	0.9600
Fe—O2	2.041 (3)	C3—H3A	0.9600
Fe—N3	2.016 (4)	C3—H3B	0.9600
Fe—N2	1.997 (4)	C3—H3C	0.9600
S1—O1	1.529 (3)	C5—H5A	0.9600
S1—C1	1.759 (5)	C5—H5B	0.9600
S1—C2	1.768 (4)	C5—H5C	0.9600
O3—S3	1.527 (3)	C6—H6A	0.9600
S3—C3	1.755 (5)	C6—H6B	0.9600
S3—C4	1.731 (6)	C6—H6C	0.9600
S2—O2	1.538 (3)	C31—S31	1.584 (5)

S2—C5	1.773 (5)	C11—S11	1.596 (5)
S2—C6	1.769 (5)	C4—H4A	0.9600
N1—C11	1.164 (5)	C4—H4B	0.9600
N3—C31	1.158 (5)	C4—H4C	0.9600
C1—H1A	0.9600	S21—C21	1.587 (5)
C1—H1B	0.9600	N2—C21	1.148 (5)
C1—H1C	0.9600		

O3—Fe—N1	174.70 (13)	S1—C2—H2A	109.5
O3—Fe—O1	87.64 (12)	S1—C2—H2B	109.5
O3—Fe—O2	85.20 (11)	S1—C2—H2C	109.5
N1—Fe—O1	89.85 (14)	H2A—C2—H2B	109.5
N1—Fe—O2	90.08 (13)	H2A—C2—H2C	109.5
O2—Fe—O1	88.64 (11)	H2B—C2—H2C	109.5
N3—Fe—O3	90.20 (15)	S3—C3—H3A	109.5
N3—Fe—N1	92.26 (17)	S3—C3—H3B	109.5
N3—Fe—O1	177.81 (14)	S3—C3—H3C	109.5
N3—Fe—O2	90.79 (13)	H3A—C3—H3B	109.5
N2—Fe—O3	91.36 (13)	H3A—C3—H3C	109.5
N2—Fe—N1	93.23 (15)	H3B—C3—H3C	109.5
N2—Fe—O1	88.32 (13)	S2—C5—H5A	109.5
N2—Fe—O2	175.50 (13)	S2—C5—H5B	109.5
N2—Fe—N3	92.13 (15)	S2—C5—H5C	109.5
O1—S1—C1	103.3 (2)	H5A—C5—H5B	109.5
O1—S1—C2	105.5 (2)	H5A—C5—H5C	109.5
C1—S1—C2	97.6 (2)	H5B—C5—H5C	109.5
S3—O3—Fe	122.26 (16)	S2—C6—H6A	109.5
O3—S3—C3	104.5 (2)	S2—C6—H6B	109.5
O3—S3—C4	104.9 (2)	S2—C6—H6C	109.5
C4—S3—C3	100.5 (3)	H6A—C6—H6B	109.5
O2—S2—C5	102.7 (2)	H6A—C6—H6C	109.5
O2—S2—C6	105.63 (19)	H6B—C6—H6C	109.5
C6—S2—C5	99.1 (3)	N3—C31—S31	179.3 (4)
C11—N1—Fe	170.6 (4)	N1—C11—S11	178.5 (4)
S1—O1—Fe	125.96 (15)	S3—C4—H4A	109.5
S2—O2—Fe	128.93 (17)	S3—C4—H4B	109.5
C31—N3—Fe	160.1 (4)	S3—C4—H4C	109.5
S1—C1—H1A	109.5	H4A—C4—H4B	109.5
S1—C1—H1B	109.5	H4A—C4—H4C	109.5
S1—C1—H1C	109.5	H4B—C4—H4C	109.5
H1A—C1—H1B	109.5	C21—N2—Fe	155.5 (4)
H1A—C1—H1C	109.5	N2—C21—S21	177.3 (4)
H1B—C1—H1C	109.5		

Fe—O3—S3—C3	147.3 (3)	C2—S1—O1—Fe	−99.5 (2)
Fe—O3—S3—C4	−107.4 (3)	C5—S2—O2—Fe	−166.8 (2)
C1—S1—O1—Fe	158.6 (2)	C6—S2—O2—Fe	89.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···S31^{i}	0.96	2.84	3.751 (6)	159

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