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trans-Bis[2,5-bis(pyridin-2-yl)-1,3,4-thiadiazole- κ^2N^2,N^3]bis(methanol- κO)-iron(II) bis(perchlorate)

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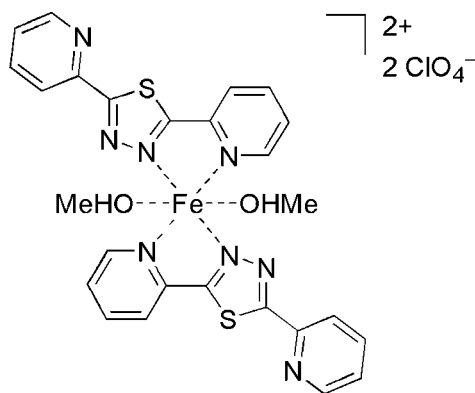
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.027; wR factor = 0.062; data-to-parameter ratio = 13.8.

The title compound, $[Fe(C_{12}H_8N_4S)_2(CH_3OH)_2](ClO_4)_2$, crystallized in the solvent-free form from a methanol solution. The Fe^{II} ion is located on a centre of inversion. The distorted N_4O_2 octahedral coordination geometry is formed by two N,N' -chelating equatorial 2,5-bis(pyridin-2-yl)-1,3,4-thiadiazole ligands and axially coordinating methanol coligands, resulting in the mononuclear *trans*-(N^2,N^3,O)₂ coordination mode. The methanol co-ligand is involved in a hydrogen bond to the perchlorate counter-ion.

Related literature

For other 3d metal structures of 2,5-bis(pyridin-2-yl)-1,3,4-thiadiazole, see: Klingele *et al.* (2010, 2012); Bentiss, Lagrenee, Mentre *et al.* (2004); Bentiss, Lagrenee, Vezin *et al.* (2004); Zheng *et al.* (2006); Bentiss *et al.* (2002); Wan *et al.* (2007). For related compounds, see: Guionneau *et al.* (2004). For the bridging capability of 4,4'-bispyridine- N,N' -dioxide, see: Jia *et al.* (2008).



Experimental

Crystal data

$[Fe(C_{12}H_8N_4S)_2(CH_3OH)_2](ClO_4)_2$ $\gamma = 74.735$ (2) $^\circ$
 $M_r = 799.40$ $V = 780.61$ (5) Å³
 Triclinic, $P\bar{1}$ $Z = 1$
 $a = 8.8410$ (3) Å Mo $K\alpha$ radiation
 $b = 9.5579$ (4) Å $\mu = 0.86$ mm⁻¹
 $c = 9.5875$ (4) Å $T = 100$ K
 $\alpha = 87.169$ (2) $^\circ$ $0.18 \times 0.08 \times 0.03$ mm
 $\beta = 88.945$ (2) $^\circ$

Data collection

Bruker APEXII CCD area-detector diffractometer 18025 measured reflections
 3128 independent reflections
 Absorption correction: multi-scan (SADABS; Bruker, 2001) 2789 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.019$
 $T_{min} = 0.861$, $T_{max} = 0.975$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$ H atoms treated by a mixture of independent and constrained refinement
 $wR(F^2) = 0.062$ $\Delta\rho_{max} = 0.49$ e Å⁻³
 $S = 1.05$ $\Delta\rho_{min} = -0.38$ e Å⁻³
 3128 reflections
 227 parameters

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O20-H20\cdots O11$	0.78 (3)	1.91 (3)	2.690 (2)	178 (3)

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: OLEX2.refine (Puschmann *et al.*, 2013); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008) and OLEX2.refine (Puschmann *et al.*, 2013); molecular graphics: DIAMOND (Brandenburg & Putz, 2011); software used to prepare material for publication: SHELXL97.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: LR2128).

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supporting information

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***trans*-Bis[2,5-bis(pyridin-2-yl)-1,3,4-thiadiazole- κ^2N^2,N^3]bis(methanol- κO)iron(II) bis(perchlorate)**

Dominic Kaase and Julia Klingele

S1. Introduction

The ligand 2,5-bis(pyridin-2-yl)-1,3,4-thiadiazole (**L**) is well known to have a suitable ligand field for the preparation of iron(II) spin crossover complexes (Klingele, *et al.*, 2010). Known examples are the 2:1-type complexes $[\text{Fe}(\text{L})_2(\text{NCS})_2]$, $[\text{Fe}(\text{L})_2(\text{NCSe})_2]$ and $[\text{Fe}(\text{L})_2(\text{NCBH}_3)_2]$ (Klingele *et al.*, 2012). 4,4'-Bispyridine-*N,N'*-dioxide is able to bridge metal ions to form multidimensional structures (Jia *et al.*, 2008). The title compound $[\text{Fe}(\text{L})_2(\text{MeOH})_2](\text{ClO}_4)_2$ was obtained unintentionally in the attempt to isolate one-dimensional chains of 4,4'-bispyridine-*N,N'*-dioxide-bridged $[\text{Fe}(\text{L})_2]^{2+}$ units.

S2. Experimental

S2.1. Synthesis and crystallization

Single crystals suitable for X-ray diffraction of the title compound were obtained unexpectedly by layering a MeOH solution of iron(II) perchlorate with a MeOH solution of 2,5-di(pyridin-2-yl)-1,3,4-thiadiazole and 4,4'-bispyridine-*N,N'*-dioxide in an argon atmosphere.

S2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in the Table below. All hydrogen atoms of the ligand and of the methyl hydrogen atoms of the methanol coligand were positioned geometrically and refined using a riding model. The hydrogen atom of the methanol hydroxyl group was located from the difference maps and refined freely and isotropically.

S3. Results and discussion

The ligand **L** was synthesized according to literature procedure (Klingele *et al.*, 2012). A single-crystal of $[\text{Fe}(\text{L})_2(\text{MeOH})_2](\text{ClO}_4)_2$ suitable for X-ray diffraction was obtained unexpectedly by layering a MeOH solution of iron(II) perchlorate with a MeOH solution of **L** and 4,4'-bispyridine-*N,N'*-dioxide. The mononuclear complex cation is formed by high-spin iron(II) ion coordinated by two bidentate ligands **L** and two MeOH coligands. The Fe—N [Fe—N_{pyr} 2.1516 (15), Fe—N_{tda} 2.2015 (15) Å] and Fe—O [2.0886 (13) Å] distances are in the expected range for high-spin iron(II) (Guionneau *et al.*, 2004).

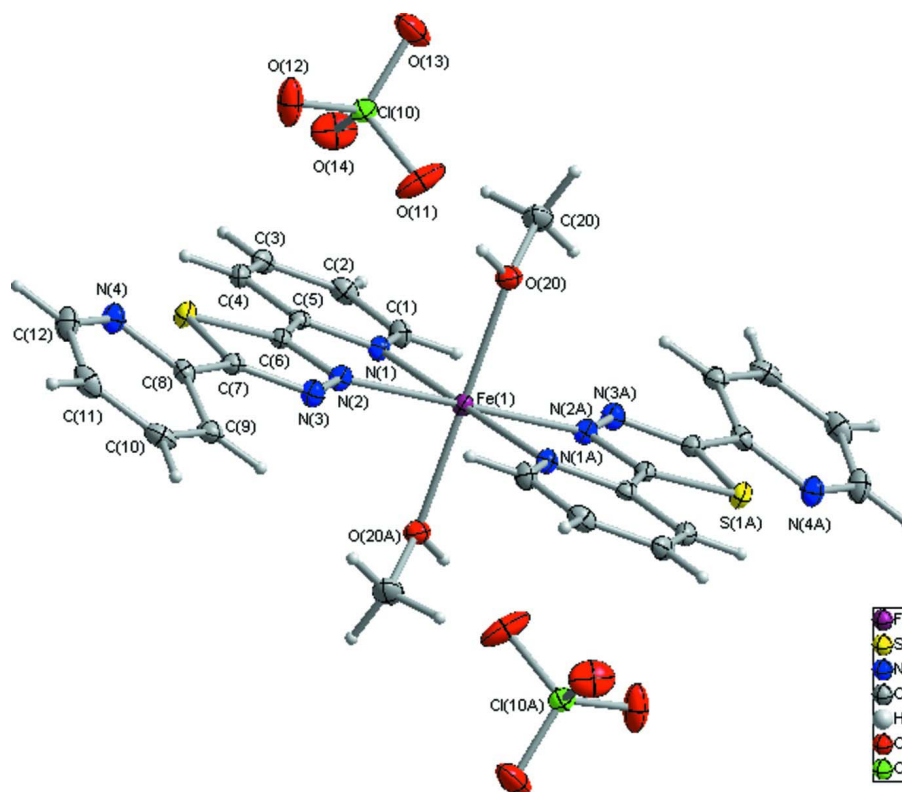


Figure 1

View of the complex $[\text{Fe}(\text{L})_2(\text{MeOH})_2](\text{ClO}_4)_2$. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn with arbitrary radii. [Symmetry code: (A) $-x, -y+2, -z$.]

trans-Bis[2,5-bis(pyridin-2-yl)-1,3,4-thiadiazole- $\kappa^2\text{N}^2, \text{N}^3$]bis(methanol- κO)iron(II) bis(perchlorate)

Crystal data

$[\text{Fe}(\text{C}_{12}\text{H}_8\text{N}_4\text{S})_2(\text{CH}_4\text{O})_2](\text{ClO}_4)_2$

$M_r = 799.40$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.8410\ (3)\ \text{\AA}$

$b = 9.5579\ (4)\ \text{\AA}$

$c = 9.5875\ (4)\ \text{\AA}$

$\alpha = 87.169\ (2)^\circ$

$\beta = 88.945\ (2)^\circ$

$\gamma = 74.735\ (2)^\circ$

$V = 780.61\ (5)\ \text{\AA}^3$

$Z = 1$

$F(000) = 408$

$D_x = 1.701\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9969 reflections

$\theta = 2.2\text{--}30.5^\circ$

$\mu = 0.86\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Plate, red

$0.18 \times 0.08 \times 0.03\ \text{mm}$

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: microfocus sealed tube

Multilayer mirror optics monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.861, T_{\max} = 0.975$

18025 measured reflections

3128 independent reflections

2789 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 26.4^\circ, \theta_{\min} = 2.1^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -11 \rightarrow 11$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.027$ $wR(F^2) = 0.062$ $S = 1.05$

3128 reflections

227 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0172P)^2 + 0.9493P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.49 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$ *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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.0000	1.0000	0.0000	0.01139 (10)
S1	0.22171 (5)	0.51392 (5)	0.06646 (5)	0.01390 (11)
N1	0.18464 (17)	0.89318 (16)	-0.14602 (15)	0.0128 (3)
N2	0.05730 (17)	0.77550 (16)	0.07183 (16)	0.0131 (3)
N3	-0.00347 (18)	0.70371 (17)	0.17709 (16)	0.0144 (3)
N4	0.14375 (19)	0.33511 (17)	0.30380 (17)	0.0171 (3)
C1	0.2469 (2)	0.9547 (2)	-0.25294 (19)	0.0154 (4)
H1	0.2034	1.0550	-0.2760	0.018*
C2	0.3724 (2)	0.8783 (2)	-0.33180 (19)	0.0162 (4)
H2	0.4130	0.9255	-0.4075	0.019*
C3	0.4371 (2)	0.7330 (2)	-0.2986 (2)	0.0154 (4)
H3	0.5228	0.6786	-0.3510	0.018*
C4	0.3748 (2)	0.6677 (2)	-0.18715 (19)	0.0138 (4)
H4	0.4174	0.5679	-0.1617	0.017*
C5	0.2495 (2)	0.75062 (19)	-0.11400 (18)	0.0115 (4)
C6	0.1740 (2)	0.69113 (19)	0.00391 (18)	0.0118 (4)
C7	0.0705 (2)	0.5668 (2)	0.18660 (19)	0.0131 (4)
C8	0.0312 (2)	0.4599 (2)	0.28666 (19)	0.0131 (4)
C9	-0.1131 (2)	0.4898 (2)	0.35465 (19)	0.0158 (4)
H9	-0.1888	0.5801	0.3387	0.019*
C10	-0.1429 (2)	0.3835 (2)	0.4465 (2)	0.0186 (4)
H10	-0.2402	0.3992	0.4949	0.022*
C11	-0.0285 (2)	0.2540 (2)	0.4665 (2)	0.0200 (4)
H11	-0.0462	0.1794	0.5288	0.024*

C12	0.1125 (2)	0.2350 (2)	0.3942 (2)	0.0201 (4)
H12	0.1908	0.1463	0.4098	0.024*
C20	-0.2991 (2)	0.9010 (2)	-0.0662 (2)	0.0234 (5)
H20A	-0.3466	0.8617	-0.1416	0.035*
H20B	-0.3792	0.9775	-0.0223	0.035*
H20C	-0.2552	0.8232	0.0036	0.035*
O20	-0.17589 (15)	0.96075 (15)	-0.12275 (15)	0.0173 (3)
H20	-0.212 (3)	1.021 (3)	-0.179 (3)	0.026*
Cl10	-0.46099 (5)	1.25579 (5)	-0.29619 (5)	0.01521 (11)
O11	-0.30426 (17)	1.16340 (19)	-0.32171 (16)	0.0353 (4)
O12	-0.47275 (19)	1.39590 (16)	-0.36152 (17)	0.0320 (4)
O13	-0.57261 (18)	1.19384 (18)	-0.35684 (18)	0.0339 (4)
O14	-0.48818 (18)	1.26721 (19)	-0.14843 (15)	0.0327 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01072 (18)	0.00969 (19)	0.01282 (19)	-0.00126 (14)	0.00130 (14)	0.00030 (14)
S1	0.0141 (2)	0.0101 (2)	0.0162 (2)	-0.00128 (17)	0.00275 (17)	0.00076 (18)
N1	0.0137 (8)	0.0124 (8)	0.0118 (8)	-0.0027 (6)	0.0007 (6)	-0.0007 (6)
N2	0.0133 (7)	0.0125 (8)	0.0128 (8)	-0.0024 (6)	0.0018 (6)	0.0005 (6)
N3	0.0159 (8)	0.0134 (8)	0.0136 (8)	-0.0042 (6)	0.0017 (6)	0.0012 (6)
N4	0.0202 (8)	0.0136 (8)	0.0171 (8)	-0.0041 (7)	0.0023 (7)	0.0009 (7)
C1	0.0184 (9)	0.0129 (9)	0.0153 (9)	-0.0048 (8)	0.0005 (7)	-0.0001 (7)
C2	0.0177 (9)	0.0198 (10)	0.0134 (9)	-0.0090 (8)	0.0025 (7)	-0.0020 (8)
C3	0.0124 (9)	0.0184 (10)	0.0163 (9)	-0.0047 (7)	0.0026 (7)	-0.0070 (8)
C4	0.0137 (9)	0.0115 (9)	0.0157 (9)	-0.0021 (7)	-0.0010 (7)	-0.0026 (7)
C5	0.0119 (8)	0.0128 (9)	0.0104 (8)	-0.0041 (7)	-0.0022 (7)	-0.0014 (7)
C6	0.0117 (8)	0.0109 (9)	0.0126 (9)	-0.0026 (7)	-0.0025 (7)	-0.0009 (7)
C7	0.0115 (9)	0.0152 (9)	0.0127 (9)	-0.0036 (7)	-0.0007 (7)	-0.0015 (7)
C8	0.0159 (9)	0.0129 (9)	0.0118 (9)	-0.0060 (7)	-0.0007 (7)	-0.0015 (7)
C9	0.0152 (9)	0.0170 (10)	0.0161 (9)	-0.0057 (8)	-0.0035 (7)	-0.0003 (8)
C10	0.0184 (10)	0.0262 (11)	0.0153 (10)	-0.0130 (8)	0.0002 (8)	-0.0026 (8)
C11	0.0301 (11)	0.0198 (10)	0.0144 (10)	-0.0145 (9)	0.0005 (8)	0.0011 (8)
C12	0.0272 (11)	0.0131 (10)	0.0189 (10)	-0.0037 (8)	-0.0001 (8)	0.0015 (8)
C20	0.0144 (10)	0.0255 (11)	0.0320 (12)	-0.0074 (8)	0.0032 (8)	-0.0068 (9)
O20	0.0145 (7)	0.0178 (7)	0.0192 (7)	-0.0037 (6)	-0.0026 (5)	0.0009 (6)
Cl10	0.0138 (2)	0.0166 (2)	0.0151 (2)	-0.00390 (17)	0.00130 (17)	0.00016 (18)
O11	0.0177 (8)	0.0490 (11)	0.0267 (9)	0.0102 (7)	0.0051 (6)	0.0129 (8)
O12	0.0452 (10)	0.0162 (8)	0.0349 (9)	-0.0095 (7)	0.0194 (7)	-0.0019 (7)
O13	0.0289 (9)	0.0383 (10)	0.0423 (10)	-0.0201 (7)	0.0035 (7)	-0.0160 (8)
O14	0.0312 (9)	0.0527 (11)	0.0135 (7)	-0.0105 (8)	0.0059 (6)	-0.0004 (7)

Geometric parameters (Å, °)

Fe1—O20	2.0886 (13)	C1—C2	1.391 (3)
Fe1—O20 ⁱ	2.0886 (13)	C2—C3	1.379 (3)
Fe1—N2 ⁱ	2.1516 (15)	C3—C4	1.389 (3)

Fe1—N2	2.1516 (15)	C4—C5	1.382 (3)
Fe1—N1 ⁱ	2.2015 (15)	C5—C6	1.468 (2)
Fe1—N1	2.2015 (15)	C7—C8	1.471 (2)
S1—C6	1.7144 (18)	C8—C9	1.389 (3)
S1—C7	1.7364 (19)	C9—C10	1.386 (3)
N1—C1	1.338 (2)	C10—C11	1.384 (3)
N1—C5	1.354 (2)	C11—C12	1.389 (3)
N2—C6	1.315 (2)	C20—O20	1.443 (2)
N2—N3	1.372 (2)	Cl10—O13	1.4232 (15)
N3—C7	1.299 (2)	Cl10—O12	1.4292 (15)
N4—C12	1.339 (2)	Cl10—O14	1.4372 (15)
N4—C8	1.342 (2)	Cl10—O11	1.4574 (15)
O20—Fe1—O20 ⁱ	180.00 (4)	C2—C3—C4	118.88 (17)
O20—Fe1—N2 ⁱ	91.48 (6)	C5—C4—C3	118.73 (17)
O20 ⁱ —Fe1—N2 ⁱ	88.52 (6)	N1—C5—C4	122.90 (16)
O20—Fe1—N2	88.52 (6)	N1—C5—C6	114.25 (16)
O20 ⁱ —Fe1—N2	91.48 (6)	C4—C5—C6	122.85 (16)
N2 ⁱ —Fe1—N2	180.0	N2—C6—C5	120.39 (16)
O20—Fe1—N1 ⁱ	87.99 (5)	N2—C6—S1	113.48 (13)
O20 ⁱ —Fe1—N1 ⁱ	92.01 (5)	C5—C6—S1	126.13 (14)
N2 ⁱ —Fe1—N1 ⁱ	76.37 (6)	N3—C7—C8	124.64 (17)
N2—Fe1—N1 ⁱ	103.63 (6)	N3—C7—S1	114.73 (13)
O20—Fe1—N1	92.01 (5)	C8—C7—S1	120.61 (14)
O20 ⁱ —Fe1—N1	87.99 (5)	N4—C8—C9	124.49 (17)
N2 ⁱ —Fe1—N1	103.63 (6)	N4—C8—C7	114.70 (16)
N2—Fe1—N1	76.37 (6)	C9—C8—C7	120.81 (17)
N1 ⁱ —Fe1—N1	180.0	C10—C9—C8	117.74 (18)
C6—S1—C7	86.84 (9)	C11—C10—C9	118.93 (18)
C1—N1—C5	117.61 (16)	C10—C11—C12	118.91 (18)
C1—N1—Fe1	127.76 (12)	N4—C12—C11	123.43 (19)
C5—N1—Fe1	114.39 (11)	C20—O20—Fe1	123.03 (12)
C6—N2—N3	113.63 (15)	O13—Cl10—O12	109.10 (10)
C6—N2—Fe1	114.27 (12)	O13—Cl10—O14	110.30 (10)
N3—N2—Fe1	132.09 (12)	O12—Cl10—O14	110.33 (10)
C7—N3—N2	111.33 (15)	O13—Cl10—O11	108.75 (10)
C12—N4—C8	116.48 (17)	O12—Cl10—O11	108.62 (9)
N1—C1—C2	122.82 (17)	O14—Cl10—O11	109.71 (9)
C3—C2—C1	119.05 (17)		
O20—Fe1—N1—C1	92.67 (15)	Fe1—N2—C6—C5	-2.5 (2)
O20 ⁱ —Fe1—N1—C1	-87.33 (15)	N3—N2—C6—S1	-0.96 (19)
N2 ⁱ —Fe1—N1—C1	0.65 (16)	Fe1—N2—C6—S1	178.04 (8)
N2—Fe1—N1—C1	-179.35 (16)	N1—C5—C6—N2	-2.2 (2)
O20—Fe1—N1—C5	-93.28 (12)	C4—C5—C6—N2	178.55 (16)
O20 ⁱ —Fe1—N1—C5	86.72 (12)	N1—C5—C6—S1	177.18 (13)
N2 ⁱ —Fe1—N1—C5	174.71 (12)	C4—C5—C6—S1	-2.0 (3)
N2—Fe1—N1—C5	-5.29 (12)	C7—S1—C6—N2	0.74 (14)

O20—Fe1—N2—C6	96.46 (13)	C7—S1—C6—C5	-178.71 (16)
O20 ⁱ —Fe1—N2—C6	-83.54 (13)	N2—N3—C7—C8	-178.46 (16)
N1 ⁱ —Fe1—N2—C6	-175.97 (12)	N2—N3—C7—S1	-0.07 (19)
N1—Fe1—N2—C6	4.03 (12)	C6—S1—C7—N3	-0.37 (15)
O20—Fe1—N2—N3	-84.78 (15)	C6—S1—C7—C8	178.09 (15)
O20 ⁱ —Fe1—N2—N3	95.22 (15)	C12—N4—C8—C9	-0.7 (3)
N1 ⁱ —Fe1—N2—N3	2.79 (16)	C12—N4—C8—C7	179.92 (17)
N1—Fe1—N2—N3	-177.21 (16)	N3—C7—C8—N4	-163.82 (17)
C6—N2—N3—C7	0.7 (2)	S1—C7—C8—N4	17.9 (2)
Fe1—N2—N3—C7	-178.11 (13)	N3—C7—C8—C9	16.8 (3)
C5—N1—C1—C2	0.7 (3)	S1—C7—C8—C9	-161.50 (14)
Fe1—N1—C1—C2	174.61 (13)	N4—C8—C9—C10	0.0 (3)
N1—C1—C2—C3	-0.5 (3)	C7—C8—C9—C10	179.33 (17)
C1—C2—C3—C4	-0.1 (3)	C8—C9—C10—C11	0.3 (3)
C2—C3—C4—C5	0.3 (3)	C9—C10—C11—C12	0.1 (3)
C1—N1—C5—C4	-0.4 (3)	C8—N4—C12—C11	1.2 (3)
Fe1—N1—C5—C4	-175.14 (13)	C10—C11—C12—N4	-0.9 (3)
C1—N1—C5—C6	-179.67 (15)	N2 ⁱ —Fe1—O20—C20	-124.06 (14)
Fe1—N1—C5—C6	5.64 (19)	N2—Fe1—O20—C20	55.94 (14)
C3—C4—C5—N1	-0.1 (3)	N1 ⁱ —Fe1—O20—C20	-47.76 (14)
C3—C4—C5—C6	179.08 (16)	N1—Fe1—O20—C20	132.24 (14)
N3—N2—C6—C5	178.53 (15)		

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

Hydrogen-bond geometry (Å, °)

<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>
O20—H20 \cdots O11	0.78 (3)	1.91 (3)	2.690 (2)	178 (3)