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Tris(4,4′-bi-1,3-thiazole-κ^2N,N')iron(II) tetrabromidoferrate(III) bromide

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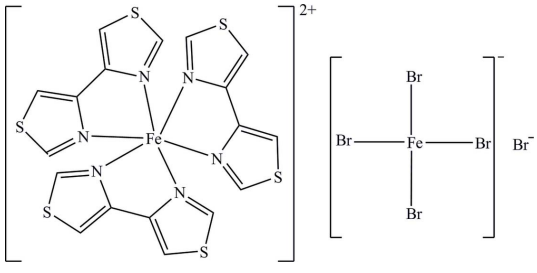
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.036; wR factor = 0.085; data-to-parameter ratio = 22.4.

In the $[Fe(4,4'\text{-bit})_3]^{2+}$ (4,4′-bit is 4,4′-bi-1,3-thiazole) cation of the title compound, $[Fe(C_6H_4N_2S_2)_3][FeBr_4]Br$, the Fe^{II} atom (3 symmetry) is six-coordinated in a distorted octahedral geometry by six N atoms from three 4,4′-bit ligands. In the $[FeBr_4]^-$ anion, the Fe^{III} atom (3 symmetry) is four-coordinated in a distorted tetrahedral geometry. In the crystal, intermolecular C—H···Br hydrogen bonds and Br···π interactions [Br···centroid distances = 3.562 (3) and 3.765 (2) Å] link the cations and anions, stabilizing the structure.

Related literature

For general background to metal complexes with 4,4′-bi-1,3-thiazole ligands, see: Baker & Goodwin (1985); Mahjoub & Morsali (2001, 2002*a*,*b*). For related structures, see: Al-Hashemi *et al.* (2009); Ali & Al-Far (2007); Amani *et al.* (2007*a*,*b*, 2009); Craig *et al.* (1988); Figgis *et al.* (1983); Jia *et al.* (2006); Khavasi *et al.* (2008); Kulkarni *et al.* (1998); Notash *et al.* (2008, 2009); Rahimi *et al.* (2009); Safari *et al.* (2009). For the synthesis of the ligand, see: Erlenmeyer & Ueberwasser (1939).



Experimental

Crystal data

$[Fe(C_6H_4N_2S_2)_3][FeBr_4]Br$
M_r = 1015.95
Trigonal, $R3$
a = 12.0638 (7) Å
c = 17.6907 (13) Å
V = 2229.7 (2) Å^3
Z = 3
Mo $K\alpha$ radiation
μ = 8.14 mm^{-1}
T = 100 K
0.45 × 0.35 × 0.30 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.031, T_{max} = 0.086
8430 measured reflections
2508 independent reflections
2427 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.085
S = 1.01
2508 reflections
112 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}
Absolute structure: Flack (1983), 1195 Friedel pairs
Flack parameter: 0.021 (9)

Table 1
Selected bond lengths (Å).

Fe1—N1	1.962 (3)	Fe2—Br1	2.3348 (5)
Fe1—N2	1.974 (3)	Fe2—Br2	2.3370 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···Br3	0.93	2.81	3.665 (5)	153
C5—H5A···Br3	0.93	2.97	3.798 (5)	149

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2404).

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Tris(4,4′-bi-1,3-thiazole-κ^2N,N')iron(II) tetrabromidoferrate(III) bromide

Anita Abedi, Vahid Amani and Nasser Safari

S1. Comment

Erlenmeyer & Ueberwasser (1939) first reported the synthesis of 4,4′-bi-1,3-thiazole (4,4′-bit) and Craig *et al.* (1988) determined the structure of this compound. Although 4,4′-bit is a good bidentate ligand, a few of its metal complexes have been prepared, such as those of nickel and iron (Baker & Goodwin, 1985), lead (Mahjoub & Morsali, 2001, 2002*a*) and bismuth (Mahjoub & Morsali, 2002*b*). We recently introduced the coordination chemistry of 2,2′-dimethyl-4,4′-bi-1,3-thiazole with copper (Al-Hashemi *et al.*, 2009), zinc and mercury (Khavasi *et al.*, 2008; Safari *et al.*, 2009), cadmium (Notash *et al.*, 2009) and thallium (Notash *et al.*, 2008). We report here the synthesis and crystal structure of the title compound.

The asymmetric unit of the title compound (Fig. 1), contains one third of an $[Fe(4,4'\text{-bit})_3]^{2+}$ cation, one third of an $[FeBr_4]^-$ anion and one third of a Br^- anion. In the $[Fe(4,4'\text{-bit})_3]^{2+}$ cation, the Fe^{II} atom (3 symmetry) is six-coordinated in a distorted octahedral geometry by six N atoms from three 4,4′-bit ligands. The Fe—N bond lengths are 1.962 (3) and 1.974 (3) Å (Table 1). The average Fe—N bond distances in high-spin iron(II) and (III) complexes with phenanthroline and bipyridine are around 2.2 Å. However, for low-spin iron(II) and (III) complexes, the Fe—N distances less than 2.0 Å have been reported (Amani *et al.*, 2007*a*,b, 2009; Figgis *et al.*, 1983; Kulkarni *et al.*, 1998; Rahimi *et al.*, 2009). Therefore, in the $[Fe(4,4'\text{-bit})_3]^{2+}$ cation, the Fe—N bond distances are unambiguous in accord with low-spin iron(II). The N—Fe—N bond angles are in the range of 82.00 (14) to 171.87 (14)°. The bond angles and distances are in good agreement to those of $[Fe(4,4'\text{-bit})_3]^{2+}$ cations, which have been found in other structures (Baker & Goodwin, 1985). In the $[FeBr_4]^-$ anion, the Fe^{III} atom (3 symmetry) is four-coordinated in a distorted tetrahedral geometry by four Br atoms. The Fe—Br bond lengths are 2.3348 (5) and 2.3370 (12) Å. The Br—Fe—Br angles, in turn, span the ranges of 108.64 (3) to 110.29 (3)°, and the bond angles and distances are in good agreement to those of $[FeBr_4]^-$ anions, which have been found in other structures (Ali & Al-Far 2007; Jia *et al.*, 2006).

Fig. 2 shows significant intermolecular C—H···Br hydrogen bonds in the title compound (Table 2). The hydrogen bonds cause the formation of a supramolecular architecture, best described as built up by $Br(thiazol)_9$ supramolecular synthons (Fig. 2) assembled *via* C—H···Br hydrogen bonds, where nine thiazole groups surround one (central) uncoordinated bromide ion. These synthons are further connected into an adamantoid-like network that extends into a three-dimensional structure. The discrete $[FeBr_4]^-$ anions occupy the cavities that result from the three-dimensional assembly of the $Br(thiazol)_9$ entities. There also exist intermolecular Br···π interactions between the $[FeBr_4]^-$ anions and thiazole rings in the crystal structure (Fig. 3), with Br1···*Cg*1 = 3.562 (3) and Br1^{i}···*Cg*2 = 3.765 (2) Å [*Cg*1 and *Cg*2 are the centroids of C1, C2, C3, N2, S2 ring and C4, C5, C6, N1, S1 ring. Symmetry code: (i) 1-x+y, 2-x, z]. The hydrogen bonds and Br···π interactions link the cations and anions, which may be effective in the stabilization of the structure.

S2. Experimental

4,4′-bi-1,3-thiazole (0.11 g, 0.63 mmol) in CH_3OH (20 ml) was added to a solution of $FeBr_3$ (0.06 g, 0.21 mmol) in CH_3OH (10 ml) and the resulting red solution was stirred at 313 K for 1 h. The red colored precipitated product was recrystallized from CH_3CN/CH_3OH (v/v 2:1). After two weeks, dark-red prismatic crystals of the title compound were isolated (yield: 0.08 g, 75.0%; m.p. 464 K).

S3. Refinement

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

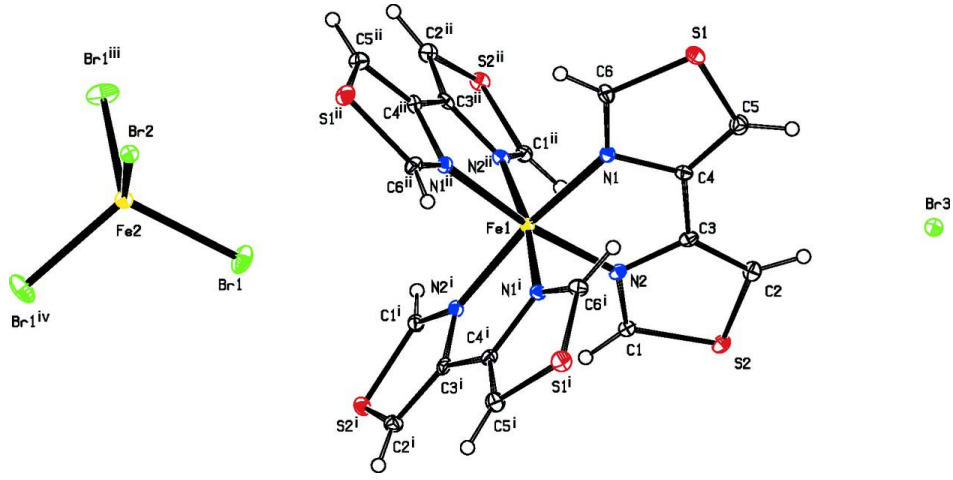

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) 1-x+y, 2-x, z; (ii) 2-y, 1+x-y, z; (iii) 1-y, 1+x-y, z; (iv) -x+y, 1-x, z.]

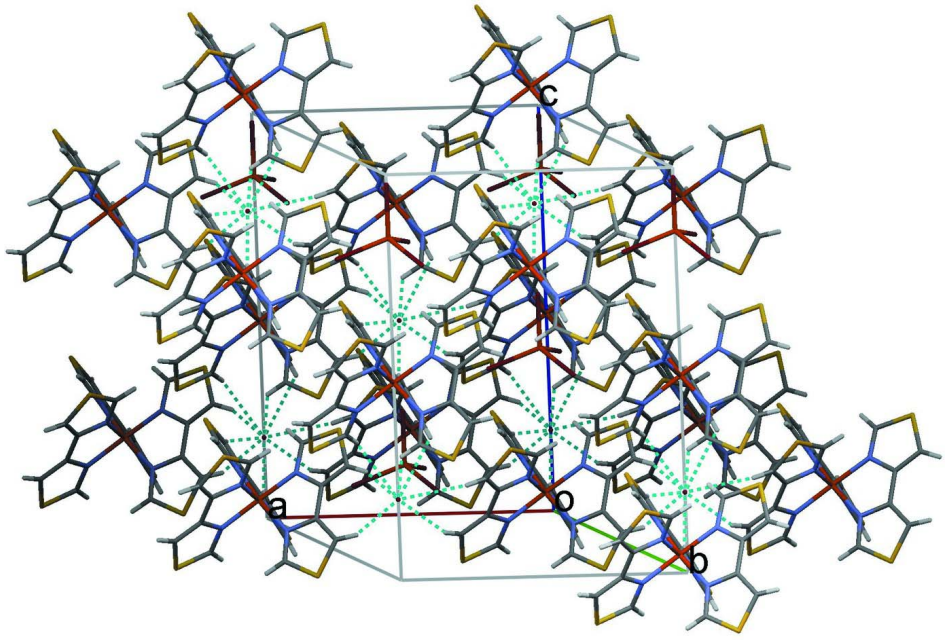

Figure 2

Crystal packing diagram for the title compound. Hydrogen bonds are shown as dashed lines.

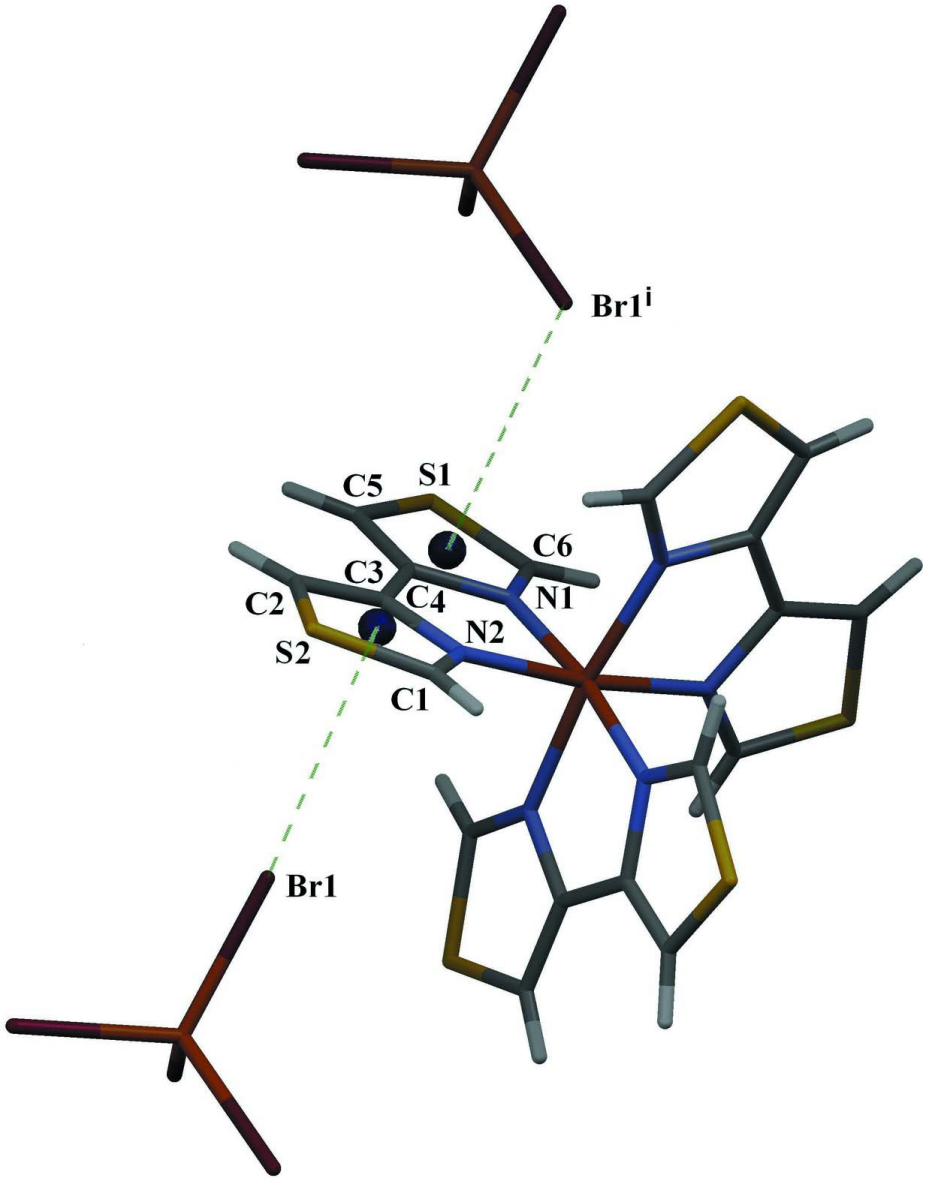

Figure 3

Intermolecular Br···π interactions (dashed lines) in the title compound. [Symmetry code: (i) 1-x+y, 2-x, z.]

Tris(4,4′-bi-1,3-thiazole-κ^2N,N')iron(II) tetrabromidoferrate(III) bromide

Crystal data

$[Fe(C_6H_4N_2S_2)_3][FeBr_4]Br$
M_r = 1015.95
Trigonal, $R3$
Hall symbol: R 3
a = 12.0638 (7) Å
c = 17.6907 (13) Å
V = 2229.7 (2) Å^3
Z = 3
$F(000)$ = 1455
D_x = 2.270 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1635 reflections
θ = 3.0–28.0°
μ = 8.14 mm^{-1}
T = 100 K
Prism, dark-red
0.45 × 0.35 × 0.30 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.031, T_{max} = 0.086
8430 measured reflections
2508 independent reflections
2427 reflections with $I > 2\sigma(I)$
R_{int} = 0.099
θ_{max} = 28.9°, θ_{min} = 2.3°
h = −16→16
k = −16→16
l = −24→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.085
S = 1.01
2508 reflections
112 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}
Absolute structure: Flack (1983), 1195 Friedel pairs
Absolute structure parameter: 0.021 (9)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.53314 (4)	0.70585 (5)	0.46767 (3)	0.02946 (13)
Br2	0.3333	0.6667	0.64196 (3)	0.01401 (14)
Br3	1.6667	1.3333	0.53208 (4)	0.01483 (14)
Fe1	1.0000	1.0000	0.48640 (5)	0.00941 (17)
Fe2	0.3333	0.6667	0.50986 (6)	0.01351 (18)
S1	1.25908 (10)	1.31480 (10)	0.64504 (6)	0.0182 (2)
S2	1.33303 (9)	1.07879 (10)	0.33584 (6)	0.01552 (19)
N1	1.1247 (3)	1.1426 (3)	0.54875 (19)	0.0120 (6)
N2	1.1543 (3)	1.0443 (3)	0.42603 (19)	0.0121 (6)
C1	1.1756 (4)	1.0038 (4)	0.3613 (2)	0.0141 (7)
H1A	1.1107	0.9401	0.3323	0.017*
C2	1.3758 (4)	1.1697 (4)	0.4169 (2)	0.0161 (7)
H2A	1.4589	1.2296	0.4310	0.019*
C3	1.2677 (4)	1.1394 (4)	0.4572 (2)	0.0132 (7)
C4	1.2524 (4)	1.1950 (4)	0.5268 (2)	0.0127 (7)
C5	1.3381 (4)	1.2906 (4)	0.5716 (3)	0.0185 (8)
H5A	1.4262	1.3361	0.5639	0.022*
C6	1.1159 (4)	1.1969 (4)	0.6109 (2)	0.0154 (7)
H6A	1.0383	1.1732	0.6345	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0213 (2)	0.0518 (3)	0.0176 (2)	0.0201 (2)	0.00229 (16)	−0.0064 (2)

Br2	0.01593 (18)	0.01593 (18)	0.0102 (3)	0.00796 (9)	0.000	0.000
Br3	0.01604 (19)	0.01604 (19)	0.0124 (3)	0.00802 (9)	0.000	0.000
Fe1	0.0096 (2)	0.0096 (2)	0.0090 (4)	0.00479 (11)	0.000	0.000
Fe2	0.0153 (3)	0.0153 (3)	0.0099 (4)	0.00764 (13)	0.000	0.000
S1	0.0184 (4)	0.0170 (4)	0.0170 (5)	0.0072 (4)	−0.0042 (4)	−0.0073 (4)
S2	0.0162 (4)	0.0198 (4)	0.0128 (4)	0.0107 (3)	0.0037 (3)	0.0013 (3)
N1	0.0113 (13)	0.0118 (14)	0.0122 (14)	0.0052 (12)	0.0016 (11)	0.0003 (11)
N2	0.0143 (14)	0.0143 (14)	0.0102 (13)	0.0090 (12)	0.0021 (12)	0.0016 (12)
C1	0.0135 (16)	0.0138 (16)	0.0157 (17)	0.0074 (14)	0.0000 (13)	−0.0008 (13)
C2	0.0161 (16)	0.0175 (17)	0.0139 (18)	0.0078 (14)	0.0027 (14)	0.0035 (14)
C3	0.0173 (17)	0.0131 (15)	0.0134 (16)	0.0106 (14)	0.0009 (13)	0.0036 (13)
C4	0.0156 (16)	0.0101 (15)	0.0126 (16)	0.0065 (13)	0.0010 (13)	0.0001 (12)
C5	0.0168 (17)	0.0198 (19)	0.0192 (19)	0.0092 (15)	−0.0020 (14)	−0.0002 (15)
C6	0.0135 (16)	0.0148 (17)	0.0151 (17)	0.0048 (13)	−0.0024 (14)	−0.0020 (13)

Geometric parameters (Å, º)

Fe1—N1	1.962 (3)	N2—C1	1.320 (5)
Fe1—N2	1.974 (3)	N2—C3	1.385 (5)
Fe2—Br1	2.3348 (5)	C1—H1A	0.9300
Fe2—Br2	2.3370 (12)	C2—C3	1.366 (6)
S1—C6	1.706 (4)	C2—H2A	0.9300
S1—C5	1.721 (4)	C3—C4	1.458 (5)
S2—C1	1.706 (4)	C4—C5	1.355 (6)
S2—C2	1.720 (4)	C5—H5A	0.9300
N1—C6	1.312 (5)	C6—H6A	0.9300
N1—C4	1.396 (5)		
N1—Fe1—N1^{i}	91.50 (14)	C6—N1—Fe1	133.8 (3)
N1—Fe1—N1^{ii}	91.50 (14)	C4—N1—Fe1	115.4 (3)
N1^{i}—Fe1—N1^{ii}	91.50 (14)	C1—N2—C3	111.0 (3)
N1—Fe1—N2^{i}	171.87 (13)	C1—N2—Fe1	134.5 (3)
N1^{i}—Fe1—N2^{i}	82.00 (14)	C3—N2—Fe1	114.6 (3)
N1^{ii}—Fe1—N2^{i}	93.53 (13)	N2—C1—S2	113.8 (3)
N1—Fe1—N2	82.00 (14)	N2—C1—H1A	123.1
N1^{i}—Fe1—N2	93.53 (13)	S2—C1—H1A	123.1
N1^{ii}—Fe1—N2	171.87 (13)	C3—C2—S2	108.8 (3)
N2^{i}—Fe1—N2	93.49 (14)	C3—C2—H2A	125.6
N1—Fe1—N2^{ii}	93.53 (13)	S2—C2—H2A	125.6
N1^{i}—Fe1—N2^{ii}	171.87 (14)	C2—C3—N2	115.4 (3)
N1^{ii}—Fe1—N2^{ii}	82.00 (14)	C2—C3—C4	129.9 (4)
N2^{i}—Fe1—N2^{ii}	93.49 (14)	N2—C3—C4	114.7 (3)
N2—Fe1—N2^{ii}	93.49 (14)	C5—C4—N1	115.0 (4)
Br1^{iii}—Fe2—Br1^{iv}	110.29 (3)	C5—C4—C3	131.9 (4)
Br1^{iii}—Fe2—Br1	110.29 (3)	N1—C4—C3	113.0 (3)
Br1^{iv}—Fe2—Br1	110.29 (3)	C4—C5—S1	109.5 (3)
Br1^{iii}—Fe2—Br2	108.64 (3)	C4—C5—H5A	125.2
Br1^{iv}—Fe2—Br2	108.64 (3)	S1—C5—H5A	125.2

Br1—Fe2—Br2	108.64 (3)	N1—C6—S1	114.3 (3)
C6—S1—C5	90.4 (2)	N1—C6—H6A	122.8
C1—S2—C2	91.01 (19)	S1—C6—H6A	122.8
C6—N1—C4	110.7 (3)		

N1^{i}—Fe1—N1—C6	−86.9 (3)	S2—C2—C3—N2	1.7 (4)
N1^{ii}—Fe1—N1—C6	4.6 (4)	S2—C2—C3—C4	−175.8 (3)
N2—Fe1—N1—C6	179.8 (4)	C1—N2—C3—C2	−1.2 (5)
N2^{ii}—Fe1—N1—C6	86.7 (4)	Fe1—N2—C3—C2	178.8 (3)
N1^{i}—Fe1—N1—C4	88.3 (3)	C1—N2—C3—C4	176.7 (3)
N1^{ii}—Fe1—N1—C4	179.8 (3)	Fe1—N2—C3—C4	−3.3 (4)
N2—Fe1—N1—C4	−5.1 (3)	C6—N1—C4—C5	−1.7 (5)
N2^{ii}—Fe1—N1—C4	−98.1 (3)	Fe1—N1—C4—C5	−178.0 (3)
N1—Fe1—N2—C1	−175.5 (4)	C6—N1—C4—C3	−179.1 (3)
N1^{i}—Fe1—N2—C1	93.5 (4)	Fe1—N1—C4—C3	4.7 (4)
N2^{i}—Fe1—N2—C1	11.3 (4)	C2—C3—C4—C5	−0.2 (7)
N2^{ii}—Fe1—N2—C1	−82.4 (3)	N2—C3—C4—C5	−177.7 (4)
N1—Fe1—N2—C3	4.6 (3)	C2—C3—C4—N1	176.7 (4)
N1^{i}—Fe1—N2—C3	−86.5 (3)	N2—C3—C4—N1	−0.8 (5)
N2^{i}—Fe1—N2—C3	−168.6 (3)	N1—C4—C5—S1	1.4 (5)
N2^{ii}—Fe1—N2—C3	97.6 (3)	C3—C4—C5—S1	178.2 (3)
C3—N2—C1—S2	0.0 (4)	C6—S1—C5—C4	−0.6 (3)
Fe1—N2—C1—S2	−180.0 (2)	C4—N1—C6—S1	1.2 (4)
C2—S2—C1—N2	0.8 (3)	Fe1—N1—C6—S1	176.5 (2)
C1—S2—C2—C3	−1.4 (3)	C5—S1—C6—N1	−0.3 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···Br3	0.93	2.81	3.665 (5)	153
C5—H5*A*···Br3	0.93	2.97	3.798 (5)	149