Acta Cryst E STRUCTURE REPORTS

ISSN 1600-5368

Crystal structure of 3-{1′-[3,5-bis(trifluoromethyl)-phenyl]ferrocenyl}-4-bromothiophene

Elisabeth A. Poppitz, Marcus Korb and Heinrich Lang*

Technische Universität Chemnitz, Fakultät für Naturwissenschaften, Institut für Chemie, Anorganische Chemie, D-09107 Chemnitz. *Correspondence e-mail: heinrich.lang@chemie.tu-chemnitz.de

Received 8 August 2014
Accepted 15 September 2014

Edited by M. Weil, Vienna University of Technology, Austria

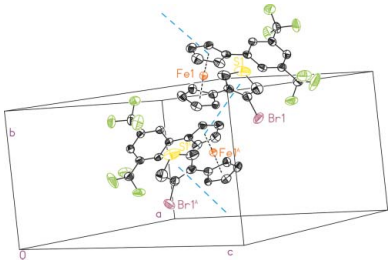
Keywords: crystal structure; ferrocenyl backbone; thiophene; Negishi cross-coupling

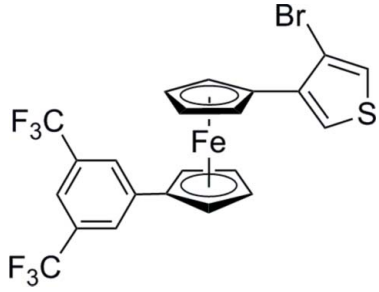
CCDC reference: 1018554
Supporting information: this article has supporting information at journals.iucr.org/e

The molecular structure of the title compound, $[Fe(C_9H_6BrS)(C_{13}H_7F_6)]$, consists of a ferrocene backbone with a bis(trifluoromethyl)phenyl group at one cyclopentadienyl ring and a thiophene heterocycle at the other cyclopentadienyl ring. The latter is disordered over two sets of sites in a 0.6:0.4 ratio. In the crystal structure, intramolecular π–π interactions between the thienyl and the phenyl substituent [centroid–centroid distance 3.695 (4) Å] and additional weak *T*-shaped π–π interactions between the thienyl and the phenyl-substituted cyclopentadienyl ring [4.688 (6) Å] consolidate the crystal packing.

1. Chemical context

The use of ferrocenyl (Fc) functionalized thiophenes as redox-active metal-based monomers offers the possibility of designing new conductive materials, such as polymers and molecular wires (see, for example: MacDiarmid *et al.*, 2001; Barsch *et al.*, 1994; Heeger *et al.*, 2001; Speck *et al.*, 2012; Pfaff *et al.*, 2013; Hildebrandt *et al.*, 2011; Hildebrandt & Lang, 2013; Wolf, 2001; Zhu & Wolf, 2000; Zotti *et al.*, 1995). The electrochemical interaction between the thiophene donor and the ferrocenyl acceptor with different conjugated 2-Fc—C≡C-(5-^{c}C$_4$H$_2$S)$_n$(^{c}C$_4$H$_3$S) (n = 0, 1, 2), 2-Fc—C≡C-[5-(3,4-OCH$_2$CH$_2$O)(^{c}C$_4$S)]$_n$(3,4-OCH$_2$CH$_2$O)^{c}C$_4$HS (n = 0, 1, 2) and 2,5-(Fc—C≡C)$_2$-(^{c}C$_4$H$_2$S)$_n$ (n = 1, 2, 3), 2,5-(Fc—C≡C)$_2$-[(3,4-OCH$_2$CH$_2$O)(^{c}C$_4$S)]$_n$ (n = 1, 2, 3) were studied by Zhu & Wolf (1999). The results of the spectro- and electrochemical measurements showed an interesting insight into the conductibility, which may lead to an improvement of sensor technology using conductive polymers. Electron-withdrawing and donating groups on the ferrocenyl or the thienyl moieties have been used to modify the charge-transfer properties. This has been shown for a series of different 2,5-diferrocenyl thiophenes (Speck *et al.*, 2014). In continuation of this work, we present herein the synthesis and crystal structure of 3-{1′-[3,5-bis(trifluoromethyl)phenyl]-1,1′-ferrocenediyl}-4-bromothiophene, $[Fe(C_9H_6BrS)(C_{13}H_7F_6)]$, (I). The synthesis of this compound was realized using typical Negishi *C,C*-cross-coupling reaction conditions.





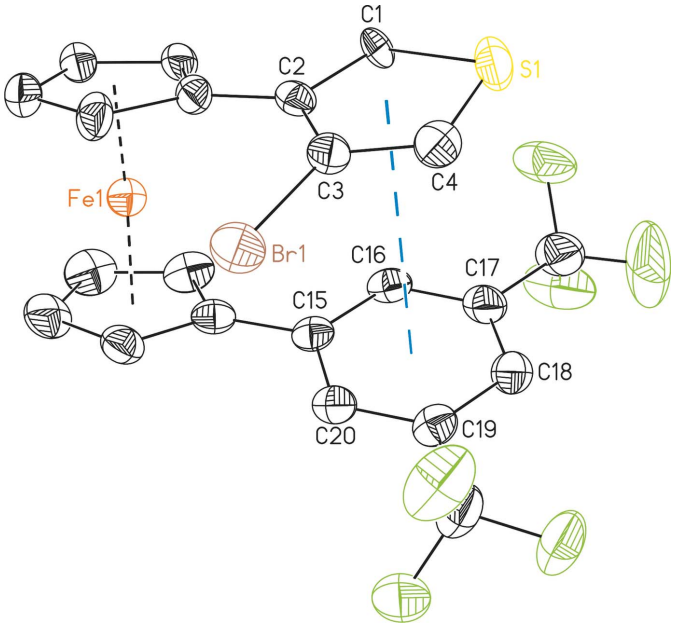


Figure 1
The molecular structure of (I) showing short intramolecular π–π interactions between the thienyl and the phenyl substituents, with displacement ellipsoids drawn at the 50% probability level. All hydrogen atoms, the minor disordered part of the structure and further π–π interactions have been omitted for clarity.

2. Structural commentary

The title compound contains one molecule in the asymmetric unit with an intramolecular π–π distance between the centroids (D) of the thiophene and the phenyl substituents (Fig. 1) of 3.695 (4) Å (Table 1) (Sinnokrot *et al.*, 2002) favoured by the nearly coplanar cylopentadienyl rings [D(C_5H_4)—Fe—D(C_5H_4): 175.84 (3) and 175.66 (3)°] in the ferrocenyl backbone. For the disordered part (′-labeled, see: *Refinement* and additional Figure in the supporting information), however, the distance of 3.871 (6) Å is too long for a π–π interaction caused by the increased torsion angle between the substituents in the 1- and 1′-position [9.2 (4)° for the main part; 16.7 (5)° for the disordered part]. The mean planes of the cyclopentadienyl rings and the bonded aromatic rings are almost coplanar with each other [C_6H_3—C_5H_4, 16.2 (3)°; C_4H_3S—C_5H_4, 17.3 (6) (main part) and 16.9 (10)° (other part)] and thus, a nearly parallel arranged stacking between the phenyl and the thiophene rings [8.9 (3)° for the main part and 9.7 (6)° for the other part] is realized.

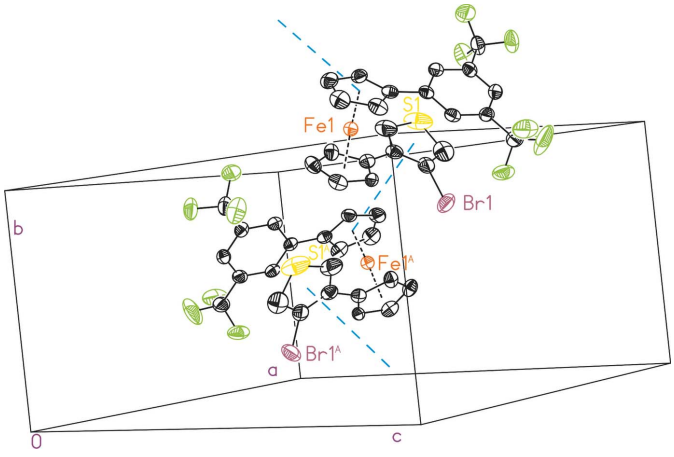


Figure 2
Intermolecular T-shaped π–π interactions between the thienyl and the phenyl-substituted cyclopentadienyl rings, with displacement ellipsoids drawn at the 50% probability level. All hydrogen atoms, the minor disordered part of the structure and further π–π distances have been omitted for clarity. [Symmetry code: (A) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.]

Table 1
T-shaped π–π interaction geometries (Å, °) for (I).

$D\cdots D$	$D\cdots D$	$\alpha^{(i)}$
$C_6H_3(CF_3)_2\cdots C_4H_2BrS^{(ii)}$	3.695 (4)	8.8 (3)
$C_4H_2BrS\cdots C_5H_4^{(iii)}$	4.943 (4)	88.3 (3)
$C_4H_2BrS^{(iv)}\cdots C_5H_4^{(iii)}$	4.688 (6)	86.8 (5)

D denotes the centroids of the respective aromatic rings. (i) The angle α is described by the intersection of the involved aromatics. (ii) Intramolecular interaction. (iii) Intermolecular interaction with symmetry code: $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$. (iv): Disordered (′-labeled) part.

3. Supramolecular features

Intermolecular T-shaped π–π interactions between the thienyl and the phenyl-substituted cyclopentadienyl rings (Fig. 2) are observed. The disordered part (labeled with ′) exhibits a stronger interaction of 4.688 (6) Å; in contrast, it is 4.943 (4) Å for the other disordered part, which is rather weak (Table 1).

4. Database survey

The only reported examples of 3-ferrocenyl-substituted five-membered group-VI heterocycles (Speck *et al.*, 2012; Hildebrandt *et al.*, 2011; Claus *et al.*, 2011) exhibit a similar coplanarity between non-sterically hindered thiophenes and the cyclopentadienyl rings [10.4 (2)°, Speck *et al.*, 2012; −6.4 (4)°, Claus *et al.*, 2011], but a high distortion for thiophenes bearing further *ortho*-substituents [40.1 (9) to 56.6 (9)°, Speck *et al.*, 2012; 70.9 (3) and 42.7 (3)°, Hildebrandt *et al.*, 2011]. The conformations of reported ferrocene derivatives bearing aromatic substituents in the 1 and 1′ positions range from antiperiplanar [180.0 (4), plane twisting 13.99 (15)°, Braga *et al.*, 2003] and anticlinal [147.02 (14), plane twisting 33.7 (9)°, Deck *et al.*, 2004] to synperiplanar [0.3 (3)°, Deck *et al.*, 2000; −0.5 (9)°, Blanchard *et al.*, 2000; 4.09 (19)°, Gallagher *et al.*, 2010; −6.5 (6)°, Hursthouse *et al.*, 2003; 14.4 (8)°, Foxman *et al.*, 1991] with plane twists from 12.8 (9) (Gallagher *et al.*, 2010) to 82.8 (4)° (Foxman *et al.*, 1993). Furthermore, for all synperiplanar examples, intramolecular interactions between the aromatic planes are present with distances smaller than 3.42 Å (Hursthouse *et al.*, 2003).

5. Synthesis and crystallization

1-Bromo-1′-(3,5-bis(trifluoromethyl)phenyl)ferrocene was prepared according to synthetic methodologies reported by Speck *et al.* (2014). The synthesis of ferrocenyl thiophene (I) was realized using typical Negishi *C,C*-cross-coupling conditions by reacting 1-bromo-1′-(3,5-bis(trifluoromethyl)phenyl)-ferrocene with 3,4-dibromothiophene (Negishi *et al.*, 1977).

Synthesis of (I): For the Negishi *C,C*-cross-coupling reaction, 1-bromo-1′-(3,5-bis(trifluoromethyl)phenyl)ferrocene (1.0 g, 2.10 mmol) was dissolved in 50 ml of tetrahydrofuran (THF) and 1.2 equivalents (0.9 ml, 2.52 mmol) of a 2.5 *M* solution of *n*-butyllithium in *n*-hexane were added dropwise at 193 K. After 1 h of stirring at this temperature, 1.2 equivalents (0.71 g, 2.52 mmol) of [$ZnCl_2$·2THF] were added in a single portion. The reaction was kept for 10 min at this temperature and was then allowed to warm to 273 K during an additional hour. Afterwards, 0.25 mol% of [P(*t*-C_4H_9)$_2$C(CH_3)$_2$$CH_2$Pd-($\mu$-Cl)]$_2$ and 1.5 equivalents (0.76 g, 3.15 mmol) of 3,4-dibromothiophene were added in a single portion. The resulting mixture was stirred for 10 h at 323 K. After evaporation of all volatiles, the crude product was dissolved in 30 ml of dichloromethane and was washed twice with 50 ml portions of water. The organic phase was dried over $MgSO_4$ and the solvent was removed with a rotary evaporator. The remaining orange solid was purified by column chromatography on silica gel using a *n*-hexane/diethyl ether 1/1 (*v*/*v*) mixture. Red crystals of (I) were obtained by slow evaporation of a saturated *n*-hexane/methanol 1/5 (*v*/*v*) solution at ambient temperature. Yield: 660 mg (1.18 mmol, 56% based on 1-bromo-1′-(3,5-bis(trifluoromethyl)phenyl)ferrocene). IR (KBr, cm^{-1}): ν = 1275 (*s*, C—F), 1504 (*s*, C=C), 1615 (*m*, C=C) 2848, 3095 (*w*, C—H). ^{1}H NMR (500.3 MHz, $CDCl_3$, 298 K, ppm): δ = 7.61 (*s*, 3H, $C_8H_3F_6$), 7.09 (*d*, 1H, $J_{H,H}$ = 3.6 Hz, C_4H_2S), 6.90 (*d*, 1H, $J_{H,H}$ = 3.6 Hz, C_4H_2S), 4.73 (*pt*, 2H, $J_{H,H}$ = 1.9 Hz, C_5H_4), 4.69 (*pt*, 2H, $J_{H,H}$ = 1.9 Hz, C_5H_4), 4.46 (*pt*, 2H, $J_{H,H}$ = 1.9 Hz, C_5H_4), 4.25 (*pt*, 2H, $J_{H,H}$ = 1.9 Hz, C_5H_4). ^{13}C{^{1}H} NMR (125.7 MHz, $CDCl_3$, 298 K, ppm): δ = 140.64 (*s*, C_i-C_6H_3), 135.56 (*s*, C_i-C_4H_2S), 131.54 (*q*, $J_{C,F}$ = 33 Hz, C_i-C_6H_3), 125,63 (*m*, C_6H_3), 124.88 (*s*, C_4H_2S), 123.50 (*q*, $J_{C,F}$ =273 Hz, CF_3), 121.12 (*s*, C_4H_2S), 119.05 (*m*, C_6H_3), 109.78 (*s*, C_i-C_4H_2S), 82.98 (*s*, C_i-C_5H_4), 82.01 (*s*, C_i-C_5H_4), 71.40 (*s*, C_5H_4), 70.17 (*s*, C_5H_4), 68.81 (*s*, C_5H_4), 68.20 (*s*, C_5H_4). HRMS (ESI–TOF, M^+): $C_{23}H_{16}F_6FeSO$: *m*/*z* = 557.9291 (calc. 557.9171).

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bonded hydrogen atoms were placed in calculated positions and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C) and a C—H distance of 0.93 Å for the aromatic protons. The thienyl and the attached cyclopentadienyl ring were refined as disordered over two sets of sites with occupancies of 0.6 and 0.4. The spatial proximity of the sulfur and the bromine atom of the disordered part required DFIX [C1—C2 1.51 (2), C2—C3 1.33 (2), C3—C4 1.35 (2) S1—C1 1.62 (2), S1—C4 1.82 (2), C3—Br1 1.94 (2) Å) and DANG (C4—Br1 2.75 (4), C1—C3 2.27 (4), C2—C4 2.38 (4), C4—Br1 2.75 (4) Å] instructions, which were used for the minor disordered part (′-labeled). For both disordered parts, some anisotropic displacement ellipsoids were rather elongated and hence SIMU/ISOR restraints (McArdle, 1995; Sheldrick, 2008) were also applied. Both cyclopentadienyl rings were generated by using the AFIX 56 command. For atom pair C9/C9′, a further EADP instruction was applied to achieve reasonable anisotropic displacement ellipsoids.

Table 2
Experimental details.

Crystal data	
Chemical formula	[Fe(C_9H_6BrS)($C_{13}H_7F_6$)]
M_r	559.14
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	110
a, *b*, *c* (Å)	18.056 (5), 10.294 (5), 21.451 (5)
β (°)	93.268 (5)
V (Å^3)	3981 (2)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	2.93
Crystal size (mm)	0.4 × 0.4 × 0.2
Data collection	
Diffractometer	Oxford Gemini CCD
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min}, T_{max}	0.436, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11002, 3687, 2887
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.125, 1.00
No. of reflections	3687
No. of parameters	357
No. of restraints	258
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.94, −0.61

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2006), *SHELXS2013*, *SHELXL2013* and *SHELXTL*(Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Acknowledgements

We are grateful to the Federal Cluster of Excellence EXC 1075 "MERGE Technologies for Multifunctional Lightweight Structures". MK thanks the Fonds der Chemischen Industrie for a Chemiefonds fellowship.

References

Barsch, U., Beck, F., Hambitzer, G., Holze, R., Lippe, J. & Stassen, I. (1994). *J. Electroanal. Chem.* **369**, 97–101.
Blanchard, M. D., Hughes, R. P., Concolino, T. E. & Rheingold, A. L. (2000). *Chem. Mater.* **12**, 1604–1610.
Braga, D., Polito, M., Bracaccini, M., D'Addario, D., Tagliavini, E., Sturba, L. & Grepioni, F. (2003). *Organometallics*, **22**, 2142–2150.
Claus, R. (2011). *Dissertation*. TU Chemnitz, Germany.
Deck, P. A., Konaté, M. M., Kelly, B. V. & Slebodnick, C. (2004). *Organometallics*, **23**, 1089–1097.

Deck, P. A., Lane, M. J., Montgomery, J. L., Slebodnick, C. & Fronczek, F. R. (2000). *Organometallics*, **19**, 1013–1024.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Foxman, B. M., Gronbeck, D. A., Khruschova, N. & Rosenblum, M. (1993). *J. Org. Chem.* **58**, 4078–4082.
Foxman, B. M., Gronbeck, D. A. & Rosenblum, M. (1991). *J. Organomet. Chem.* **413**, 287–294.
Gallagher, J. F., Alley, S., Brosnan, M. & Lough, A. J. (2010). *Acta Cryst.* B**66**, 196–205.
Heeger, A. J. (2001). *Angew. Chem. Int. Ed.* **40**, 2591–2611.
Hildebrandt, A. & Lang, H. (2013). *Organometallics*, **32**, 5640–5653.
Hildebrandt, A., Pfaff, U. & Lang, H. (2011). *Rev. Inorg. Chem.* **31**, 111–141.
Hursthouse, M. B., Light, M. E. & Butler, I. R. (2003). *Private Communication*.
MacDiarmid, A. G. (2001). *Angew. Chem. Int. Ed.* **40**, 2581–2590.
McArdle, P. (1995). *J. Appl. Cryst.* **28**, 65.
Negishi, E., King, A. O. & Okukado, N. (1977). *J. Org. Chem.* **42**, 1821–1823.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction, Abingdon, England.
Pfaff, U., Hildebrandt, A., Schaarschmidt, D., Rüffer, T., Low, P. J. & Lang, H. (2013). *Organometallics*, **32**, 6106–6117.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sinnokrot, M. O., Valeev, E. F. & Sherrill, C. D. (2002). *J. Am. Chem. Soc.* **124**, 10887–10893.
Speck, J. M., Claus, R., Hildebrandt, A., Rüffer, T., Erasmus, E., van As, L., Swarts, J. C. & Lang, H. (2012). *Organometallics*, **31**, 6373–6380.
Speck, J. M., Korb, M., Rüffer, T., Hildebrandt, A. & Lang, H. (2014). *Organometallics*, doi: 10.1021/om500062h.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Wolf, M. O. (2001). *Adv. Mater.* **13**, 545–553.
Zhu, Y. & Wolf, M. O. (1999). *Chem. Mater.* **11**, 2995–3001.
Zhu, Y. & Wolf, M. O. (2000). *J. Am. Chem. Soc.* **122**, 10121–10125.
Zotti, G., Zecchin, S., Schiavon, G., Berlin, A., Pagani, G. & Canavesi, A. (1995). *Chem. Mater.* **7**, 2309–2315.

supporting information

Acta Cryst. (2014). E**70**, 238-241 [doi:10.1107/S1600536814020674]

Crystal structure of 3-{1′-[3,5-bis(trifluoromethyl)phenyl]ferrocenyl}-4-bromothiophene

Elisabeth A. Poppitz, Marcus Korb and Heinrich Lang

Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *publCIF* (Westrip, 2010).

3-{1′-[3,5-Bis(trifluoromethyl)phenyl]ferrocenyl}-4-bromothiophene

Crystal data

$[Fe(C_9H_6BrS)(C_{13}H_7F_6)]$
$M_r = 559.14$
Monoclinic, $C2/c$
$a = 18.056$ (5) Å
$b = 10.294$ (5) Å
$c = 21.451$ (5) Å
$\beta = 93.268$ (5)°
$V = 3981$ (2) Å^3
$Z = 8$
$F(000) = 2208$
$D_x = 1.866$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3003 reflections
$\theta = 3.8$–$27.2°$
$\mu = 2.93$ mm^{-1}
$T = 110$ K
Block, orange
0.4 × 0.4 × 0.2 mm

Data collection

Oxford Gemini CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
$T_{min} = 0.436$, $T_{max} = 1.000$
11002 measured reflections
3687 independent reflections
2887 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.9°$
$h = -21 \rightarrow 21$
$k = -12 \rightarrow 12$
$l = -23 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.125$
$S = 1.00$
3687 reflections
357 parameters
258 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 7.0529P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.61$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.59952 (12)	−0.21423 (19)	0.60297 (8)	0.0419 (4)	0.6
Br1	0.63183 (5)	0.10861 (8)	0.73209 (4)	0.0409 (2)	0.6
C1	0.6910 (4)	−0.2085 (6)	0.6296 (3)	0.0323 (13)	0.6
H1	0.7272	−0.2654	0.6168	0.039*	0.6
C2	0.7045 (3)	−0.1088 (5)	0.6724 (3)	0.0259 (11)	0.6
C3	0.6392 (4)	−0.0394 (6)	0.6811 (3)	0.0297 (13)	0.6
C4	0.5776 (5)	−0.0824 (8)	0.6470 (3)	0.0342 (17)	0.6
H4	0.5307	−0.0454	0.6477	0.041*	0.6
C5	0.7792 (3)	−0.0860 (8)	0.7008 (3)	0.0274 (17)	0.6
C6	0.7990 (4)	−0.0156 (9)	0.7562 (3)	0.034 (2)	0.6
H6	0.7667	0.0301	0.7804	0.041*	0.6
C7	0.8769 (4)	−0.0272 (8)	0.7683 (3)	0.037 (2)	0.6
H7	0.9045	0.0095	0.8017	0.045*	0.6
C8	0.9052 (3)	−0.1047 (6)	0.7204 (3)	0.0367 (18)	0.6
H8	0.9546	−0.1277	0.7169	0.044*	0.6
C9	0.8449 (3)	−0.1410 (6)	0.6786 (2)	0.0303 (14)	0.6
H9	0.8478	−0.1920	0.6431	0.036*	0.6
S1′	0.56009 (19)	0.0774 (3)	0.7152 (2)	0.0816 (12)	0.4
Br1′	0.64769 (11)	−0.25200 (13)	0.61634 (6)	0.0613 (4)	0.4
C1′	0.6502 (7)	0.0577 (13)	0.7354 (8)	0.063 (4)	0.4
H1′	0.6753	0.1051	0.7669	0.076*	0.4
C2′	0.6844 (6)	−0.0381 (9)	0.6999 (5)	0.037 (2)	0.4
C3′	0.6298 (7)	−0.1011 (10)	0.6644 (5)	0.046 (3)	0.4
C4′	0.5597 (7)	−0.0537 (14)	0.6654 (7)	0.060 (4)	0.4
H4′	0.5183	−0.0866	0.6429	0.072*	0.4
C5′	0.7644 (4)	−0.0653 (12)	0.7128 (5)	0.030 (3)	0.4
C6′	0.8083 (7)	−0.0167 (14)	0.7647 (5)	0.035 (3)	0.4
H6′	0.7916	0.0346	0.7967	0.042*	0.4
C7′	0.8823 (5)	−0.0602 (13)	0.7592 (5)	0.040 (3)	0.4
H7′	0.9225	−0.0424	0.7869	0.047*	0.4
C8′	0.8841 (5)	−0.1356 (10)	0.7039 (5)	0.039 (3)	0.4
H8′	0.9257	−0.1759	0.6890	0.047*	0.4
C9′	0.8113 (5)	−0.1388 (9)	0.6752 (4)	0.0303 (14)	0.4
H9′	0.7968	−0.1814	0.6383	0.036*	0.4
C10	0.81000 (19)	0.1698 (3)	0.61277 (16)	0.0300 (8)	
C11	0.8794 (2)	0.1132 (4)	0.59760 (18)	0.0387 (9)	
H11	0.8870	0.0601	0.5635	0.046*	
C12	0.9345 (2)	0.1522 (4)	0.6438 (2)	0.0467 (10)	
H12	0.9844	0.1291	0.6451	0.056*	

C13	0.9005 (2)	0.2321 (4)	0.6870 (2)	0.0442 (10)
H13	0.9241	0.2712	0.7218	0.053*
C14	0.8247 (2)	0.2427 (3)	0.66885 (18)	0.0345 (8)
H14	0.7898	0.2896	0.6899	0.041*
C15	0.73864 (19)	0.1567 (3)	0.57697 (14)	0.0271 (7)
C16	0.7274 (2)	0.0608 (3)	0.53160 (15)	0.0311 (8)
H16	0.7651	0.0018	0.5247	0.037*
C17	0.6609 (2)	0.0524 (3)	0.49668 (16)	0.0356 (9)
C18	0.6033 (2)	0.1366 (4)	0.50595 (16)	0.0345 (8)
H18	0.5585	0.1296	0.4825	0.041*
C19	0.6138 (2)	0.2321 (4)	0.55113 (15)	0.0318 (8)
C20	0.6805 (2)	0.2420 (3)	0.58615 (15)	0.0299 (8)
H20	0.6865	0.3067	0.6163	0.036*
C21	0.6527 (3)	−0.0494 (4)	0.44666 (19)	0.0481 (11)
C22	0.5538 (2)	0.3269 (4)	0.56256 (17)	0.0434 (10)
F1	0.67577 (17)	−0.1660 (2)	0.46565 (11)	0.0628 (8)
F2	0.6945 (2)	−0.0225 (3)	0.39867 (11)	0.0786 (10)
F3	0.5850 (2)	−0.0629 (4)	0.42356 (19)	0.1139 (16)
F4	0.52097 (15)	0.3028 (3)	0.61561 (11)	0.0669 (8)
F5	0.50019 (14)	0.3292 (3)	0.51730 (11)	0.0582 (7)
F6	0.57912 (16)	0.4492 (2)	0.56767 (14)	0.0655 (8)
Fe1	0.85187 (3)	0.05282 (5)	0.68322 (2)	0.02830 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0414 (11)	0.0476 (11)	0.0357 (9)	−0.0166 (9)	−0.0064 (8)	−0.0030 (8)
Br1	0.0436 (5)	0.0359 (4)	0.0437 (4)	0.0049 (3)	0.0063 (3)	−0.0053 (3)
C1	0.025 (3)	0.029 (3)	0.042 (3)	−0.017 (3)	−0.007 (3)	0.003 (2)
C2	0.029 (3)	0.022 (2)	0.028 (2)	−0.005 (2)	0.005 (2)	0.002 (2)
C3	0.031 (3)	0.029 (3)	0.030 (3)	−0.004 (3)	0.002 (3)	0.003 (3)
C4	0.028 (4)	0.039 (4)	0.036 (4)	−0.004 (3)	0.005 (3)	0.007 (3)
C5	0.033 (3)	0.029 (3)	0.020 (3)	−0.005 (3)	0.001 (3)	0.001 (3)
C6	0.038 (4)	0.043 (4)	0.021 (3)	−0.008 (3)	−0.002 (3)	0.001 (3)
C7	0.039 (4)	0.037 (4)	0.035 (3)	−0.007 (3)	−0.009 (3)	0.002 (3)
C8	0.039 (4)	0.029 (3)	0.040 (4)	0.001 (3)	−0.011 (3)	−0.003 (3)
C9	0.024 (4)	0.0264 (19)	0.039 (2)	−0.003 (3)	−0.005 (3)	0.0004 (18)
S1′	0.0422 (18)	0.0499 (17)	0.156 (4)	0.0105 (14)	0.037 (2)	0.023 (2)
Br1′	0.0844 (11)	0.0503 (8)	0.0479 (7)	−0.0304 (8)	−0.0074 (7)	−0.0028 (5)
C1′	0.062 (7)	0.044 (6)	0.085 (7)	0.010 (5)	0.007 (5)	0.006 (6)
C2′	0.033 (4)	0.032 (4)	0.048 (4)	−0.002 (4)	0.006 (4)	0.011 (4)
C3′	0.039 (5)	0.043 (5)	0.056 (5)	−0.013 (4)	−0.009 (4)	0.020 (4)
C4′	0.043 (6)	0.071 (7)	0.064 (7)	−0.018 (5)	−0.001 (5)	0.028 (5)
C5′	0.028 (4)	0.031 (5)	0.032 (5)	−0.010 (4)	0.010 (4)	0.007 (4)
C6′	0.035 (5)	0.044 (5)	0.026 (5)	−0.007 (4)	0.005 (4)	0.006 (4)
C7′	0.033 (5)	0.047 (6)	0.039 (5)	0.003 (4)	0.004 (4)	0.011 (4)
C8′	0.038 (6)	0.039 (5)	0.042 (6)	0.007 (5)	0.013 (5)	0.007 (5)
C9′	0.024 (4)	0.0264 (19)	0.039 (2)	−0.003 (3)	−0.005 (3)	0.0004 (18)

C10	0.031 (2)	0.0257 (17)	0.0336 (18)	−0.0006 (14)	0.0084 (15)	0.0061 (14)
C11	0.039 (2)	0.042 (2)	0.036 (2)	0.0058 (18)	0.0173 (17)	0.0097 (17)
C12	0.028 (2)	0.051 (2)	0.062 (3)	−0.0058 (19)	0.0121 (19)	0.012 (2)
C13	0.030 (2)	0.038 (2)	0.064 (3)	−0.0095 (17)	−0.0013 (19)	0.0023 (19)
C14	0.033 (2)	0.0271 (18)	0.043 (2)	−0.0035 (15)	0.0017 (16)	0.0000 (15)
C15	0.0324 (19)	0.0267 (17)	0.0229 (16)	0.0003 (15)	0.0074 (14)	0.0068 (13)
C16	0.041 (2)	0.0266 (18)	0.0267 (17)	0.0064 (15)	0.0072 (15)	0.0029 (14)
C17	0.054 (3)	0.0280 (18)	0.0248 (17)	0.0008 (17)	0.0014 (17)	−0.0025 (14)
C18	0.041 (2)	0.0336 (19)	0.0281 (18)	0.0007 (16)	−0.0017 (16)	−0.0015 (15)
C19	0.036 (2)	0.0347 (19)	0.0249 (17)	0.0057 (16)	0.0043 (15)	0.0016 (14)
C20	0.040 (2)	0.0271 (17)	0.0235 (17)	0.0034 (15)	0.0065 (15)	−0.0001 (13)
C21	0.069 (3)	0.037 (2)	0.038 (2)	0.006 (2)	−0.002 (2)	−0.0067 (18)
C22	0.043 (2)	0.055 (3)	0.031 (2)	0.0147 (19)	−0.0054 (18)	−0.0054 (18)
F1	0.116 (2)	0.0309 (13)	0.0419 (13)	0.0021 (13)	0.0113 (14)	−0.0070 (10)
F2	0.161 (3)	0.0460 (15)	0.0316 (13)	0.0019 (17)	0.0266 (16)	−0.0061 (11)
F3	0.087 (3)	0.115 (3)	0.133 (3)	0.034 (2)	−0.053 (2)	−0.093 (3)
F4	0.0594 (17)	0.101 (2)	0.0415 (14)	0.0347 (16)	0.0151 (12)	−0.0019 (14)
F5	0.0474 (15)	0.0777 (18)	0.0474 (14)	0.0252 (13)	−0.0145 (11)	−0.0153 (13)
F6	0.0636 (18)	0.0427 (15)	0.088 (2)	0.0220 (13)	−0.0152 (15)	−0.0183 (13)
Fe1	0.0262 (3)	0.0287 (3)	0.0302 (3)	−0.0004 (2)	0.0033 (2)	0.0008 (2)

Geometric parameters (Å, º)

S1—C1	1.717 (6)	C7′—Fe1	2.052 (12)
S1—C4	1.713 (8)	C7′—H7′	0.9300
Br1—C3	1.885 (7)	C8′—C9′	1.4200
C1—C2	1.389 (8)	C8′—Fe1	2.066 (9)
C1—H1	0.9300	C8′—H8′	0.9300
C2—C3	1.399 (8)	C9′—Fe1	2.107 (9)
C2—C5	1.469 (7)	C9′—H9′	0.9300
C3—C4	1.370 (10)	C10—C14	1.430 (5)
C4—H4	0.9300	C10—C11	1.436 (5)
C5—C9	1.4200	C10—C15	1.468 (5)
C5—C6	1.4200	C10—Fe1	2.043 (3)
C5—Fe1	1.990 (8)	C11—C12	1.422 (6)
C6—C7	1.4200	C11—Fe1	2.027 (4)
C6—Fe1	2.007 (9)	C11—H11	0.9300
C6—H6	0.9300	C12—C13	1.407 (6)
C7—C8	1.4200	C12—Fe1	2.033 (4)
C7—Fe1	2.029 (8)	C12—H12	0.9300
C7—H7	0.9300	C13—C14	1.406 (5)
C8—C9	1.4200	C13—Fe1	2.043 (4)
C8—Fe1	2.026 (6)	C13—H13	0.9300
C8—H8	0.9300	C14—Fe1	2.035 (4)
C9—Fe1	2.002 (6)	C14—H14	0.9300
C9—H9	0.9300	C15—C16	1.392 (5)
S1′—C1′	1.672 (13)	C15—C20	1.391 (5)
S1′—C4′	1.721 (13)	C16—C17	1.381 (5)

Br1′—C3′	1.902 (11)	C16—H16	0.9300
C1′—C2′	1.410 (14)	C17—C18	1.377 (5)
C1′—H1′	0.9300	C17—C21	1.501 (5)
C2′—C3′	1.373 (13)	C18—C19	1.386 (5)
C2′—C5′	1.483 (13)	C18—H18	0.9300
C3′—C4′	1.359 (14)	C19—C20	1.386 (5)
C4′—H4′	0.9300	C19—C22	1.489 (5)
C5′—C6′	1.4200	C20—H20	0.9300
C5′—C9′	1.4200	C21—F3	1.300 (6)
C5′—Fe1	2.118 (11)	C21—F1	1.327 (5)
C6′—C7′	1.4200	C21—F2	1.339 (5)
C6′—Fe1	2.084 (14)	C22—F5	1.332 (4)
C6′—H6′	0.9300	C22—F4	1.336 (5)
C7′—C8′	1.4200	C22—F6	1.341 (5)

C1—S1—C4	92.1 (4)	C13—C12—H12	126.0
C2—C1—S1	112.0 (5)	C11—C12—H12	126.0
C2—C1—H1	124.0	Fe1—C12—H12	126.1
S1—C1—H1	124.0	C12—C13—C14	108.5 (4)
C1—C2—C3	110.4 (6)	C12—C13—Fe1	69.4 (2)
C1—C2—C5	121.0 (6)	C14—C13—Fe1	69.5 (2)
C3—C2—C5	128.5 (6)	C12—C13—H13	125.8
C4—C3—C2	115.3 (6)	C14—C13—H13	125.8
C4—C3—Br1	119.3 (5)	Fe1—C13—H13	126.9
C2—C3—Br1	125.4 (5)	C13—C14—C10	108.9 (3)
C3—C4—S1	110.2 (6)	C13—C14—Fe1	70.1 (2)
C3—C4—H4	124.9	C10—C14—Fe1	69.8 (2)
S1—C4—H4	124.9	C13—C14—H14	125.6
C9—C5—C6	108.0	C10—C14—H14	125.6
C9—C5—C2	124.2 (5)	Fe1—C14—H14	126.1
C6—C5—C2	127.7 (5)	C16—C15—C20	117.7 (3)
C9—C5—Fe1	69.6 (3)	C16—C15—C10	121.3 (3)
C6—C5—Fe1	69.8 (3)	C20—C15—C10	121.0 (3)
C2—C5—Fe1	129.5 (5)	C17—C16—C15	120.7 (3)
C7—C6—C5	108.0	C17—C16—H16	119.6
C7—C6—Fe1	70.3 (3)	C15—C16—H16	119.6
C5—C6—Fe1	68.5 (3)	C18—C17—C16	121.5 (3)
C7—C6—H6	126.0	C18—C17—C21	119.9 (4)
C5—C6—H6	126.0	C16—C17—C21	118.6 (4)
Fe1—C6—H6	126.8	C17—C18—C19	118.2 (4)
C6—C7—C8	108.0	C17—C18—H18	120.9
C6—C7—Fe1	68.6 (3)	C19—C18—H18	120.9
C8—C7—Fe1	69.4 (3)	C18—C19—C20	120.8 (3)
C6—C7—H7	126.0	C18—C19—C22	120.5 (3)
C8—C7—H7	126.0	C20—C19—C22	118.7 (3)
Fe1—C7—H7	127.6	C19—C20—C15	121.1 (3)
C9—C8—C7	108.0	C19—C20—H20	119.5
C9—C8—Fe1	68.4 (3)	C15—C20—H20	119.5

C7—C8—Fe1	69.6 (3)	F3—C21—F1	107.0 (4)
C9—C8—H8	126.0	F3—C21—F2	106.7 (4)
C7—C8—H8	126.0	F1—C21—F2	104.0 (3)
Fe1—C8—H8	127.5	F3—C21—C17	113.5 (4)
C8—C9—C5	108.0	F1—C21—C17	113.3 (3)
C8—C9—Fe1	70.3 (3)	F2—C21—C17	111.6 (4)
C5—C9—Fe1	68.7 (3)	F5—C22—F4	106.5 (3)
C8—C9—H9	126.0	F5—C22—F6	105.9 (3)
C5—C9—H9	126.0	F4—C22—F6	105.7 (3)
Fe1—C9—H9	126.6	F5—C22—C19	113.4 (3)
C1′—S1′—C4′	92.0 (7)	F4—C22—C19	112.4 (3)
C2′—C1′—S1′	113.2 (11)	F6—C22—C19	112.4 (4)
C2′—C1′—H1′	123.4	C5—Fe1—C9	41.68 (12)
S1′—C1′—H1′	123.4	C5—Fe1—C6	41.62 (17)
C3′—C2′—C1′	107.9 (11)	C9—Fe1—C6	69.9 (2)
C3′—C2′—C5′	132.5 (10)	C5—Fe1—C11	126.2 (2)
C1′—C2′—C5′	118.8 (10)	C9—Fe1—C11	106.21 (19)
C4′—C3′—C2′	117.5 (11)	C6—Fe1—C11	165.1 (2)
C4′—C3′—Br1′	119.3 (9)	C5—Fe1—C8	69.79 (16)
C2′—C3′—Br1′	123.2 (8)	C9—Fe1—C8	41.28 (10)
C3′—C4′—S1′	108.7 (10)	C6—Fe1—C8	69.5 (2)
C3′—C4′—H4′	125.6	C11—Fe1—C8	117.8 (2)
S1′—C4′—H4′	125.6	C5—Fe1—C7	69.7 (2)
C6′—C5′—C9′	108.0	C9—Fe1—C7	69.49 (16)
C6′—C5′—C2′	125.1 (9)	C6—Fe1—C7	41.19 (17)
C9′—C5′—C2′	126.8 (9)	C11—Fe1—C7	152.3 (2)
C6′—C5′—Fe1	69.0 (4)	C8—Fe1—C7	40.99 (13)
C9′—C5′—Fe1	70.0 (4)	C5—Fe1—C14	124.2 (2)
C2′—C5′—Fe1	124.8 (8)	C9—Fe1—C14	159.5 (2)
C5′—C6′—C7′	108.0	C6—Fe1—C14	109.5 (2)
C5′—C6′—Fe1	71.5 (4)	C11—Fe1—C14	68.76 (15)
C7′—C6′—Fe1	68.7 (4)	C8—Fe1—C14	159.0 (2)
C5′—C6′—H6′	126.0	C7—Fe1—C14	124.4 (2)
C7′—C6′—H6′	126.0	C5—Fe1—C12	161.4 (2)
Fe1—C6′—H6′	125.3	C9—Fe1—C12	121.8 (2)
C8′—C7′—C6′	108.0	C6—Fe1—C12	153.4 (2)
C8′—C7′—Fe1	70.4 (4)	C11—Fe1—C12	40.99 (16)
C6′—C7′—Fe1	71.2 (4)	C8—Fe1—C12	102.9 (2)
C8′—C7′—H7′	126.0	C7—Fe1—C12	116.6 (3)
C6′—C7′—H7′	126.0	C14—Fe1—C12	68.27 (17)
Fe1—C7′—H7′	124.1	C5—Fe1—C13	158.0 (2)
C9′—C8′—C7′	108.0	C9—Fe1—C13	158.2 (2)
C9′—C8′—Fe1	71.7 (4)	C6—Fe1—C13	120.5 (2)
C7′—C8′—Fe1	69.3 (5)	C11—Fe1—C13	68.45 (17)
C9′—C8′—H8′	126.0	C8—Fe1—C13	120.9 (2)
C7′—C8′—H8′	126.0	C7—Fe1—C13	104.9 (2)
Fe1—C8′—H8′	124.6	C14—Fe1—C13	40.33 (15)
C8′—C9′—C5′	108.0	C12—Fe1—C13	40.38 (18)

C8′—C9′—Fe1	68.6 (4)	C5—Fe1—C10	110.1 (2)
C5′—C9′—Fe1	70.8 (4)	C9—Fe1—C10	122.11 (19)
C8′—C9′—H9′	126.0	C6—Fe1—C10	127.7 (2)
C5′—C9′—H9′	126.0	C11—Fe1—C10	41.30 (14)
Fe1—C9′—H9′	126.2	C8—Fe1—C10	155.5 (2)
C14—C10—C11	106.3 (3)	C7—Fe1—C10	163.4 (2)
C14—C10—C15	127.1 (3)	C14—Fe1—C10	41.06 (14)
C11—C10—C15	126.5 (3)	C12—Fe1—C10	69.21 (16)
C14—C10—Fe1	69.2 (2)	C13—Fe1—C10	68.75 (16)
C11—C10—Fe1	68.8 (2)	C11—Fe1—C7′	145.6 (3)
C15—C10—Fe1	127.6 (2)	C14—Fe1—C7′	135.8 (3)
C12—C11—C10	108.2 (3)	C12—Fe1—C7′	116.5 (3)
C12—C11—Fe1	69.7 (2)	C13—Fe1—C7′	112.7 (3)
C10—C11—Fe1	69.93 (19)	C10—Fe1—C7′	173.1 (3)
C12—C11—H11	125.9	C11—Fe1—C8′	113.7 (3)
C10—C11—H11	125.9	C14—Fe1—C8′	175.6 (3)
Fe1—C11—H11	126.0	C12—Fe1—C8′	110.9 (3)
C13—C12—C11	108.1 (4)	C13—Fe1—C8′	136.4 (3)
C13—C12—Fe1	70.2 (2)	C10—Fe1—C8′	143.1 (3)
C11—C12—Fe1	69.3 (2)	C7′—Fe1—C8′	40.34 (19)

C4—S1—C1—C2	1.1 (5)	Fe1—C7′—C8′—C9′	−61.6 (4)
S1—C1—C2—C3	−0.8 (6)	C6′—C7′—C8′—Fe1	61.6 (4)
S1—C1—C2—C5	−179.7 (5)	C7′—C8′—C9′—C5′	0.0
C1—C2—C3—C4	0.1 (8)	Fe1—C8′—C9′—C5′	−60.0 (5)
C5—C2—C3—C4	178.8 (7)	C7′—C8′—C9′—Fe1	60.0 (5)
C1—C2—C3—Br1	−177.0 (4)	C6′—C5′—C9′—C8′	0.0
C5—C2—C3—Br1	1.7 (9)	C2′—C5′—C9′—C8′	177.7 (12)
C2—C3—C4—S1	0.7 (8)	Fe1—C5′—C9′—C8′	58.6 (4)
Br1—C3—C4—S1	178.0 (4)	C6′—C5′—C9′—Fe1	−58.6 (4)
C1—S1—C4—C3	−1.0 (6)	C2′—C5′—C9′—Fe1	119.1 (12)
C1—C2—C5—C9	14.0 (10)	C14—C10—C11—C12	−0.2 (4)
C3—C2—C5—C9	−164.6 (6)	C15—C10—C11—C12	178.8 (3)
C1—C2—C5—C6	−161.0 (6)	Fe1—C10—C11—C12	−59.4 (3)
C3—C2—C5—C6	20.4 (10)	C14—C10—C11—Fe1	59.2 (2)
C1—C2—C5—Fe1	104.9 (7)	C15—C10—C11—Fe1	−121.7 (3)
C3—C2—C5—Fe1	−73.8 (8)	C10—C11—C12—C13	−0.1 (4)
C9—C5—C6—C7	0.0	Fe1—C11—C12—C13	−59.7 (3)
C2—C5—C6—C7	175.7 (8)	C10—C11—C12—Fe1	59.6 (2)
Fe1—C5—C6—C7	−59.4 (3)	C11—C12—C13—C14	0.4 (5)
C9—C5—C6—Fe1	59.4 (3)	Fe1—C12—C13—C14	−58.7 (3)
C2—C5—C6—Fe1	−125.0 (7)	C11—C12—C13—Fe1	59.1 (3)
C5—C6—C7—C8	0.0	C12—C13—C14—C10	−0.6 (4)
Fe1—C6—C7—C8	−58.3 (2)	Fe1—C13—C14—C10	−59.2 (2)
C5—C6—C7—Fe1	58.3 (2)	C12—C13—C14—Fe1	58.6 (3)
C6—C7—C8—C9	0.0	C11—C10—C14—C13	0.5 (4)
Fe1—C7—C8—C9	−57.8 (3)	C15—C10—C14—C13	−178.6 (3)
C6—C7—C8—Fe1	57.8 (3)	Fe1—C10—C14—C13	59.4 (3)

C7—C8—C9—C5	0.0	C11—C10—C14—Fe1	−59.0 (2)
Fe1—C8—C9—C5	−58.5 (3)	C15—C10—C14—Fe1	122.0 (3)
C7—C8—C9—Fe1	58.5 (3)	C14—C10—C15—C16	−165.3 (3)
C6—C5—C9—C8	0.0	C11—C10—C15—C16	15.8 (5)
C2—C5—C9—C8	−175.9 (8)	Fe1—C10—C15—C16	−74.2 (4)
Fe1—C5—C9—C8	59.5 (3)	C14—C10—C15—C20	16.3 (5)
C6—C5—C9—Fe1	−59.5 (3)	C11—C10—C15—C20	−162.5 (3)
C2—C5—C9—Fe1	124.6 (7)	Fe1—C10—C15—C20	107.4 (3)
C4′—S1′—C1′—C2′	7.1 (12)	C20—C15—C16—C17	0.7 (5)
S1′—C1′—C2′—C3′	−8.6 (14)	C10—C15—C16—C17	−177.7 (3)
S1′—C1′—C2′—C5′	179.8 (9)	C15—C16—C17—C18	−1.0 (5)
C1′—C2′—C3′—C4′	6.2 (16)	C15—C16—C17—C21	177.6 (3)
C5′—C2′—C3′—C4′	176.2 (12)	C16—C17—C18—C19	0.7 (5)
C1′—C2′—C3′—Br1′	−172.1 (9)	C21—C17—C18—C19	−177.9 (3)
C5′—C2′—C3′—Br1′	−2.1 (17)	C17—C18—C19—C20	−0.2 (5)
C2′—C3′—C4′—S1′	−1.2 (15)	C17—C18—C19—C22	179.2 (3)
Br1′—C3′—C4′—S1′	177.2 (6)	C18—C19—C20—C15	0.0 (5)
C1′—S1′—C4′—C3′	−3.4 (12)	C22—C19—C20—C15	−179.4 (3)
C3′—C2′—C5′—C6′	−159.0 (11)	C16—C15—C20—C19	−0.2 (5)
C1′—C2′—C5′—C6′	10.1 (15)	C10—C15—C20—C19	178.1 (3)
C3′—C2′—C5′—C9′	23.6 (18)	C18—C17—C21—F3	−11.8 (6)
C1′—C2′—C5′—C9′	−167.3 (11)	C16—C17—C21—F3	169.6 (4)
C3′—C2′—C5′—Fe1	113.6 (12)	C18—C17—C21—F1	−134.1 (4)
C1′—C2′—C5′—Fe1	−77.3 (13)	C16—C17—C21—F1	47.3 (5)
C9′—C5′—C6′—C7′	0.0	C18—C17—C21—F2	108.9 (5)
C2′—C5′—C6′—C7′	−177.8 (12)	C16—C17—C21—F2	−69.7 (5)
Fe1—C5′—C6′—C7′	−59.3 (4)	C18—C19—C22—F5	−14.8 (5)
C9′—C5′—C6′—Fe1	59.3 (4)	C20—C19—C22—F5	164.6 (3)
C2′—C5′—C6′—Fe1	−118.5 (10)	C18—C19—C22—F4	106.1 (4)
C5′—C6′—C7′—C8′	0.0	C20—C19—C22—F4	−74.5 (5)
Fe1—C6′—C7′—C8′	−61.1 (4)	C18—C19—C22—F6	−134.8 (4)
C5′—C6′—C7′—Fe1	61.1 (4)	C20—C19—C22—F6	44.6 (5)
C6′—C7′—C8′—C9′	0.0		