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Molecular and crystal structures of six poly(arylsulfinyl)- and poly(arylsulfanyl)ferrocenes

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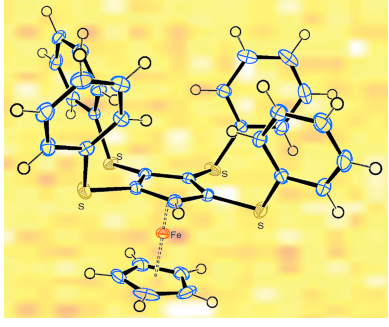
Starting from (*p*-tolylsulfinyl)ferrocene (**1**), a mixture of the complete series [CpFe{C_5H_{5-n}(SOTol-*p*)$_n$}] (n = 2–4) (**2**–**4**) in all regioisomers was obtained. After chromatographic separation, crystals of 1,2-bis[(4-methylbenzene)sulfinyl]ferrocene, **2a**, and 1,3-bis[(4-methylbenzene)sulfinyl]ferrocene, **2b**, both [Fe(C_5H_5)($C_{19}H_{17}O_2S_2$)], as well as of 1,2,3-tris[(4-methylbenzene)sulfinyl]ferrocene, [Fe(C_5H_5)($C_{26}H_{23}O_3S_3$)], **3a**, and 1,2,3,4-tetrakis[(4-methylbenzene)sulfinyl]ferrocene ethyl acetate 0.75-solvate, [Fe(C_5H_5)($C_{33}H_{29}O_4S_4$)]·0.75$C_4H_8O_2$, **4**, could be isolated. Their molecular and crystal structures are compared with each other and also with the so far unreported structures of related 1,2-bis(phenylsulfanyl)ferrocene, [Fe(C_5H_5)($C_{17}H_{13}S_2$)], **5**, and 1,2,3,4-tetrakis(phenylsulfanyl)ferrocene, [Fe(C_5H_5)($C_{29}H_{21}S_4$)], **6**. In all the sulfinyl structures, the O atoms of the S=O groups are in equatorial positions, except for that in tetrasubstituted **4**. All the arene rings of these compounds (except for one ring in **4**) are in axial positions directed away from the Fe atom, mostly in a near perpendicular orientation with respect to the plane of the cyclopentadienyl ring. The main intermolecular interactions in the crystals are C—H···H—C, C—H···π and C—H···O, while C—H···S interactions are much less important, except for tetrasulfanyl compound **6**. π–π interactions (intramolecular) are only important in compound **3a**. Hirshfeld analysis shows that dispersion terms are dominant for the interaction energies of all six compounds. In general, the calculated total interaction energies increase with increasing number of substituents and are higher for the sulfinyl than for the sulfanyl groups.

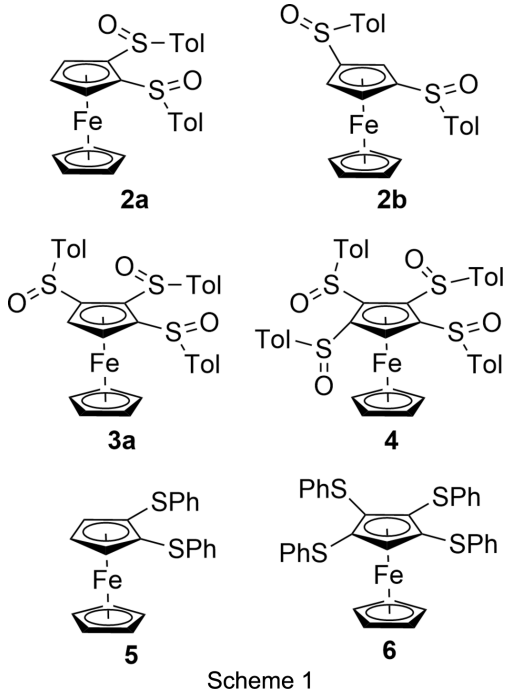
1. Introduction

(R_S)-(*p*-Tolylsulfinyl)ferrocene [CpFe(C_5H_4SOTol-*p*)] (**1**) was first reported by Rebiere *et al.* (1990). It was obtained by treatment of lithioferrocene with the Andersen reagent, *i.e.* (+)-(R_S,1*S*)-menthyl *p*-toluenesulfinate (Andersen, 1964). An alternative approach, also introduced by the group of Kagan, used the enantioselective oxidation of the corresponding ferrocenyl sulfide (Diter *et al.*, 1994). Treating this compound with lithium diisopropylamide (LDA) led to diastereoselective *ortho*-lithiation (Rebière *et al.*, 1993) and, after quenching with appropriate electrophiles, a selective synthesis of planar–chiral ferrocenes was possible (Ferber & Kagan, 2007; Schaarschmidt & Lang, 2013). While numerous unsymmetrically disubstituted and, therefore, planar–chiral ferrocenes have been reported, there are very few reports on disubstituted ferrocenes, [CpFe($C_5H_3R_2$)], with two identical substituents carrying the same chirality on the α-atom of the substituent: R = CHMe(OH) (Moïse & Mugnier, 1972), CHPh(OAc), CHPh(N_3) and CHPh(NH_2) (Fukuzawa & Suzuki, 2006), CHMe(PPh_2BH_3) (Fukuzawa *et al.*, 2000), and, more recently, R = SO(*t*-Bu) or SO(Tol-*p*) (Wen *et al.*, 2022). The latter article described the synthesis of (S_S,$S_{S'}$)-[CpFe{C_5H_3(SOTol-*p*)}$_2$-1,2)] (**2a**). Apparently, no metallocenes



with more than two arylsulfinyl substituents have been reported so far. A search in the Cambridge Structural Database (CSD, accessed on March 10, 2024; Groom *et al.*, 2016) shows 35 entries for the search mask '[CpFe{C_5(SOPh)}]', including three sulfone compounds. Nine of the 35 contained a {C_5H_4SOPh} ring, while 26 were 1,2-disubstituted. None contains more than one sulfinyl substituent and no 1,3-disubstituted structure was reported.

Structurally related to arylsulfinyl groups are arylsulfanyl groups, which create interesting electrical properties on the molecules to which they are bound. It was found that 'phenylthiol substituents attached to aromatic cores result in a reduction of the HOMO–LUMO gap' (HOMO is the highest occupied molecular orbital and LUMO is the lowest unoccupied molecular orbital) (Gingras *et al.*, 2006; Deng *et al.*, 2017). Previously, we described the synthesis of the arylsulfanylferrocenes [CpFe{C_5H_{5-n}(SPh)$_n$}] (n = 1–5) (Blockhaus *et al.*, 2019) and reported the crystal structure of the penta-substituted compound. We found it worthwhile to study the synthesis of poly(arylsulfinyl)ferrocenes [CpFe{C_5H_{5-n}(SOAr)$_n$}] with $n \geq 2$ and compare their crystal and molecular structures with the corresponding poly(arylsulfanyl)ferrocenes. Scheme 1 shows the compounds discussed in the present study. To the best of our knowledge, there is only one systematic study comparing organic sulfides and sulfoxides with respect to the intermolecular interactions in the crystal (Zhou *et al.*, 2021).



Scheme 1

2. Experimental

2.1. Synthesis and crystallization

Reactions were carried out under an argon atmosphere using standard Schlenk techniques. The anhydrous solvents and LDA (1.0 *M* in THF/hexane, Sigma–Aldrich) were used as provided. Andersen's reagent was prepared according to the literature (Andersen, 1964)

Column chromatography was performed on silica gel (Acros Organics) using petroleum ether (PE), diethyl ether (Et_2O), dichloromethane (CH_2Cl_2) or ethyl acetate (EA), or mixtures thereof, as eluents.

2.1.1. Synthesis of (S_S)-(*p*-tolylsulfinyl)ferrocene, 1

A solution of ferrocene (6.52 g, 35.1 mmol) and KO*t*-Bu (0.47 g, 4.21 mmol) in THF (100 ml) was treated at −78 °C with *tert*-butyllithium solution (22 ml), with stirring for 30 min at −78 °C and 30 min at room temperature. Then, at −78 °C, Andersen's reagent (10.32 g, 35.05 mmol) was added and stirring continued for 18 h. After evaporation of the solvents *in vacuo*, the residue was placed on top of a silica-gel column and extracted with dichloromethane (5 × 100 ml). After removal of the solvents *in vacuo*, the desired product was obtained after chromatography on silica gel, using a 1:1 (*v*/*v*) PE/Et_2O mixture as eluent (yield: 6.56 g, 20.3 mmol, 58%). For the ^{1}H NMR spectrum, see Fig. S17 of the supporting information.

2.1.2. Reaction of 1 with LDA and Andersen's reagent

A solution of **1** (2.400 g, 7.41 mmol) in THF (75 ml) was treated at −78°C with 1.0 *M* LDA solution (8.90 ml, 8.90 mmol) with stirring for 45 min. Then, after addition of solid Andersen reagent (2.620 g, 8.90 mmol) with continuous stirring, the reaction mixture was warmed gradually to room temperature (20 °C) within 16 h. After evaporation of the obtained suspension, the residue was taken up in the minimum amount of ethyl acetate and placed on top of a silica-gel column. Repeated chromatography was necessary to afford separations of the products.

(1S_S,2S_S)-1,2-Bis[(4-methylbenzene)sulfinyl]ferrocene (2a). ^{1}H NMR (400 MHz, $CDCl_3$, Fig. S8): δ 7.46 (*m*, 4H), 7.22 (*m*, 2H), 7.10 (*m*, 2H), 4.91 (*m*, 1H), 4.55 (*s*, 5H), 4.48 (*m*, 1H), 4.23 (*m*, 1H), 2.40 (*s*, 3H), 2.32 (*s*, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, Fig. S9): δ 141.8, 141.1, 129.7, 125.3, 125.2, (87.8, assignment dubious), 72.2, 70.8, 67.2, 21.6, 21.5; HRMS (+p ESI): *m*/*z* 463.04871 (M + H^+; calculated for $C_{24}H_{23}O_2FeS_2$: 463.04891); IR (ATR, cm^{-1}): ν(SO) 1733, 1714.

(1S_S,3S_S)-1,3-Bis[(4-methylbenzene)sulfinyl]ferrocene (2b). ^{1}H NMR (270 MHz, $CDCl_3$, Fig. S10): δ 7.50 (*m*, 2H), 7.47 (*m*, 2H), 7.28 (*m*, 2H), 7.26 (*m*, overlapped with solvent), 4.80 (*m*, 1H), 4.78 (*m*, 1H), 4.54 (*s*, 5H), 4.49 (*m*, 1H), 2.39 (*s*, 6H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, Fig. S11): δ 142.0, 141.9, 141.8, 130.03, 129.99, 124.63, 124.55, 86.4, 96.3, 72.0, 69.3, 67.5, 66.2, 21.6; HRMS (+p ESI): *m*/*z* 501.00495 (M + K^+, calculated for $C_{24}H_{22}KO_2FeS_2$: 501.00481); IR (ATR, cm^{-1}): ν(SO) 1736, 1718.

(1S_S,2S_S,3S_S)-1,2,3-Tris[(4-methylbenzene)sulfinyl]ferrocene (3a). ^{1}H NMR (270 MHz, $CDCl_3$ Fig. S12): δ 7.48 (*m*, 2H), 7.25 (*m*, overlapped with solvent), 7.13 (*m*, 2H), 6.96–6.86 (*m*, 6H), 5.13 (*m*, 1H), 4.79 (*s*, 5H), 4.36 (*m*, 1H), 2.40 (*s*, 3H), 2.27 (*s*, 3H), 2.25 (*s*, 3H); ^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2, Fig. S13): δ 143.7, 142.7, 142.5, 141.6, 141.3, 139.9, 130.1, 129.70, 129.66,

Table 1
Experimental details.

Experiments were carried out with Mo $K\alpha$ radiation using a Bruker D8 VENTURE diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Krause *et al.*, 2015). H-atom parameters were constrained.

	2a	**2b**	**3a**
Crystal data			
Chemical formula	$[Fe(C_5H_5)(C_{19}H_{17}O_2S_2)]$	$[Fe(C_5H_5)(C_{19}H_{17}O_2S_2)]$	$[Fe(C_5H_5)(C_{26}H_{23}O_3S_3)]$
M_r	462.38	462.38	600.56
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1$	Triclinic, $P1$
Temperature (K)	297	296	110
a, b, c (Å)	7.8964 (2), 12.9064 (3), 11.0124 (3)	17.1882 (10), 6.0383 (4), 20.4271 (12)	7.8298 (5), 9.8573 (6), 17.4937 (11)
α, β, γ (°)	90, 109.467 (1), 90	90, 95.995 (2), 90	93.379 (2), 91.120 (2), 98.051 (2)
V (Å^3)	1058.16 (5)	2108.5 (2)	1334.02 (14)
Z	2	4	2
μ (mm^{-1})	0.93	0.93	0.83
Crystal size (mm)	0.07 × 0.05 × 0.04	0.10 × 0.02 × 0.02	0.10 × 0.03 × 0.02
Data collection			
T_{min}, T_{max}	0.679, 0.746	0.648, 0.746	0.809, 0.862
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11282, 4815, 4393	34842, 10422, 8415	21012, 10957, 9889
R_{int}	0.020	0.032	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649	0.667	0.634
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.084, 1.14	0.042, 0.095, 1.02	0.034, 0.073, 1.02
No. of reflections	4815	10422	10957
No. of parameters	264	573	691
No. of restraints	13	8	6
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.34	0.50, −0.23	0.41, −0.30
Absolute structure	Flack x determined using 1876 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 3063 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 4237 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.014 (6)	0.019 (7)	0.014 (8)

	4	**5**	**6**
Crystal data			
Chemical formula	$[Fe(C_5H_5)(C_{33}H_{29}O_4S_4)]\cdot 0.75C_4H_8O_2$	$[Fe(C_5H_5)(C_{17}H_{13}S_2)]$	$[Fe(C_5H_5)(C_{29}H_{21}S_4)]$
M_r	804.82	402.33	618.64
Crystal system, space group	Monoclinic, $P2_1$	Orthorhombic, $Pmn2_1$	Triclinic, $P\overline{1}$
Temperature (K)	107	110	110
a, b, c (Å)	12.8893 (7), 8.2225 (4), 36.500 (2)	14.0977 (11), 7.1607 (5), 8.8504 (5)	8.4836 (4), 10.3028 (5), 16.7210 (8)
α, β, γ (°)	90, 97.106 (2), 90	90, 90, 90	90.730 (2), 103.948 (2), 94.999 (2)
V (Å^3)	3838.6 (4)	893.44 (11)	1412.15 (12)
Z	4	2	2
μ (mm^{-1})	0.66	1.08	0.85
Crystal size (mm)	0.07 × 0.02 × 0.02	0.10 × 0.08 × 0.05	0.06 × 0.05 × 0.02
Data collection			
T_{min}, T_{max}	0.811, 0.862	0.682, 0.746	0.691, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	59999, 15634, 13598	9831, 2561, 2426	23494, 7023, 5898
R_{int}	0.074	0.041	0.046
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.694	0.667
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.141, 1.12	0.025, 0.060, 1.05	0.034, 0.088, 1.04
No. of reflections	15634	2561	7023
No. of parameters	936	118	352
No. of restraints	77	1	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.69, −0.56	0.30, −0.31	0.42, −0.39
Absolute structure	Flack x determined using 4943 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1069 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	–
Absolute structure parameter	0.053 (8)	0.018 (9)	–

Computer programs: *APEX2* (Bruker, 2011), *SAINT* (Bruker, 2011), *SHELXT2014/SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018/SHELXL2019* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020) and *PLATON* (Spek, 2020).

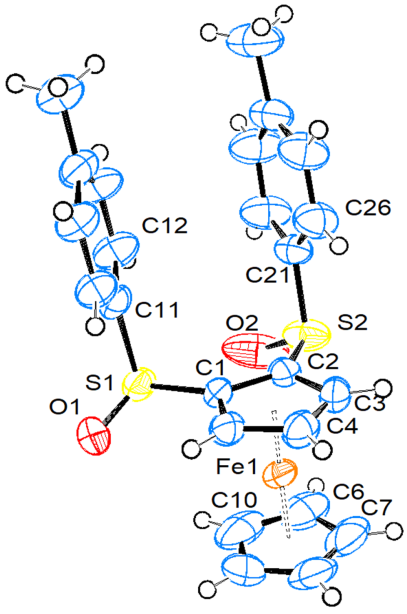


Figure 1
View of the molecular structure of compound **2a**. Displacement ellipsoids are drawn at the 50% probability level.

125.8, 125.5, 125.4, 98.6, 97.1, 95.4, 74.5, 70.8, 68.0, 21.6, 21.41, 21.39; HRMS (+p ESI): *m*/*z* 601.06268 ($M + H^+$, calculated for $C_{31}H_{29}O_3FeS_3$: 601.06285); IR (ATR, cm^{-1}): ν(SO) 1736.

(1*S*$_S$,2*S*$_S$,3*S*$_S$,4*S*$_S$)-1,2,3,4-Tetrakis[(4-methylbenzene)sulfinyl]ferrocene (4). ^{1}H NMR (400 MHz, $CDCl_3$, Fig. S14): δ 7.75 (*m*, 2H), 7.41 (*m*, 2H), 7.21 (*m*, 2H), 7.17 (*m*, 2H), 6.90 (*m*, 2H), 6.80 (*m*, 2H), 6.51 (*m*, 2H), 6.21 (*m*, 2H), 5.16 (*s*, 1H), 4.96 (*s*, 5H), 2.50 (*s*, 3H), 2.26 (*s*, 3H),2.19 (*s*, 3H), 2.16 (*s*, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$, Fig. S15): δ 143.5, 142.8, 141.8, 141.7, 141.6, 141.3, 141.0, 140.8, 140.0, 138.1, 130.4, 129.7, 129.50. 129.48, 129.0, 126.34, 126.25, 125.8, 125.5, 125.0, 98.6, 98.4, 97.3, 94.3, 92.8, 71.9, 21.8, 21.6, 21.5, 21.3; HRMS (+p ESI): *m*/*z* 739.07683 ($M + H^+$, calculated for $C_{38}H_{35}O_4FeS_4$: 739.07682).

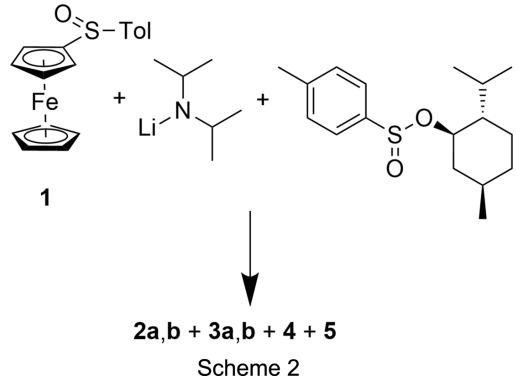
2.2. Refinement

Some remarks are necessary with regard to the structure of compound **4**. The crystals of this compound contain in their voids ethyl acetate solvent molecules. One of them is 'well behaved', with no sign of disorder, while the other shows a disorder of the kind that the terminal methyl groups are screw-related, *i.e.* the CH_3CO methyl group coincides with the screw-related $(-x, y + \frac{1}{2}, -z)$ OCH_2CH_3 methyl group of the next molecule. Since this is chemically impossible, the site-occupancy factor (s.o.f.) was restricted to 0.5. It was also necessary to restrain all bonds within the disordered molecules to be the same as the corresponding bonds of the ordered solvent molecule (five SADI instructions in *SHELXL*). The refinement showed also some problems with the anisotropic displacement parameters of the cyclopentadienyl (Cp) ring of molecule *A* (most likely unresolved disorder, combined with strong librations). To overcome this problem, further restraints were necessary (ISOR and DELU instructions were applied for all five Cp C atoms, *i.e.* the U^{ij} components were modelled approximately isotropically and rigid-bond restraints were applied). Further crystal data, data collection and structure refinement details are summarized in Table 1.

3. Results and discussion

3.1. Synthesis

We decided to use the original procedure of Kagan, with only slight modifications, for the synthesis of (S_S)-(*p*-tolylsulfinyl)ferrocene [(S_S)-**1**]. We did not check the enantiomeric purity, as we hoped that necessary purifications would be easier at a later stage. In this context, we also became aware of a report on 'problems with the accurate determination of the stereochemical outcome' of such reactions (Han *et al.*, 2018). We then treated the isolated product with 1.2 equivalents of LDA and 1.2 equivalents of Andersen's reagent in THF at −78 °C, followed by warming to room temperature (Scheme 2).



Scheme 2

A ^{1}H NMR spectrum of the crude product showed a myriad of signals. After several chromatographic separations, regio-

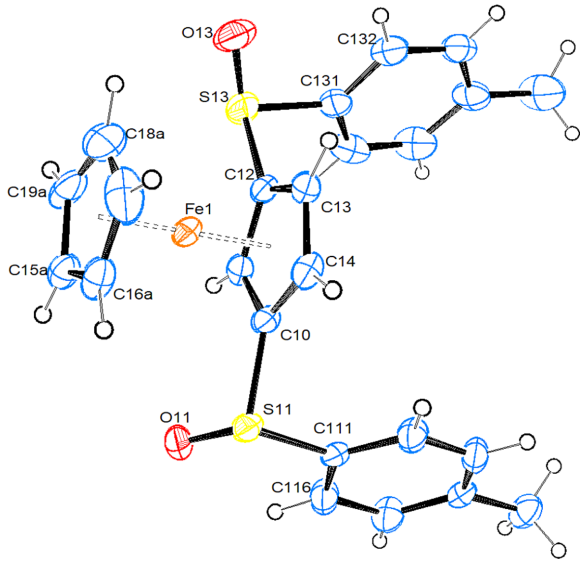


Figure 2
View of the molecular structure of molecule *A* of compound **2b**. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Important bond parameters (Å, °) for **2a**, **2b** and **5** in comparison with some related compounds from the literature.

CT is the centroid of a Cp ring, the subscript 'sub' refers to the substituted Cp ring, the subscript 'C5H5' refers to the unsubstituted Cp ring, C_i is an arene *ipso*-C atom and C_o is an arene *ortho*-C atom.

Distances/angles	**2a**	**2b** (molecule *A*)	**2b** (molecule *B*)	**1** (VEZPUM)	HEZMIJ	TELHOH	**5**
Fe—CT_{sub}	1.629 (2)	1.634 (2)	1.631 (2)	1.647/1.643	1,647/1.641	1.634 (3)	1.6305 (11)
Fe—CT_{C5H5}	1.653 (2)	1.644 (4)	1.660 (4)	1.657/1.656	1.654/1.650	1.650 (3)	1.6512 (13)
C_{sub}—CT_{sub}—CT_{C5H5}—C_{C5H5}	5.2	14.0	9.9	0.2/1.7	15.2/10.6	6.4 (5)	0.2
C_{sub}—S	1.770 (3)	1.779 (4)	1.778 (4)	1.779 (2)/	1.770 (3)/	1.774 (6)	1.752 (2)
	1.757 (3)	1.764 (4)	1.779 (4)	1.777 (2)	1.768 (3)		
S—O	1.478 (4)	1.490 (4)	1.479 (5)	1.496 (2)/	1.498 (2)/	1.502 (5)	
	1.498 (4)	1.476 (4)	1.488 (4)	1.496 (1)	1.491 (2)		
Fe···O	3.694 (3)	3.777 (3)	3.772 (4)	3.803 (2)/	4.589 (1)/	4.555 (5)	
	3.725 (3)	3.686 (4)	3.822 (3)	3.782 (2)	4.581 (1)		
Fe···S	3.333 (1)	3.365 (1)	3.340 (1)	3.3634 (8)	3.4042 (6)	3.409 (2)	3.3038 (7)
	3.288 (1)	3.334 (1)	3.345 (1)	3.3180 (8)	3.4062 (6)		
C_{sub}—S—O	103.4 (2)	105.4 (6)	105.7 (2)	107.1 (1)/	107.9 (2)/	105.6 (3)	
	108.6 (2)	106.7 (3)	107.0 (2)	106.9 (1)	106.5 (1)		
CT_{C5H5}—CT_{sub}—S—O	73.6	61.4	73.5	66.3/	172.4/	170.1	
	62.9	66.3	71.4	74.0	176.1		
O—S—C_i—C_o	37.8 (4)	14.3 (4)	28.8 (4)	21.3 (2)/	21.1 (2)/	14.0 (6)	
	27.7 (4)	12.4 (6)	32.2 (5)	19,7(2)	24.9 (2)		
O—S—C_{sub}—C	14.9 (3)	20.6 (4)	12.8 (4)	23.6 (3)/	86.0 (2)/	79.6 (3)	
	23.2 (3)	27.8 (5)	14.9 (5)	13.2 (2)	82.7 (2)		
C_{sub}—S—C_i—C_o	44.0 (4)	84.9 (5)	82.8 (4)	85.7 (2)/	91.1 (1)/	90.4 (6)	7.0 (2)
	69.4 (4)	59.3 (4)	72.5 (4)	88.9 (2)	89.6 (1)		
∠(Cp, Ph)	80.9 (2)	85.6 (3)	81.6 (2)	82.6/	86.4/	84.7	89.63 (12)
	86.4 (2)	86.3 (3)	81.4 (3)	84.0	78.5		
∠(Ph, Ph)	32.3 (3)	17.2 (2)	37.6 (2)				60.59 (6)

isomers **2a** and **2b**, as well as **3a** and **4**, could be isolated in pure forms, albeit in low yields.

The syntheses of the poly(phenylsulfanyl)ferrocenes [CpFe{$C_5H_3(SPh)_2$-1,2}] (**5**) and [CpFe{$C_5H(SPh)_4$}] (**6**) were reported by us previously (Blockhaus *et al.*, 2019).

3.2. Molecular structures

3.2.1. Disubstituted ferrocenes

(1*S*$_S$,2*S*$_S$)-1,2-Bis[(4-methylbenzene)sulfinyl]ferrocene (2a) and (1*S*$_S$,3*S*$_S$)-1,3-bis[(4-methylbenzene)sulfinyl]ferrocene (2b). Compound **2a** crystallizes in the monoclinic space group $P2_1$ with one molecule in the asymmetric unit. Fig. 1 shows a side view of the molecule (a top view is shown in Fig. S1 of the supporting information). Compound **2b** also crystallizes in the monoclinic space group $P2_1$, however, with two molecules in the asymmetric unit. Fig. 2 shows a side view of molecule *A*, while top views of molecules *A* and *B* can be found in the supporting information (Fig. S2).

1,2-Bis(phenylsulfanyl)ferrocene (5). Compound **5**, [FeCp{$C_5H_3(SPh)_2$-1,2}], crystallizes in the orthorhombic space group $Pmn2_1$, with half a molecule in the asymmetric unit. Fig. 3 shows a side view of one complete molecule.

The Fe1, C3 and C4 atoms are located on the mirror plane. The Cp rings are exactly eclipsed and all bond parameters occur necessarily pairwise.

Important bond parameters are collected in Table 2, together with literature data for the mono(tolylsulfinyl)ferrocene (**1**) (CSD refcode VEZPUM) and the 1,2-disubstituted [CpFe{$C_5H_3(CH_2NMe_2)$(SOTol-*p*)}] (HEZMIJ) (both in Heinemann *et al.*, 2007), and [CpFe{$C_5H_3(CH_2OH)$(SOTol-*p*)}] (TELHOH; Robinson *et al.*, 1996).

As can be seen from Table 2, the distances from Fe to the unsubstituted Cp ring are slightly longer than from Fe to the substituted Cp ring. The relative orientation of the Cp rings is close to eclipsed in **1**, **2a** and the CH_2OH-substituted compound TELHOH. The C—S bonds from the Cp rings are slightly shorter in **2a** than in all the other compounds, while the S—O bonds in disulfinyl complexes **2a** and **2b** are slightly shorter than in the monosulfinyl compounds. The ring C—S bond in **5** is slightly shorter than in the sulfinyl compounds, and lies exactly in the arene plane. The O atoms on sulfur are in equatorial positions directed towards the Fe atom in compounds **1**, **2a** and **2b** (the Fe···O distances are between 3.66

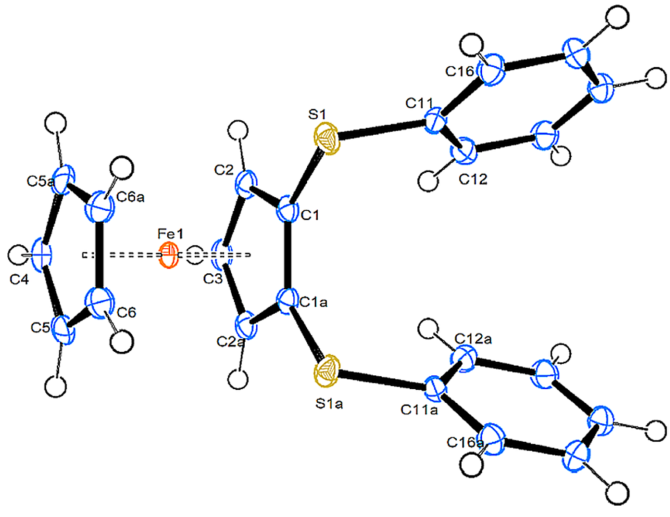


Figure 3
View of the molecular structure of the whole molecule of compound **5**. Displacement ellipsoids are drawn at the 50% probability level.

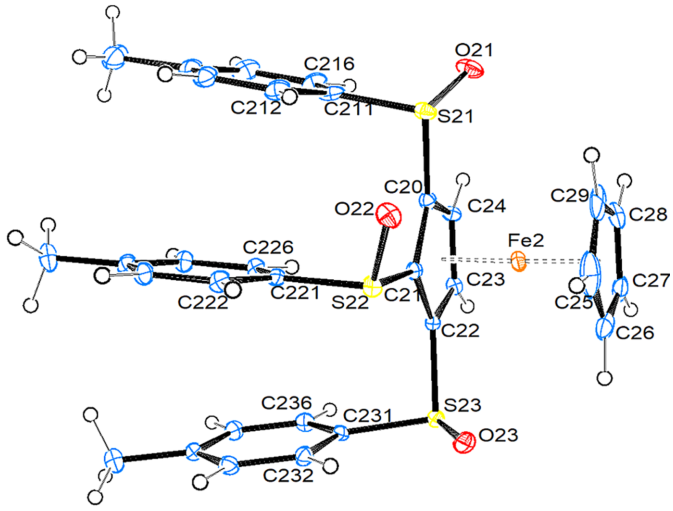


Figure 4
View of the molecular structure of molecule *B* of compound **3a**. Displacement ellipsoids are drawn at the 50% probability level.

and 3.82 Å, and torsion angles CT—CT—S—O (CT is as defined in Tables 2 and 3) are in the range 61–74°), while they are in axial positions directed away from Fe in the remaining two compounds (Fe···O distance > 4.5 Å and torsion angles CT—CT—S—O in the range 170–176°). The C—S—O angles are all between 103 and 109°, with no recognizable trends. The arene rings on sulfur are always close to being perpendicular with respect to the plane of the Cp ring, spanning a range from *ca* 81° to nearly 90° (in sulfanyl compound **5**). Whenever the O atom is in an equatorial position, the S—O bond assumes an angle between 13 and 28° with respect to the arene plane, while the S—O bond orients itself nearly perpendicular when the O atom is in an axial position. In all the title compounds, the Fe···S distance is significantly shorter than the sum of the van der Waals radii (3.80 Å), with the shortest distance being observed for compound **5**.

3.2.2. Trisubstituted ferrocene

Compound **3a** crystallizes in the triclinic space group *P*1, with two molecules in the asymmetric unit. Fig. 4 shows a side view of molecule *B*. Top views of molecules *A* and *B* can be found in the supporting information (Fig. S3). Table 3 collects important bond parameters for compounds **3a**, **4** and **6**.

There is a slight tendency for the distances between Fe and the substituted Cp ring to decrease with increasing degree of substitution, while the distance to the unsubstituted ring remains unchanged. There seems to be no effect of the number of sulfinyl substituents on the relative orientation of the Cp rings. Both molecules of **3a** have nearly perfectly eclipsed Cp rings, as in compounds **1** and **2a**. The C—S bonds become gradually longer with increasing degree of substitution, while there is no observable trend in the S—O bond lengths. All O atoms are in equatorial positions (Fe···O distances between 3.59 and 3.86 Å and torsion angles CT—CT—S—O in the range 49–84.5°). All arene rings adopt a nearly perpendicular orientation with respect to the plane of the Cp ring, and are close to being parallel to each other. The relative orientation of the S—O bond and the plane of the arene ring spans the whole range from coplanar to nearly perpendicular. Quite interestingly, in both molecules, the ring C—S vector of the 'middle' bond lies in the plane of the corresponding arene ring, while for the 'outer' two C—S bonds, these vectors and the arene planes are at a 70 ± 5° angle. The Fe···S distances are well below the sum of the van der Waals radii, spanning, however, a relative large range between 3.319 (1) and 3.441 (1) Å.

3.2.3. Tetrasubstituted ferrocene

1,2,3,4-Tetrakis[(4-methylbenzene)sulfinyl]ferrocene (4). Compound **4** crystallizes in the monoclinic space group $P2_1$ with two molecules in the asymmetric unit. In addition, there is one molecule of ethyl acetate, which shows no disorder, and another half molecule of this solvent, which shows disorder. Fig. 5 shows a side view of molecule *B*. Top views of molecules *A* and *B* can be found in the supporting information (Fig. S4).

The Cp rings are more staggered than in the other compounds, and the substituted ring is closer to the Fe atom than in the less substituted complexes. Compound **4** is the only one of the studied compounds where one sulfinyl O atom is in an axial position. The other three O atoms are – as usual – in equatorial positions. However, in literature compounds HEZMIJ and TELHOH, the O atom is also in an axial position. As these compounds are only disubstituted ferrocenes with only one sulfinyl substituent, it becomes clear that shifting the O atom into an axial position is not a consequence of steric congestion in compound **4**. The Fe···S distances are – as in all other compounds described in this study – well below the sum of the van der Waals radii, spanning a range from 3.302 (2) to 3.407 (2) Å. All arene rings – except for one in molecule *A* – are close to being perpendicular with respect to

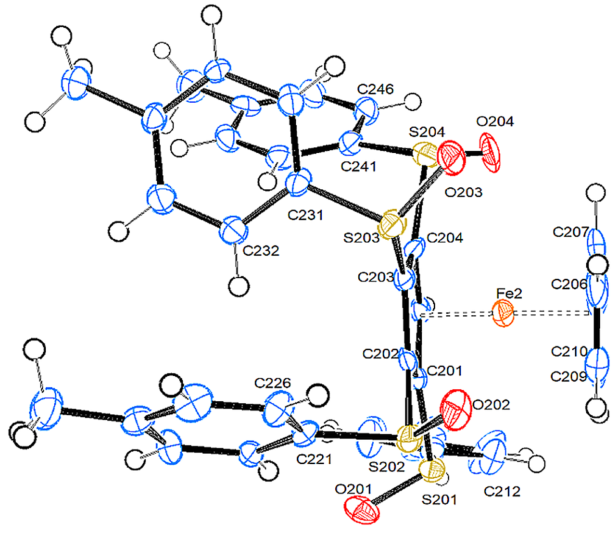


Figure 5
View of the molecular structure of molecule *B* of compound **4**. Displacement ellipsoids are drawn at the 50% probability level.

Table 3
Important bond parameters (Å, °) in compounds **3a**, **4** and **6**.

CT is the centroid of a Cp ring, the subscript 'sub' refers to the substituted Cp ring, the subscript 'C5H5' refers to the unsubstituted Cp ring, C_i is an arene *ipso*-C atom and C_o is an arene *ortho*-C atom.

Distances/angles	**3a** (molecule *A*)	**3a** (molecule *B*)	**4** (molecule *A*)	**4** (molecule *B*)	**6**
$Fe-CT_{sub}$	1.629 (2)	1.623 (2)	1.621 (3)	1.622 (3)	1.6196 (8)
$Fe-CT_{C5H5}$	1.653 (2)	1.661 (3)	1.664 (4)	1.660 (4)	1.6668 (11)
$C_{sub}-CT_{sub}-CT_{C5H5}-C_{C5H5}$	2.5	0.88	20.9	8.6	18.4
$C_{sub}-S$	1.779 (4)	1.788 (4)	1.791 (7)	1.784 (8)	1.756 (2)
	1.773 (4)	1.776 (4)	1.786 (7)	1.795 (8)	1.753 (2)
	1.791 (4)	1.791 (4)	1.793 (7)	1.801 (8)	1.754 (2)
			1.786 (8)	1.801 (8)	1.756 (2)
S—O	1.486 (3)	1.492 (3)	1.486 (6)	1.488 (6)	
	1.496 (3)	1.495 (3)	1.480 (6)	1.490 (6)	
	1.494 (3)	1.486 (3)	1.485 (6)	1.480 (6)	
			1.490 (6)	1.490 (7)	
Fe···O	3.856 (3)	3.850 (3)	4.518 (6)	4.455 (6)	
	3.800 (3)	3.698 (3)	3.550 (5)	3.643 (6)	
	3.613 (2)	3.593 (3)	3.671 (6)	3.665 (6)	
			3.480 (6)	3.470 (7)	
Fe···S	3.370 (1)	3.319 (1)	3.407 (2)	3.302 (2)	3.3339 (6)
	3.386 (1)	3.441 (1)	3.305 (2)	3.404 (2)	3.3336 (6)
	3.337 (1)	3.324 (1)	3.400 (2)	3.341 (2)	3.2381 (5)
			3.356 (2)	3.340 (2)	3.3717 (6)
$C_{sub}-S-O$	107.9 (2)	103.6 (2)	107.4 (3)	104.8 (3)	,
	105.9 (2)	105.9 (2)	108.8 (3)	108.2 (3)	
	103.0 (2)	108.5 (2)	107.6 (3)	108.8 (4)	
			104.7 (3)	107.2 (4)	
$CT_{C5H5}-CT_{sub}-S-O$	84.5	72.1	34.9	42.7	
	69.2	67.2	44.0	44.3	
	49.8	49.0	46.8	51.6	
			156.4	152.1	
$O-S-C_i-C_o$	3.1 (5)	34.8 (5)	12.2 (7)	31.8 (7)	
	74.0 (4)	66.5 (3)	12.0 (7)	1.5 (7)	
	40.7 (4)	5.4 (4)	2.5 (7)	8.0 (7)	
			35.1 (9)	22.8 (8)	
$O-S-C_{sub}-C$	36.4 (4)	14.2 (4)	53.6 (8)	67.3 (7)	
	20.9 (4)	25.8 (4)	47.5 (7)	35.9 (8)	
	4.4 (4)	37.2 (4)	36.7 (7)	44.7 (8)	
			70.7 (7)	41.4 (8)	
$C_{sub}-S-C_i-C_o$	65.1 (4)	71.6 (4)	66.0 (7)	53.8 (8)	8.1 (2)
	1.3 (5)	5.0 (4)	61.3 (6)	64.3 (7)	15.8 (2)
	74.2 (4)	74.4 (4)	72.2 (7)	66.6 (6)	57.2 (2)
			73.3 (7)	77.0 (7)	13.7 (2)
∠(Cp,Ph)	84.5 (2)	81.6 (2)	87.9 (4)	80.6 (4)	67.27 (11)
	89.8 (2)	81.4 (2)	81.8 (4)	88.6 (4)	87.37 (10)
	87.4 (2)	86.0 (2)	85.6 (4)	86.1 (4)	67.32 (10)
			73.0 (4)	86.1 (4)	71.45 (10)
∠(Ph,Ph)	6.4 (2)	6.4 (2)	71.4 (4)	22.7 (4)	42.81 (11)
	18.6 (2)	15.9 (2)	46.8 (4)	88.5 (4)	25.13 (10)
	14.1 (2)	12.8 (2)	22.2 (4)	33.3 (4)	58.66 (10)
			62.8 (4)	69.2 (4)	66.05 (10)
			85.9 (4)	52.7 (4)	34.45 (10)
			40.8 (4)	56.5 (4)	83.19 (9)

the plane of the Cp ring. In contrast to compound **3a**, there is no tendency of the arene rings to orient themselves parallel to each other.

1,2,3,4-Tetrakis(phenylsulfanyl)ferrocene (6). Compound **6** crystallizes in the triclinic space group $P\overline{1}$ with one molecule in the asymmetric unit. Fig. 6 shows a side view of its molecular structure, while a top view is shown in Fig. S5.

The distance of the substituted Cp ring is nearly the same as in compound **4** and the staggering of the rings is also very similar. All arene rings are in axial positions, which is rather surprising, and only one is in the 'usual' close to perpendicular orientation with respect to the Cp ring. As in compound **4**, there is no observable tendency of the arene rings to orient themselves parallel to each other. The Fe···S distances in **6** are slightly shorter than in compound **4**, which parallels the observation made for compound **5** in comparison with compounds **2a** and **2b**.

3.3. Packing plots

Besides the bond parameters within a single molecule, it also seemed interesting to look at the intermolecular interactions. For this purpose, we examined the packing plots. Figs. 7–12 show the packing plots of compounds **2a**, **2b**, **3a**, **4**, **5** and **6**, respectively. Although there are many different 'noncovalent interactions', the plots show only the intermolecular

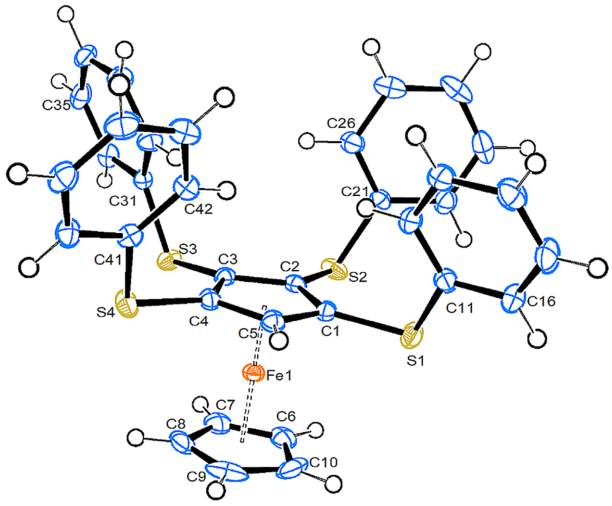


Figure 6
View of the molecular structure of compound **6**. Displacement ellipsoids are drawn at the 50% probability level.

interactions that involve O or S atoms. For other types of interactions, see Sections 3.4 and 3.6.

In **2a**, the ferrocene cores are perpendicular to the *bc* plane, while the arene rings are close to being parallel to it. A chain consisting of alternating ferrocene cores and arene rings propagates in the *c* direction. O···*X* and S···*X* contacts connect the molecules in all directions.

Compound **2b** shows a very different arrangement. Parallel to the *ac* diagonal run chains that contain either exclusively ferrocene cores with their molecular axes arranged anti-parallel to each other, or arene rings with their planes oriented nearly perpendicular to the *ac* plane. The ferrocene 'cores' are

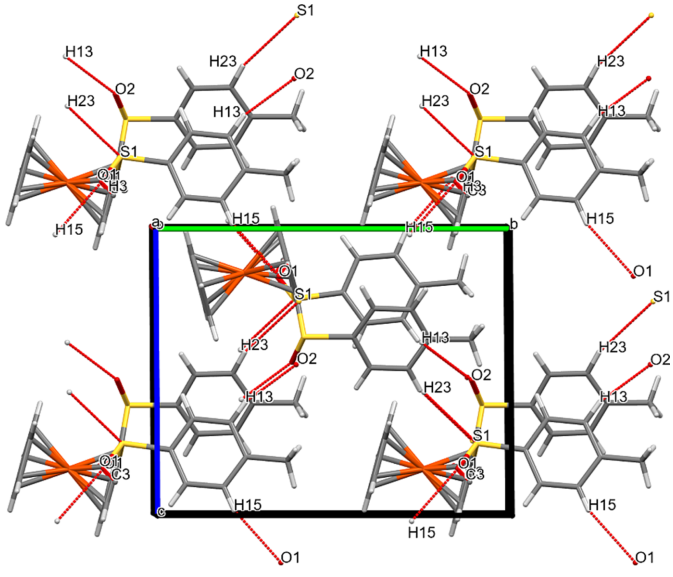


Figure 7
Packing plot of compound **2a**, viewed along *a*. The red and blue (colour coding according to the standard settings of *Mercury*: red is 'hanging', *i.e.* non-complete, and cyan is 'not-hanging', *i.e.* complete) coloured lines show weak interactions involving O and/or S atoms. Generic atoms labels without symmetry codes have been used.

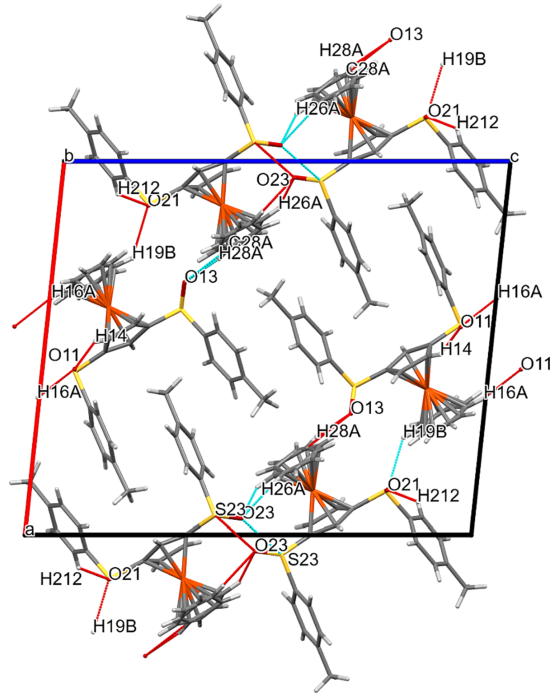


Figure 8
Packing plot of compound **2b**, viewed along *b*. The red and blue lines (for definition of colours, see Fig. 7) show weak interactions involving O and/or S atoms. Generic atoms labels without symmetry codes have been used.

joined in the direction of the *ac* diagonal *via* S···*X* and O···*X* interactions.

In compound **3a**, as can also be seen in Fig. S3, the ferrocene axis of all the molecules in the crystal are parallel to each other, and all the arene rings orient themselves perpendicular

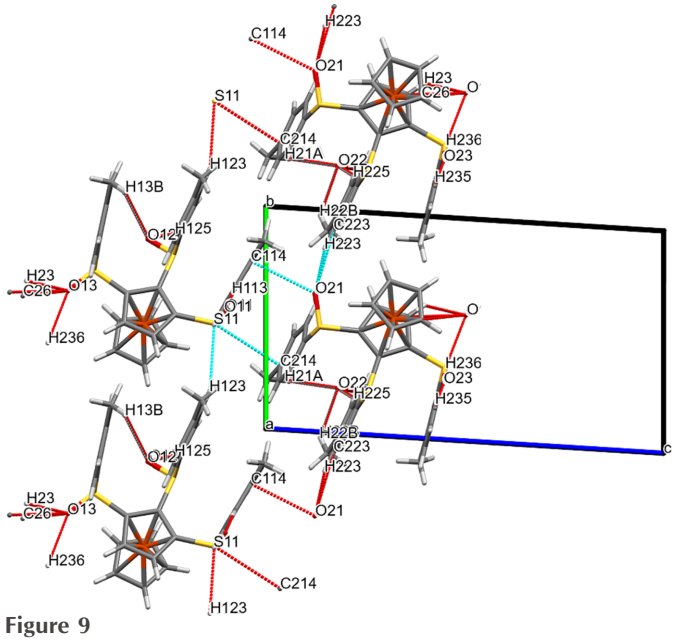


Figure 9
Packing plot of compound **3a**, viewed perpendicular to the Cp ring planes. The red and blue coloured lines (for definition of colours, see Fig. 7) show weak interactions involving O and/or S atoms. Generic atoms labels without symmetry codes have been used.

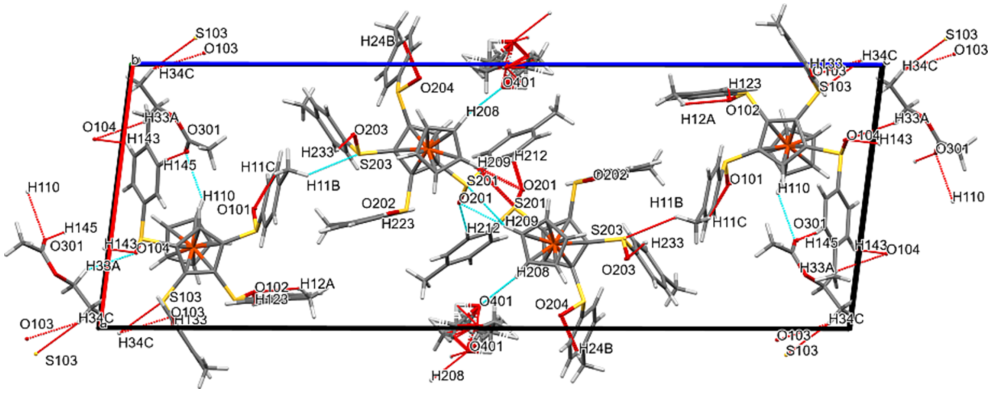


Figure 10
Packing plot of compound **4**, viewed along *b*. The red and blue coloured lines (for definition of colours, see Fig. 7) show weak interactions involving O or S atoms. Generic atoms labels without symmetry codes have been used.

to the planes of the Cp rings. Thus, a kind of 'mixed-layer' structure develops. All layers are interconnected *via* O···*X* and/or S···*X* contacts.

Figs. 10 and S6 show the packing plots for compound **4**. S···*X* and O···*X* contacts join the *A* molecules with each other, the *B* molecules with each other, as well as with *A* molecules, the *A* molecules with the ordered ethyl acetate solvent molecules and the *B* molecules with the disordered ethyl acetate solvent molecules. Fig. S6 shows the 'polymeric' arrangement of the disordered solvent molecules running at $z = 0.5$ along the *y* direction.

Compounds **5** and **6** do not contain O atoms. While **5** does not show any weak interactions involving the S atoms, there are several such contacts in the crystals of **6**. Inversion- and translation-related molecules are thus joined in the *a* and *b* directions. As the ferrocene cores are situated close to $z = 0$ and $z = 1$, the space between them is filled by arene rings. Therefore, there are no contacts involving the S atoms in the 'long' *c* direction.

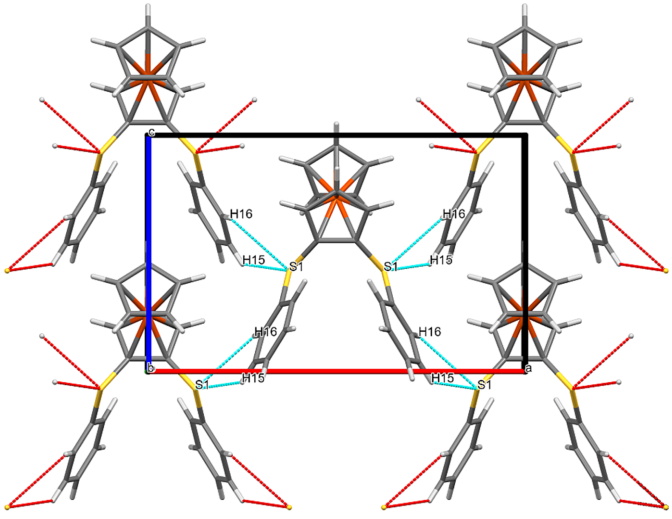


Figure 11
Packing plot of compound **5**, viewed along the *b* axis. Generic atoms labels without symmetry codes have been used.

3.4. Hydrogen bonding: C—H···O, C—H···S and C—H···C contacts

For a more detailed discussion, including numerical values for these contacts, see the supporting information (chapter 2 and Tables S1–S4).

In all the sulfinyl-substituted compounds, all the O atoms, except for O23 in compound **2b**, accept hydrogen bonds. Both intra- and intermolecular C—H···O hydrogen bonds are found, in most cases involving arene C—H bonds. The shortest H···O contact of 2.19 Å occurs for compound **3a**. The observed C—H···O angles range between 104 (intramolecular hydrogen bond) and 173° (intermolecular hydrogen bond).

S atoms rarely act as hydrogen-bond acceptors for the sulfinyl compounds (one intermolecular hydrogen bond each in compounds **2a** and **3a**, and none in **2b** and **4**). Quite astonishingly, the S atoms of compound **5** also do not accept any hydrogen bonds, while the two 'inner' S atoms of **6** accept one intermolecular hydrogen bond each. In the latter compound, the shortest H···S distance is 2.86 Å, while the C—H···S angles are in the range 143–163°.

C—H···C contacts of the C—H···π type (Mishra *et al.*, 2014) are found for all compounds except **2a** and **5**. There is one intramolecular interaction between an arene *ortho*-H atom and the attached substituted Cp ring for compound **3a**, and one intermolecular interaction between a tolylsulfanyl methyl group and an unsubstituted Cp ring for compound **2b**. In all other cases, the arene rings act as acceptors, mostly from other arene rings. The observed H···centroid distances range from 2.54 to 2.93 Å, both extrema being found in compound **4**.

3.5. Chalcogen bonding: O···O, O···S and S···S contacts

We examined the structures of the six title compounds for the existence of chalcogen bonding, using *Mercury* (Macrae *et al.*, 2020); however, only **2b** showed such interactions. In this compound, the molecules are joined into a helix along the crystallographic 2_1 screw axis *via* an S23···O23 interaction. The intermolecular S···O distance is 3.278 (4) Å, with an S—O···S angle of 152.4 (2)° and an O—S···O angle of 82.5 (2)°. Another much weaker S···O interaction, supporting

Table 4
Percentages of the individual contributions to the interactions across the Hirshfeld surface.

	C···C	H···H	O···O	S···S	S···O	C···H	O···H	S···H
2a	1.5	59.6	0	0	0	19.6	13.7	5.6
2b (molecule *A*)	0.2	57.0	0	0	0.5	26.8	10.3	5.3
2b (molecule *B*)	0.2	54.9	0.3	0	0.8	27.2	13.5	3.5
3a (molecule *A*)	2.9	65.5	0	0	0	9.5	14.6	5.6
3a (molecule *B*)	2.9	64.5	0	0	0	8.5	16.8	5.3
4	0.7	58.5	0	0	0	19.1	15.5	4.6
5	0.0	57.2	–	0	–	32.4	–	10.4
6	0.0	52.7	–	0.9	–	31.9	–	13.1

this helical arrangement, involves S11 and O11; the corresponding parameters are S···O = 3.779 (4) Å, S—O···S = 117.0 (2)° and O—S···O = 110.9 (2)°. These interactions can been seen in Fig. 8; however, for a clearer understanding, Fig. 13 shows these interactions more explicitly.

3.6. C···C contacts and short ring–ring interactions

This analysis was performed using *PLATON* (Spek, 2020). There are many 'short' distances between ring centroids below the *PLATON* limit of 6.0 Å, which might indicate some kind of π–π interactions. We restrict the present discussion to such interactions below the 4.5 Å distance limit. There are no such interactions for compounds **2b**, **4**, **5** and **6**.

In compound **2a**, there is a rather long intramolecular interaction of 4.156 (3) Å between the ring centroids. Quite interestingly, in corresponding disulfanyl compound **5**, the distance between the centroids is much longer at 4.716 (3) Å. However, there is an interesting C···C interaction in the latter compound between a Cp C atom of the substituted ring with two Cp atoms of the unsubstituted ring of the next molecule in the *b* direction, producing a 'polymeric' arrangement (Fig. 14).

In compound **3a**, there are close intramolecular contacts between arene rings within molecule *A* and within molecule *B*, as well as close intermolecular contacts between molecules *A* and *B* (Table S5). Most distances between centroids range from 3.70 to 3.90 Å, with only one long distance of *ca* 4.30 Å. Fig. S7 shows these interactions and a closer inspection shows that some C atoms still do not take part, with molecule *B* having a higher number of such 'unbound' C atoms.

3.7. Hirshfeld analysis

In order to gain further insight into the intermolecular interactions, we performed a Hirshfeld analysis using the program *CrystalExplorer* (Spackman *et al.*, 2021), which allows not only the calculation of the Hirshfeld surfaces, but also of so-called 'fingerprint plots' (Spackman & McKinnon, 2002) and 'interaction energies' (Spackman, 2015; Mackenzie *et al.*, 2017).

3.7.1. Fingerprint plots

Analysis of the fingerprint plots allows the relative contributions of element-pair interactions across the Hirshfeld surface to be determined (Figs. S8–S10 and Table 4). Within the graphical representations, grey areas represent the absence of any close interactions, while dark-blue and light-blue areas represent an increasing number of interactions. A

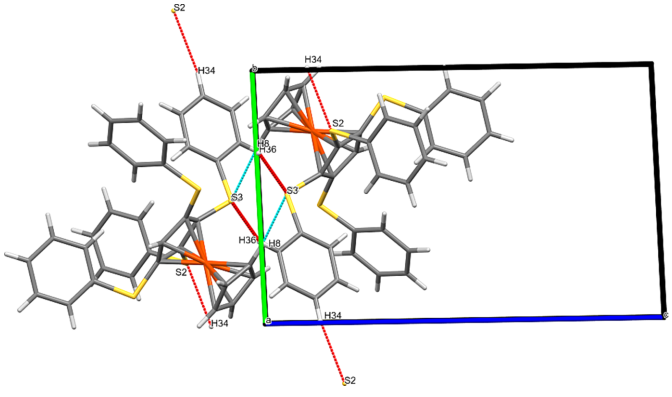


Figure 12
Packing plot of compound **6**, viewed along *a*. The red and blue coloured lines (for definition of colours, see Fig. 7) show weak interactions involving S atoms. Generic atoms labels without symmetry codes have been used.

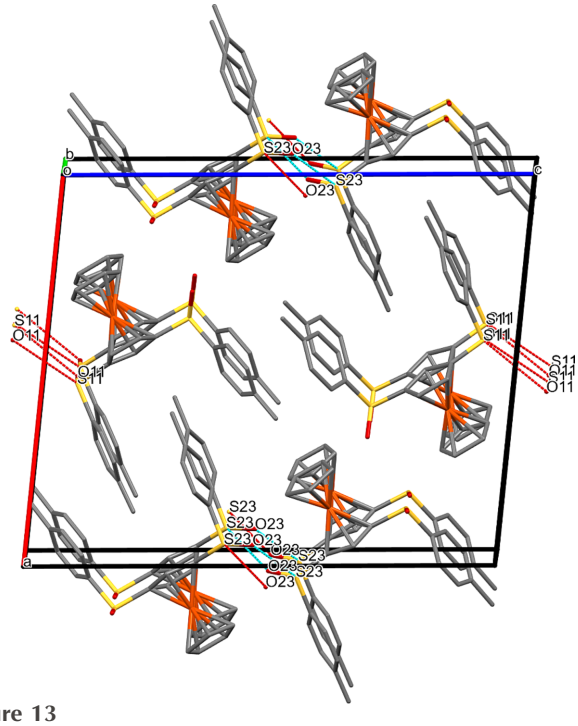


Figure 13
Packing plot of compound **2b**, viewed along *b*, showing four helices joined by S—O···S contacts in the *b* direction. H atoms have been omitted for clarity. Generic atoms labels without symmetry codes have been used.

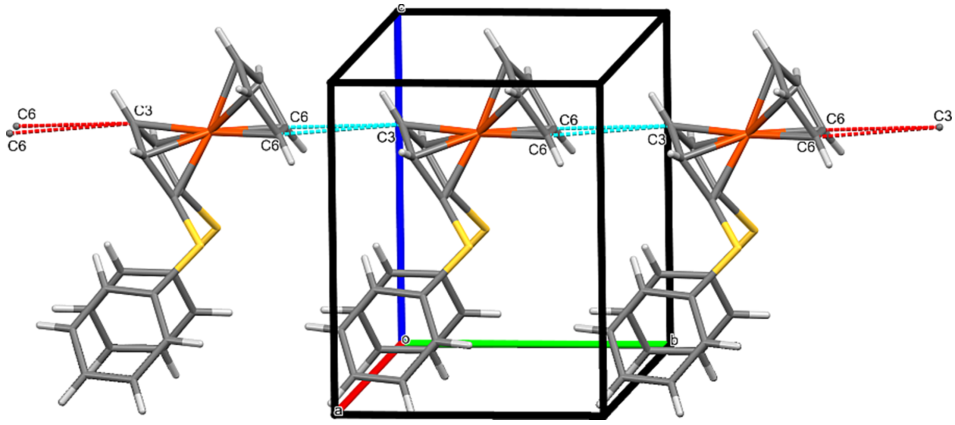


Figure 14
The polymeric arrangement of ferrocene cores in compound **5**. Generic atoms labels without symmetry codes have been used.

first quick look at Fig. S8 shows that several plots of molecules *A* and *B* of compound **2b** look quite different from each other, and also different from the plots of the stereoisomeric **2a**, and particularly different from sulfanyl compound **5**. For example, the closest H···H contacts in **2a** occur at $d_i + d_e$ = 2.15 Å, in molecule *A* of **2b** at *ca* 2.10 Å, while in molecule *B* they are at *ca* 2.00 Å and in compound **5** at 2.5 Å. Similar differences occur between the two molecules of compounds **4** and **6** (Fig. S10). While there are some subtle differences between the two molecules of compound **3a**, they are not as obvious as in the other compounds (Fig. S9).

As can be seen from Table 4, for all compounds, the major interactions are of the H···H type, followed by C···H interactions, except for compound **3a**, where O···H interactions are the second most common. It is astonishing that S···S interactions are not significant for any compound, and O···O and S···O interactions provide only small contributions in compound **2b**, while they are not significant for the other compounds. By far the largest contribution comes from H···H interactions in both molecules of compound **3a**, making up for nearly two thirds of all contributions. The largest values for the C···H and S···H contributions are found for polysulfanyl compounds **5** and **6**, where they make up for nearly one-third and approximately one-ninth, respectively. There are no recognizable trends with respect to the degree of substitution.

3.7.2. Interaction energies

Interaction energies were calculated using the program *CrystalExplorer*, using *TONTO* at the HF/3-21G level. For the discussion, only contributions with $|E_{tot}| > 10$ kJ mol^{-1} were used, usually between six and nine contributors (see Tables S6–S8 in the supporting information). For all compounds, the dispersion term was the most important, and in only a few cases was the electronic term of similar importance. When comparing only the strongest interactions (Type A) of all compounds, the following 'ranking' of the $|E_{tot}|$ values results: **4** > **2b** ≃ **6** > **3a** > **2a** > **5**. When considering only the electronic terms, there are only five contributors with $|E_{ele}| >$ 25 kJ mol^{-1}, with a ranking of **4** (types A and B) > **3a** (types B and A) > **2b** (type C). There is a general trend of increasing interaction energies with increasing degree of substitution, with the surprising exception of 1,3-disubstituted compound **2b**, and stronger interactions for the sulfinyl compounds compared with the sulfanyl compounds with the same degree of substitution.

It is quite difficult to compare these results with the literature data, as hardly any Hirshfeld analysis data with respect to interaction energies have been reported, either for metallocenes or for sulfanyl or sulfinyl compounds. For the former, only 1,1′-dimethylferrocene is reported (Mackenzie *et al.*, 2017), while for the latter, only the above-mentioned article by Zhou *et al.* (2021) applies. In both cases, the observed interaction energies were much lower than the maximal values found here {$|E_{ele}| < 9$ kJ mol^{-1} for [Fe(C_5H_4-Me)$_2$]}. However, we found a series of structurally related aromatic thioethers of the type [C_6(SPh)$_4$(CN)$_2$] in the Cambridge Structural Database (CSD; Groom *et al.*, 2016), and chose one of them (VOHFOR; Schmiedtchen *et al.*, 2023) for examination by *CrystalExplorer*. And, indeed, it turned out that similar high interaction energies were calculated with this compound ($E_{ele} \simeq -40$ kJ mol^{-1} and $E_{tot} \simeq -70$ kJ mol^{-1}; Table S9). A detailed comparison of the latter structure with compound **4** can be found in the supporting information. It seems therefore most likely that the large number of interacting –SPh groups is responsible for the observed large interaction energies.

4. Conclusion

We have shown that even with only a slight excess of LDA, compound **1** undergoes reactions that involve polyfunctionalization of the Cp ring. Chromatography allows isolation of pure disubstituted (1,2- and 1,3-isomers), trisubstituted (1,2,3-isomer) and tetrasubstituted products.

The molecular structures of all the compounds show a relatively small influence of the degree of substitution on the typical metallocene bond parameters (Fe–centroid distances and relative orientations of the Cp rings), while there seems to be no difference between the corresponding sulfinyl and sul-

fanyl compounds. In all the sulfinylferrocenes, the O atoms are in equatorial positions, except for one O atom in compound **4**, while all the arene rings (again except for one) orient themselves perpendicular to the plane of the Cp ring.

Many C—H···O hydrogen bonds are observed in all of the sulfinyl compounds, while C—H···S contacts are seen rarely in compounds **2a**, **2b**, **3a** and **4**, while they gain some importance for tetrasulfanylferrocene **6**. C—H···π interactions occur for all the compounds except the 1,2-disubstituted ones. Chalcogen bonding is seen only in 1,3-disubstituted sulfinylferrocene **2b**. Significant π–ring interactions are only observed for compound **3a** and are mainly intramolecular.

Hirshfeld analysis shows that H···H and C···H interactions are the most important, except for trisulfinylferrocene **3a**, where H···H and H···O interactions are of the highest importance. Calculation of the interaction energies shows that for all compounds the dispersion terms are the most important. A 'ranking' of the total energies shows a general trend of increasing interaction energies (absolute values) with increasing degree of substitution, and with higher values for sulfinyl than for sulfanyl compounds.

Although the optical purity was not checked for any of the compounds, the values for the Flack parameters in the structures of **2a**, **2b**, **3a** and **4** suggest that the observed stereochemical outcome of the reactions resembles the expectation, *i.e.* always S_S. Therefore, it seems to us worthwhile to study the outcome of reactions when using either the opposite enantiomer or racemates.

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supporting information

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Molecular and crystal structures of six poly(arylsulfinyl)- and poly(arylsulfanyl)ferrocenes

Tobias Blockhaus and Karlheinz Sünkel

Computing details

1,2-Bis[(4-methylbenzene)sulfinyl]ferrocene (comp_2a)

Crystal data

$[Fe(C_5H_5)(C_{19}H_{17}O_2S_2)]$
M_r = 462.38
Monoclinic, $P2_1$
a = 7.8964 (2) Å
b = 12.9064 (3) Å
c = 11.0124 (3) Å
β = 109.467 (1)°
V = 1058.16 (5) Å^3
Z = 2
$F(000)$ = 480
D_x = 1.451 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6560 reflections
θ = 5.0–27.5°
μ = 0.93 mm^{-1}
T = 297 K
Block, brown
0.07 × 0.05 × 0.04 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.3910 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.679, T_{max} = 0.746
11282 measured reflections
4815 independent reflections
4393 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5°, θ_{min} = 3.2°
h = −10→10
k = −16→16
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.084
S = 1.14
4815 reflections
264 parameters
13 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.2017P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack x determined using 1876 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.014 (6)

Special details

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. All crystal structure determinations were performed on a Bruker D8 VENTURE system. Structures were solved by SHELXT (Sheldrick, 2015a) and refined by SHELXL (Sheldrick, 2015b). Structure evaluation was performed with PLATON (Spek, 2020) structure plots were made with ORTEP-3 for Windows and Mercury (Macrae *et al.*, 2020), all as part of the WinGX program suite. CCDC 2330910–2330913 contain the supplementary crystallographic data for **2a**, **2b**, **3a**, **4**.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7340 (4)	0.3902 (3)	0.1731 (3)	0.0357 (7)
C2	0.5865 (5)	0.3999 (3)	0.2231 (4)	0.0397 (7)
C3	0.4241 (5)	0.3759 (3)	0.1208 (4)	0.0479 (9)
H3	0.309241	0.375323	0.126613	0.057*
C4	0.4682 (5)	0.3532 (3)	0.0101 (4)	0.0484 (9)
H4	0.387042	0.335938	−0.070202	0.058*
C5	0.6567 (5)	0.3611 (3)	0.0414 (4)	0.0436 (8)
H5	0.719835	0.349264	−0.015019	0.052*
C6	0.6167 (8)	0.1559 (4)	0.3067 (7)	0.0818 (11)
H6	0.616680	0.175080	0.388056	0.098*
C7	0.4680 (8)	0.1320 (4)	0.2020 (7)	0.0799 (16)
H7	0.350270	0.131767	0.202000	0.096*
C8	0.5198 (8)	0.1084 (4)	0.0967 (7)	0.0790 (16)
H8	0.443710	0.090050	0.015076	0.095*
C9	0.7054 (8)	0.1169 (4)	0.1346 (7)	0.0817 (12)
H9	0.776227	0.105979	0.083190	0.098*
C10	0.7673 (8)	0.1459 (4)	0.2680 (7)	0.0831 (11)
H10	0.886184	0.156157	0.319415	0.100*
C11	0.9862 (5)	0.5387 (3)	0.2297 (4)	0.0443 (8)
C12	1.0268 (7)	0.6012 (4)	0.3372 (4)	0.0610 (11)
H12	1.044430	0.572275	0.417855	0.073*
C13	1.0412 (8)	0.7069 (4)	0.3243 (5)	0.0685 (13)
H13	1.066819	0.748998	0.396752	0.082*
C14	1.0182 (5)	0.7513 (4)	0.2058 (4)	0.0542 (9)
C15	0.9805 (7)	0.6873 (3)	0.0998 (4)	0.0566 (11)
H15	0.965955	0.715920	0.019430	0.068*
C16	0.9637 (6)	0.5810 (3)	0.1109 (4)	0.0520 (10)
H16	0.937554	0.538774	0.038515	0.062*
C17	1.0323 (8)	0.8667 (4)	0.1932 (5)	0.0711 (13)
H17A	0.987817	0.885622	0.103857	0.107*
H17B	1.155708	0.887402	0.229871	0.107*
H17C	0.962445	0.900734	0.237998	0.107*
C21	0.5993 (6)	0.5622 (3)	0.3816 (4)	0.0455 (9)
C22	0.7081 (8)	0.6110 (4)	0.4897 (5)	0.0708 (14)

H22	0.777193	0.572577	0.560229	0.085*
C23	0.7144 (9)	0.7177 (4)	0.4932 (5)	0.0782 (15)
H23	0.785744	0.750675	0.567797	0.094*
C24	0.6186 (7)	0.7762 (3)	0.3900 (4)	0.0577 (11)
C25	0.5038 (7)	0.7261 (4)	0.2856 (5)	0.0703 (13)
H25	0.431880	0.764802	0.216351	0.084*
C26	0.4923 (7)	0.6193 (4)	0.2809 (5)	0.0633 (12)
H26	0.412284	0.586525	0.209497	0.076*
C27	0.6394 (10)	0.8941 (4)	0.3903 (6)	0.0902 (19)
H27A	0.681413	0.918813	0.477443	0.135*
H27B	0.525421	0.925180	0.344837	0.135*
H27C	0.724509	0.912206	0.348615	0.135*
Fe1	0.59864 (6)	0.25510 (3)	0.15872 (5)	0.04371 (15)
O1	1.0482 (4)	0.3476 (3)	0.1648 (4)	0.0729 (10)
O2	0.7682 (7)	0.3906 (3)	0.4715 (3)	0.0970 (14)
S1	0.96672 (12)	0.40195 (7)	0.25231 (10)	0.0482 (2)
S2	0.59171 (19)	0.42311 (8)	0.38146 (11)	0.0617 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0315 (16)	0.0308 (16)	0.0452 (18)	−0.0058 (13)	0.0132 (14)	−0.0017 (14)
C2	0.0442 (18)	0.0295 (16)	0.0499 (19)	−0.0008 (15)	0.0216 (16)	0.0017 (15)
C3	0.0346 (18)	0.041 (2)	0.068 (3)	0.0012 (15)	0.0178 (18)	0.0029 (18)
C4	0.041 (2)	0.046 (2)	0.049 (2)	−0.0028 (16)	0.0034 (17)	−0.0004 (17)
C5	0.0452 (19)	0.0427 (19)	0.0455 (19)	−0.0054 (15)	0.0186 (16)	−0.0053 (16)
C6	0.084 (2)	0.0374 (16)	0.114 (3)	−0.0013 (17)	0.019 (2)	0.0133 (18)
C7	0.080 (4)	0.047 (3)	0.111 (5)	−0.021 (3)	0.030 (3)	0.006 (3)
C8	0.085 (4)	0.037 (2)	0.107 (5)	−0.016 (3)	0.022 (3)	−0.014 (3)
C9	0.081 (2)	0.0381 (16)	0.119 (3)	0.0051 (17)	0.023 (2)	0.0060 (18)
C10	0.082 (2)	0.0374 (15)	0.118 (3)	0.0021 (16)	0.017 (2)	0.0108 (17)
C11	0.0354 (18)	0.0416 (19)	0.052 (2)	−0.0089 (15)	0.0090 (16)	−0.0028 (16)
C12	0.079 (3)	0.052 (2)	0.046 (2)	−0.019 (2)	0.012 (2)	−0.0049 (19)
C13	0.093 (4)	0.049 (2)	0.059 (3)	−0.021 (2)	0.019 (3)	−0.015 (2)
C14	0.052 (2)	0.045 (2)	0.062 (2)	−0.011 (2)	0.0143 (17)	0.000 (2)
C15	0.065 (3)	0.052 (2)	0.051 (2)	−0.010 (2)	0.017 (2)	0.0021 (18)
C16	0.055 (2)	0.050 (2)	0.046 (2)	−0.0097 (18)	0.0097 (18)	−0.0079 (16)
C17	0.082 (3)	0.050 (3)	0.080 (3)	−0.014 (2)	0.026 (3)	−0.005 (2)
C21	0.060 (2)	0.0375 (18)	0.044 (2)	0.0022 (17)	0.0242 (18)	0.0003 (15)
C22	0.102 (4)	0.047 (2)	0.048 (2)	0.013 (3)	0.005 (2)	0.003 (2)
C23	0.101 (4)	0.055 (3)	0.062 (3)	−0.001 (3)	0.004 (3)	−0.011 (2)
C24	0.082 (3)	0.039 (2)	0.063 (3)	0.0069 (19)	0.040 (2)	0.0013 (18)
C25	0.089 (4)	0.054 (3)	0.062 (3)	0.020 (2)	0.018 (3)	0.014 (2)
C26	0.068 (3)	0.051 (2)	0.059 (3)	0.010 (2)	0.007 (2)	0.003 (2)
C27	0.149 (6)	0.043 (3)	0.103 (4)	0.005 (3)	0.074 (4)	0.005 (3)
Fe1	0.0417 (3)	0.0285 (2)	0.0587 (3)	−0.0047 (2)	0.0136 (2)	−0.0026 (2)
O1	0.0441 (16)	0.061 (2)	0.121 (3)	−0.0016 (15)	0.0369 (18)	−0.0205 (19)
O2	0.167 (4)	0.0544 (19)	0.0495 (18)	0.036 (2)	0.009 (2)	0.0094 (15)

S1	0.0359 (4)	0.0395 (5)	0.0625 (6)	−0.0040 (4)	0.0073 (4)	−0.0014 (4)
S2	0.1046 (9)	0.0380 (5)	0.0565 (6)	0.0013 (5)	0.0455 (6)	0.0053 (4)

Geometric parameters (Å, º)

C1—C5	1.424 (5)	C11—C12	1.379 (6)
C1—C2	1.450 (5)	C11—S1	1.796 (4)
C1—S1	1.758 (3)	C12—C13	1.381 (7)
C1—Fe1	2.024 (3)	C12—H12	0.9300
C2—C3	1.431 (5)	C13—C14	1.381 (7)
C2—S2	1.756 (4)	C13—H13	0.9300
C2—Fe1	2.013 (3)	C14—C15	1.379 (6)
C3—C4	1.406 (6)	C14—C17	1.503 (7)
C3—Fe1	2.030 (4)	C15—C16	1.388 (6)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.415 (5)	C16—H16	0.9300
C4—Fe1	2.054 (4)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C5—Fe1	2.036 (4)	C17—H17C	0.9600
C5—H5	0.9300	C21—C26	1.365 (6)
C6—C7	1.378 (8)	C21—C22	1.368 (6)
C6—C10	1.396 (9)	C21—S2	1.796 (4)
C6—Fe1	2.040 (6)	C22—C23	1.378 (7)
C6—H6	0.9300	C22—H22	0.9300
C7—C8	1.386 (9)	C23—C24	1.363 (7)
C7—Fe1	2.035 (5)	C23—H23	0.9300
C7—H7	0.9300	C24—C25	1.366 (7)
C8—C9	1.387 (9)	C24—C27	1.531 (6)
C8—Fe1	2.039 (5)	C25—C26	1.382 (7)
C8—H8	0.9300	C25—H25	0.9300
C9—C10	1.435 (10)	C26—H26	0.9300
C9—Fe1	2.027 (6)	C27—H27A	0.9600
C9—H9	0.9300	C27—H27B	0.9600
C10—Fe1	2.035 (5)	C27—H27C	0.9600
C10—H10	0.9300	O1—S1	1.499 (4)
C11—C16	1.374 (6)	O2—S2	1.477 (4)
C5—C1—C2	106.5 (3)	H17A—C17—H17B	109.5
C5—C1—S1	123.4 (3)	C14—C17—H17C	109.5
C2—C1—S1	130.0 (3)	H17A—C17—H17C	109.5
C5—C1—Fe1	69.9 (2)	H17B—C17—H17C	109.5
C2—C1—Fe1	68.54 (19)	C26—C21—C22	119.9 (4)
S1—C1—Fe1	123.39 (19)	C26—C21—S2	121.8 (3)
C3—C2—C1	107.8 (3)	C22—C21—S2	118.2 (3)
C3—C2—S2	122.5 (3)	C21—C22—C23	119.4 (4)
C1—C2—S2	129.5 (3)	C21—C22—H22	120.3
C3—C2—Fe1	69.9 (2)	C23—C22—H22	120.3
C1—C2—Fe1	69.36 (19)	C24—C23—C22	121.7 (5)

S2—C2—Fe1	121.32 (19)	C24—C23—H23	119.2
C4—C3—C2	108.2 (3)	C22—C23—H23	119.2
C4—C3—Fe1	70.8 (2)	C25—C24—C23	117.9 (4)
C2—C3—Fe1	68.6 (2)	C25—C24—C27	120.8 (5)
C4—C3—H3	125.9	C23—C24—C27	121.3 (5)
C2—C3—H3	125.9	C24—C25—C26	121.4 (4)
Fe1—C3—H3	126.2	C24—C25—H25	119.3
C3—C4—C5	108.6 (3)	C26—C25—H25	119.3
C3—C4—Fe1	68.9 (2)	C21—C26—C25	119.5 (4)
C5—C4—Fe1	69.1 (2)	C21—C26—H26	120.2
C3—C4—H4	125.7	C25—C26—H26	120.2
C5—C4—H4	125.7	C24—C27—H27A	109.5
Fe1—C4—H4	127.8	C24—C27—H27B	109.5
C1—C5—C4	109.0 (3)	H27A—C27—H27B	109.5
C1—C5—Fe1	69.0 (2)	C24—C27—H27C	109.5
C4—C5—Fe1	70.4 (2)	H27A—C27—H27C	109.5
C1—C5—H5	125.5	H27B—C27—H27C	109.5
C4—C5—H5	125.5	C2—Fe1—C1	42.10 (14)
Fe1—C5—H5	126.7	C2—Fe1—C9	159.0 (2)
C7—C6—C10	107.4 (6)	C1—Fe1—C9	122.44 (18)
C7—C6—Fe1	70.1 (3)	C2—Fe1—C3	41.45 (15)
C10—C6—Fe1	69.8 (4)	C1—Fe1—C3	70.07 (15)
C7—C6—H6	126.3	C9—Fe1—C3	158.7 (2)
C10—C6—H6	126.3	C2—Fe1—C10	122.2 (2)
Fe1—C6—H6	125.4	C1—Fe1—C10	109.03 (19)
C6—C7—C8	110.0 (6)	C9—Fe1—C10	41.4 (3)
C6—C7—Fe1	70.4 (3)	C3—Fe1—C10	156.8 (2)
C8—C7—Fe1	70.2 (3)	C2—Fe1—C7	123.7 (2)
C6—C7—H7	125.0	C1—Fe1—C7	161.8 (2)
C8—C7—H7	125.0	C9—Fe1—C7	67.0 (3)
Fe1—C7—H7	126.0	C3—Fe1—C7	106.6 (2)
C7—C8—C9	107.9 (6)	C10—Fe1—C7	66.7 (2)
C7—C8—Fe1	70.0 (3)	C2—Fe1—C5	69.30 (14)
C9—C8—Fe1	69.6 (3)	C1—Fe1—C5	41.06 (14)
C7—C8—H8	126.1	C9—Fe1—C5	108.5 (2)
C9—C8—H8	126.1	C3—Fe1—C5	68.56 (16)
Fe1—C8—H8	125.9	C10—Fe1—C5	126.8 (2)
C8—C9—C10	107.1 (6)	C7—Fe1—C5	155.8 (2)
C8—C9—Fe1	70.5 (3)	C2—Fe1—C6	107.5 (2)
C10—C9—Fe1	69.6 (3)	C1—Fe1—C6	125.7 (2)
C8—C9—H9	126.4	C9—Fe1—C6	68.3 (3)
C10—C9—H9	126.4	C3—Fe1—C6	120.5 (2)
Fe1—C9—H9	125.1	C10—Fe1—C6	40.1 (3)
C6—C10—C9	107.6 (6)	C7—Fe1—C6	39.5 (2)
C6—C10—Fe1	70.1 (3)	C5—Fe1—C6	163.4 (2)
C9—C10—Fe1	69.0 (3)	C2—Fe1—C8	159.3 (2)
C6—C10—H10	126.2	C1—Fe1—C8	157.1 (2)
C9—C10—H10	126.2	C9—Fe1—C8	39.9 (2)

Fe1—C10—H10	126.2	C3—Fe1—C8	122.3 (2)
C16—C11—C12	120.3 (4)	C10—Fe1—C8	67.8 (2)
C16—C11—S1	122.2 (3)	C7—Fe1—C8	39.8 (3)
C12—C11—S1	117.5 (3)	C5—Fe1—C8	121.3 (2)
C11—C12—C13	119.6 (4)	C6—Fe1—C8	67.5 (3)
C11—C12—H12	120.2	C2—Fe1—C4	68.77 (16)
C13—C12—H12	120.2	C1—Fe1—C4	69.07 (15)
C14—C13—C12	121.2 (4)	C9—Fe1—C4	123.9 (2)
C14—C13—H13	119.4	C3—Fe1—C4	40.26 (17)
C12—C13—H13	119.4	C10—Fe1—C4	162.5 (2)
C13—C14—C15	118.3 (4)	C7—Fe1—C4	120.6 (2)
C13—C14—C17	120.5 (4)	C5—Fe1—C4	40.48 (15)
C15—C14—C17	121.2 (4)	C6—Fe1—C4	155.0 (2)
C14—C15—C16	121.2 (4)	C8—Fe1—C4	106.8 (2)
C14—C15—H15	119.4	O1—S1—C1	104.03 (18)
C16—C15—H15	119.4	O1—S1—C11	107.2 (2)
C11—C16—C15	119.4 (4)	C1—S1—C11	98.01 (17)
C11—C16—H16	120.3	O2—S2—C2	108.8 (2)
C15—C16—H16	120.3	O2—S2—C21	105.1 (2)
C14—C17—H17A	109.5	C2—S2—C21	99.25 (17)
C14—C17—H17B	109.5		

C5—C1—C2—C3	0.4 (4)	S1—C11—C12—C13	−179.3 (4)
S1—C1—C2—C3	−175.8 (3)	C11—C12—C13—C14	−1.0 (8)
Fe1—C1—C2—C3	−59.6 (3)	C12—C13—C14—C15	−0.1 (8)
C5—C1—C2—S2	174.1 (3)	C12—C13—C14—C17	179.3 (5)
S1—C1—C2—S2	−2.1 (5)	C13—C14—C15—C16	0.7 (7)
Fe1—C1—C2—S2	114.2 (3)	C17—C14—C15—C16	−178.7 (4)
C5—C1—C2—Fe1	60.0 (2)	C12—C11—C16—C15	−0.7 (7)
S1—C1—C2—Fe1	−116.2 (3)	S1—C11—C16—C15	180.0 (3)
C1—C2—C3—C4	−0.8 (4)	C14—C15—C16—C11	−0.4 (7)
S2—C2—C3—C4	−175.0 (3)	C26—C21—C22—C23	−3.0 (8)
Fe1—C2—C3—C4	−60.0 (3)	S2—C21—C22—C23	−179.0 (5)
C1—C2—C3—Fe1	59.2 (2)	C21—C22—C23—C24	−1.9 (10)
S2—C2—C3—Fe1	−115.0 (3)	C22—C23—C24—C25	5.2 (9)
C2—C3—C4—C5	0.8 (5)	C22—C23—C24—C27	−174.4 (5)
Fe1—C3—C4—C5	−57.8 (3)	C23—C24—C25—C26	−3.9 (8)
C2—C3—C4—Fe1	58.7 (3)	C27—C24—C25—C26	175.8 (5)
C2—C1—C5—C4	0.1 (4)	C22—C21—C26—C25	4.3 (8)
S1—C1—C5—C4	176.7 (3)	S2—C21—C26—C25	−179.8 (4)
Fe1—C1—C5—C4	59.2 (3)	C24—C25—C26—C21	−0.8 (8)
C2—C1—C5—Fe1	−59.1 (2)	C5—C1—S1—O1	−15.3 (4)
S1—C1—C5—Fe1	117.4 (3)	C2—C1—S1—O1	160.3 (3)
C3—C4—C5—C1	−0.6 (5)	Fe1—C1—S1—O1	71.4 (3)
Fe1—C4—C5—C1	−58.3 (3)	C5—C1—S1—C11	94.8 (3)
C3—C4—C5—Fe1	57.7 (3)	C2—C1—S1—C11	−89.6 (4)
C10—C6—C7—C8	−0.8 (6)	Fe1—C1—S1—C11	−178.5 (2)
Fe1—C6—C7—C8	59.2 (4)	C16—C11—S1—O1	38.0 (4)

C10—C6—C7—Fe1	−60.1 (4)	C12—C11—S1—O1	−141.4 (4)
C6—C7—C8—C9	0.2 (6)	C16—C11—S1—C1	−69.4 (4)
Fe1—C7—C8—C9	59.5 (4)	C12—C11—S1—C1	111.2 (4)
C6—C7—C8—Fe1	−59.3 (4)	C3—C2—S2—O2	150.0 (3)
C7—C8—C9—C10	0.5 (6)	C1—C2—S2—O2	−23.0 (4)
Fe1—C8—C9—C10	60.3 (4)	Fe1—C2—S2—O2	65.1 (3)
C7—C8—C9—Fe1	−59.7 (4)	C3—C2—S2—C21	−100.5 (3)
C7—C6—C10—C9	1.1 (6)	C1—C2—S2—C21	86.5 (4)
Fe1—C6—C10—C9	−59.1 (4)	Fe1—C2—S2—C21	174.6 (2)
C7—C6—C10—Fe1	60.2 (4)	C26—C21—S2—O2	156.5 (4)
C8—C9—C10—C6	−1.0 (6)	C22—C21—S2—O2	−27.6 (5)
Fe1—C9—C10—C6	59.8 (3)	C26—C21—S2—C2	44.0 (4)
C8—C9—C10—Fe1	−60.8 (4)	C22—C21—S2—C2	−140.1 (4)
C16—C11—C12—C13	1.3 (7)		

1,3-Bis[(4-methylbenzene)sulfinyl]ferrocene (compd_2b)

Crystal data

$[Fe(C_5H_5)(C_{19}H_{17}O_2S_2)]$
M_r = 462.38
Monoclinic, $P2_1$
a = 17.1882 (10) Å
b = 6.0383 (4) Å
c = 20.4271 (12) Å
β = 95.995 (2)°
V = 2108.5 (2) Å^3
Z = 4
$F(000)$ = 960
D_x = 1.457 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9908 reflections
θ = 3.0–28.3°
μ = 0.93 mm^{-1}
T = 296 K
Rod, yellow
0.10 × 0.02 × 0.02 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.3910 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.648, T_{max} = 0.746
34842 measured reflections
10422 independent reflections
8415 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 28.3°, θ_{min} = 2.7°
h = −22→22
k = −7→8
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.095
S = 1.02
10422 reflections
573 parameters
8 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.8351P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack x determined using 3063 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.019 (7)

Special details

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. All crystal structure determinations were performed on a Bruker D8 VENTURE system. Structures were solved by SHELXT (Sheldrick, 2015a) and refined by SHELXL (Sheldrick, 2015b). Structure evaluation was performed with PLATON (Spek, 2020) structure plots were made with ORTEP-3 for Windows and Mercury (Macrae *et al.*, 2020), all as part of the WinGX program suite. CCDC 2330910–2330913 contain the supplementary crystallographic data for **2a**, **2b**, **3a**, **4**.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C10	0.5093 (2)	0.6792 (8)	0.1370 (2)	0.0382 (10)	
C11	0.4876 (2)	0.8068 (8)	0.1899 (2)	0.0423 (11)	
H11	0.500529	0.954121	0.198740	0.051*	
C12	0.4420 (2)	0.6667 (8)	0.2275 (2)	0.0416 (11)	
C13	0.4364 (3)	0.4567 (9)	0.1974 (2)	0.0506 (12)	
H13	0.409920	0.335061	0.212077	0.061*	
C14	0.4778 (2)	0.4617 (8)	0.1407 (3)	0.0483 (12)	
H14	0.483272	0.345486	0.111637	0.058*	
C15A	0.3430 (4)	0.9532 (14)	0.0758 (6)	0.048 (4)	0.45 (3)
H15A	0.368006	1.082245	0.064628	0.058*	0.45 (3)
C16A	0.3414 (4)	0.755 (2)	0.0418 (3)	0.050 (5)	0.45 (3)
H16A	0.365230	0.727323	0.003818	0.060*	0.45 (3)
C17A	0.2983 (5)	0.6053 (12)	0.0743 (5)	0.075 (9)	0.45 (3)
H17A	0.288017	0.459056	0.061976	0.090*	0.45 (3)
C18A	0.2732 (3)	0.711 (2)	0.1283 (4)	0.078 (10)	0.45 (3)
H18A	0.243076	0.648176	0.158727	0.093*	0.45 (3)
C19A	0.3008 (6)	0.9259 (18)	0.1292 (4)	0.068 (7)	0.45 (3)
H19A	0.292511	1.033328	0.160369	0.082*	0.45 (3)
C15B	0.3277 (5)	0.9628 (11)	0.0997 (6)	0.066 (4)	0.55 (3)
H15B	0.340516	1.110524	0.107916	0.079*	0.55 (3)
C16B	0.3505 (4)	0.832 (2)	0.0464 (4)	0.056 (4)	0.55 (3)
H16B	0.380682	0.880364	0.013956	0.068*	0.55 (3)
C17B	0.3187 (6)	0.6150 (15)	0.0519 (5)	0.052 (4)	0.55 (3)
H17B	0.324601	0.496903	0.023578	0.062*	0.55 (3)
C18B	0.2763 (4)	0.6111 (18)	0.1085 (6)	0.057 (5)	0.55 (3)
H18B	0.249774	0.490077	0.123481	0.068*	0.55 (3)
C19B	0.2819 (5)	0.826 (2)	0.1380 (3)	0.062 (5)	0.55 (3)
H19B	0.259618	0.869314	0.175606	0.075*	0.55 (3)
C111	0.6594 (2)	0.7200 (9)	0.11568 (19)	0.0375 (9)	
C112	0.6799 (3)	0.5062 (8)	0.1352 (2)	0.0486 (12)	
H112	0.645068	0.389850	0.125968	0.058*	
C113	0.7528 (3)	0.4683 (9)	0.1684 (2)	0.0512 (12)	
H113	0.766215	0.325137	0.182149	0.061*	
C114	0.8068 (2)	0.6382 (8)	0.1820 (2)	0.0405 (10)	

C115	0.7858 (3)	0.8452 (9)	0.1586 (3)	0.0564 (13)	
H115	0.821670	0.960386	0.165217	0.068*	
C116	0.7123 (3)	0.8881 (8)	0.1252 (3)	0.0537 (12)	
H116	0.699609	1.029691	0.109656	0.064*	
C117	0.8844 (3)	0.5945 (10)	0.2199 (2)	0.0587 (14)	
H11A	0.910161	0.732565	0.230930	0.088*	
H11B	0.915975	0.507366	0.193565	0.088*	
H11C	0.876897	0.515376	0.259519	0.088*	
C131	0.4679 (3)	0.6318 (9)	0.3575 (2)	0.0535 (13)	
C132	0.4543 (3)	0.4296 (11)	0.3842 (2)	0.0569 (14)	
H132	0.408518	0.352457	0.371080	0.068*	
C133	0.5100 (3)	0.3409 (10)	0.4314 (2)	0.0593 (14)	
H133	0.500957	0.202260	0.448948	0.071*	
C134	0.5781 (3)	0.4520 (11)	0.4529 (2)	0.0611 (15)	
C135	0.5882 (3)	0.6587 (12)	0.4258 (3)	0.0721 (18)	
H135	0.632843	0.739617	0.439823	0.086*	
C136	0.5346 (3)	0.7477 (11)	0.3790 (3)	0.0679 (14)	
H136	0.543259	0.886893	0.361621	0.082*	
C137	0.6378 (4)	0.3522 (16)	0.5030 (3)	0.097 (3)	
H13A	0.680807	0.296307	0.481495	0.146*	
H13B	0.614441	0.233163	0.525230	0.146*	
H13C	0.656441	0.463186	0.534495	0.146*	
C20	0.0685 (2)	0.2826 (8)	0.2720 (2)	0.0393 (10)	
C21	0.0250 (2)	0.1246 (8)	0.3052 (2)	0.0398 (10)	
H21	0.015118	−0.021861	0.292886	0.048*	
C22	−0.0005 (2)	0.2355 (9)	0.36093 (19)	0.0391 (9)	
C23	0.0273 (2)	0.4595 (8)	0.3621 (2)	0.0427 (10)	
H23	0.018840	0.566381	0.393374	0.051*	
C24	0.0700 (2)	0.4884 (8)	0.3068 (2)	0.0433 (11)	
H24	0.094551	0.617822	0.295306	0.052*	
C25A	0.1747 (5)	−0.0229 (10)	0.4093 (5)	0.084 (10)	0.50 (3)
H25A	0.158313	−0.169619	0.406157	0.101*	0.50 (3)
C26A	0.1567 (5)	0.129 (2)	0.4569 (4)	0.071 (7)	0.50 (3)
H26A	0.126227	0.101776	0.491032	0.085*	0.50 (3)
C27A	0.1925 (6)	0.3301 (16)	0.4442 (5)	0.064 (5)	0.50 (3)
H27A	0.190021	0.459845	0.468467	0.076*	0.50 (3)
C28A	0.2326 (4)	0.3020 (13)	0.3888 (5)	0.063 (7)	0.50 (3)
H28A	0.261542	0.409744	0.369653	0.076*	0.50 (3)
C29A	0.2216 (4)	0.0839 (16)	0.3672 (3)	0.078 (9)	0.50 (3)
H29A	0.241941	0.020712	0.331143	0.094*	0.50 (3)
C25B	0.2008 (5)	−0.0141 (13)	0.3759 (5)	0.053 (4)	0.50 (3)
H25B	0.200453	−0.144022	0.351374	0.063*	0.50 (3)
C26B	0.1645 (4)	0.0174 (15)	0.4342 (5)	0.052 (5)	0.50 (3)
H26B	0.136154	−0.088154	0.454870	0.062*	0.50 (3)
C27B	0.1790 (5)	0.2378 (19)	0.4557 (3)	0.055 (5)	0.50 (3)
H27B	0.161852	0.302490	0.492955	0.066*	0.50 (3)
C28B	0.2243 (5)	0.3425 (11)	0.4106 (5)	0.044 (4)	0.50 (3)
H28B	0.242043	0.488051	0.413006	0.053*	0.50 (3)

C29B	0.2377 (3)	0.1868 (19)	0.3613 (4)	0.041 (3)	0.50 (3)
H29B	0.265900	0.212097	0.325500	0.050*	0.50 (3)
C211	0.0415 (2)	0.3108 (8)	0.1406 (2)	0.0413 (11)	
C212	0.0455 (3)	0.5199 (9)	0.1144 (2)	0.0491 (12)	
H212	0.087483	0.612358	0.127757	0.059*	
C213	−0.0137 (3)	0.5911 (9)	0.0680 (2)	0.0501 (12)	
H213	−0.010608	0.731449	0.049673	0.060*	
C214	−0.0769 (3)	0.4586 (10)	0.0484 (2)	0.0498 (12)	
C215	−0.0793 (3)	0.2498 (11)	0.0745 (2)	0.0552 (12)	
H215	−0.121233	0.157627	0.060789	0.066*	
C216	−0.0214 (3)	0.1731 (9)	0.1205 (2)	0.0509 (11)	
H216	−0.024236	0.031311	0.137876	0.061*	
C217	−0.1423 (3)	0.5376 (13)	−0.0012 (3)	0.0757 (18)	
H21A	−0.138392	0.465928	−0.042685	0.114*	
H21B	−0.138420	0.695024	−0.006582	0.114*	
H21C	−0.191783	0.502110	0.014097	0.114*	
C231	−0.1487 (2)	0.1566 (8)	0.3807 (2)	0.0432 (11)	
C232	−0.1886 (3)	−0.0132 (10)	0.3469 (3)	0.0654 (14)	
H232	−0.166369	−0.153217	0.345295	0.078*	
C233	−0.2633 (3)	0.0288 (11)	0.3152 (3)	0.0722 (17)	
H233	−0.290210	−0.084932	0.291964	0.087*	
C234	−0.2979 (2)	0.2321 (11)	0.3175 (2)	0.0529 (12)	
C235	−0.2569 (3)	0.3971 (10)	0.3516 (3)	0.0623 (14)	
H235	−0.279026	0.537158	0.353510	0.075*	
C236	−0.1828 (3)	0.3591 (9)	0.3835 (3)	0.0559 (13)	
H236	−0.156285	0.472843	0.407076	0.067*	
C237	−0.3783 (3)	0.2760 (13)	0.2824 (3)	0.0785 (19)	
H23A	−0.417253	0.240325	0.311127	0.118*	
H23B	−0.385990	0.186115	0.243529	0.118*	
H23C	−0.382582	0.429537	0.270360	0.118*	
Fe1	0.39158 (3)	0.69826 (9)	0.13410 (3)	0.04035 (17)	
Fe2	0.11783 (3)	0.23801 (10)	0.36529 (3)	0.03966 (16)	
O11	0.55703 (18)	1.0230 (6)	0.07242 (18)	0.0653 (10)	
O13	0.3244 (2)	0.6186 (9)	0.2980 (2)	0.0916 (15)	
O21	0.1187 (2)	−0.0267 (7)	0.19813 (18)	0.0763 (11)	
O23	−0.04328 (18)	0.2446 (7)	0.48090 (14)	0.0643 (9)	
S11	0.56413 (6)	0.7774 (2)	0.07347 (5)	0.0466 (3)	
S13	0.39663 (8)	0.7506 (3)	0.29697 (6)	0.0676 (4)	
S21	0.11674 (6)	0.2175 (3)	0.20180 (6)	0.0534 (3)	
S23	−0.05234 (7)	0.1036 (2)	0.42073 (6)	0.0459 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C10	0.0289 (17)	0.048 (3)	0.038 (2)	0.0051 (19)	0.0057 (15)	0.004 (2)
C11	0.037 (2)	0.042 (3)	0.048 (3)	0.0057 (18)	0.0018 (18)	0.005 (2)
C12	0.0351 (19)	0.051 (3)	0.040 (2)	0.0116 (19)	0.0090 (16)	0.005 (2)
C13	0.039 (2)	0.048 (3)	0.067 (3)	0.006 (2)	0.010 (2)	0.016 (3)

C14	0.037 (2)	0.045 (3)	0.062 (3)	0.005 (2)	0.001 (2)	−0.006 (2)
C15A	0.040 (6)	0.054 (8)	0.050 (9)	0.012 (6)	0.003 (6)	−0.003 (7)
C16A	0.052 (9)	0.054 (11)	0.042 (7)	0.014 (8)	−0.006 (5)	−0.013 (7)
C17A	0.044 (12)	0.057 (10)	0.12 (2)	−0.020 (8)	−0.019 (12)	0.023 (11)
C18A	0.032 (7)	0.12 (3)	0.078 (14)	0.014 (16)	0.011 (8)	0.010 (18)
C19A	0.048 (12)	0.093 (15)	0.062 (12)	0.023 (10)	0.003 (8)	−0.001 (12)
C15B	0.052 (9)	0.054 (6)	0.086 (13)	0.018 (5)	−0.015 (7)	0.007 (6)
C16B	0.045 (6)	0.065 (9)	0.058 (8)	0.006 (6)	0.000 (5)	0.029 (6)
C17B	0.032 (6)	0.066 (10)	0.055 (7)	−0.003 (6)	−0.006 (5)	−0.002 (7)
C18B	0.020 (6)	0.075 (7)	0.077 (13)	0.004 (5)	0.007 (6)	0.008 (8)
C19B	0.045 (9)	0.080 (12)	0.062 (7)	0.040 (9)	0.004 (6)	0.004 (8)
C111	0.0284 (16)	0.046 (2)	0.040 (2)	0.003 (2)	0.0099 (14)	0.003 (2)
C112	0.037 (2)	0.041 (3)	0.067 (3)	−0.0016 (19)	0.006 (2)	0.003 (2)
C113	0.044 (2)	0.042 (3)	0.066 (3)	0.012 (2)	0.003 (2)	0.007 (2)
C114	0.031 (2)	0.048 (3)	0.043 (2)	0.0032 (18)	0.0097 (17)	−0.0032 (19)
C115	0.037 (2)	0.050 (3)	0.081 (4)	−0.009 (2)	0.001 (2)	0.000 (3)
C116	0.043 (3)	0.043 (3)	0.074 (3)	0.003 (2)	0.003 (2)	0.009 (2)
C117	0.040 (2)	0.078 (4)	0.057 (3)	0.009 (2)	0.000 (2)	−0.004 (3)
C131	0.060 (3)	0.058 (3)	0.046 (3)	0.008 (2)	0.022 (2)	0.002 (2)
C132	0.045 (3)	0.078 (4)	0.048 (3)	−0.007 (3)	0.010 (2)	0.000 (3)
C133	0.053 (3)	0.072 (4)	0.055 (3)	−0.002 (3)	0.016 (2)	0.009 (3)
C134	0.065 (3)	0.082 (4)	0.037 (3)	−0.007 (3)	0.011 (2)	0.002 (3)
C135	0.069 (3)	0.091 (5)	0.056 (3)	−0.021 (3)	0.005 (3)	−0.010 (3)
C136	0.084 (4)	0.062 (3)	0.061 (3)	−0.018 (4)	0.024 (3)	−0.001 (3)
C137	0.069 (4)	0.163 (8)	0.056 (4)	−0.015 (4)	−0.010 (3)	0.023 (4)
C20	0.0295 (18)	0.047 (3)	0.041 (2)	0.0046 (18)	0.0023 (15)	0.004 (2)
C21	0.033 (2)	0.042 (3)	0.044 (2)	0.0028 (18)	0.0005 (17)	−0.007 (2)
C22	0.0306 (17)	0.045 (2)	0.041 (2)	0.002 (2)	0.0037 (15)	−0.001 (2)
C23	0.043 (2)	0.039 (2)	0.046 (3)	0.008 (2)	0.0041 (19)	−0.005 (2)
C24	0.038 (2)	0.038 (2)	0.052 (3)	0.0014 (19)	−0.0038 (19)	0.004 (2)
C25A	0.074 (16)	0.037 (7)	0.13 (2)	0.006 (8)	−0.055 (15)	0.006 (10)
C26A	0.050 (7)	0.095 (18)	0.064 (10)	−0.022 (9)	−0.019 (6)	0.040 (11)
C27A	0.045 (8)	0.075 (11)	0.065 (11)	−0.012 (7)	−0.023 (7)	0.006 (9)
C28A	0.025 (5)	0.121 (18)	0.043 (9)	−0.004 (7)	0.001 (5)	0.019 (10)
C29A	0.050 (12)	0.10 (2)	0.077 (12)	0.036 (14)	−0.022 (8)	−0.029 (13)
C25B	0.034 (8)	0.060 (10)	0.063 (9)	0.007 (6)	0.000 (6)	0.003 (7)
C26B	0.034 (6)	0.052 (9)	0.066 (11)	0.005 (6)	−0.004 (6)	0.017 (8)
C27B	0.057 (9)	0.066 (10)	0.040 (6)	0.013 (8)	−0.002 (5)	−0.006 (8)
C28B	0.041 (7)	0.043 (6)	0.049 (9)	−0.007 (5)	0.003 (6)	0.002 (6)
C29B	0.032 (5)	0.046 (8)	0.046 (7)	0.002 (5)	0.002 (5)	−0.003 (5)
C211	0.039 (2)	0.054 (3)	0.032 (2)	0.0008 (19)	0.0118 (17)	−0.002 (2)
C212	0.046 (2)	0.055 (3)	0.048 (3)	−0.009 (2)	0.011 (2)	−0.004 (2)
C213	0.060 (3)	0.049 (3)	0.042 (3)	−0.008 (2)	0.010 (2)	0.002 (2)
C214	0.048 (3)	0.069 (3)	0.033 (2)	−0.006 (2)	0.004 (2)	−0.002 (2)
C215	0.058 (3)	0.061 (3)	0.045 (3)	−0.020 (3)	0.003 (2)	−0.010 (3)
C216	0.061 (3)	0.044 (3)	0.048 (3)	−0.005 (2)	0.010 (2)	0.000 (2)
C217	0.073 (4)	0.095 (5)	0.057 (3)	−0.004 (4)	−0.004 (3)	0.013 (3)
C231	0.044 (2)	0.047 (3)	0.041 (2)	0.000 (2)	0.0139 (18)	0.0003 (19)

C232	0.055 (3)	0.053 (3)	0.088 (4)	−0.003 (2)	0.010 (3)	−0.016 (3)
C233	0.060 (3)	0.077 (4)	0.078 (4)	−0.021 (3)	0.001 (3)	−0.017 (3)
C234	0.041 (2)	0.073 (3)	0.046 (2)	−0.002 (3)	0.0123 (18)	0.008 (3)
C235	0.050 (3)	0.060 (3)	0.076 (4)	0.009 (3)	0.005 (3)	0.000 (3)
C236	0.058 (3)	0.048 (3)	0.060 (3)	−0.004 (2)	0.000 (2)	−0.007 (3)
C237	0.047 (3)	0.120 (6)	0.069 (3)	−0.013 (3)	0.002 (2)	0.000 (4)
Fe1	0.0266 (2)	0.0497 (4)	0.0450 (3)	0.0039 (3)	0.0054 (2)	0.0044 (3)
Fe2	0.0320 (3)	0.0434 (4)	0.0424 (3)	0.0017 (3)	−0.0019 (2)	0.0032 (3)
O11	0.0487 (18)	0.062 (2)	0.086 (3)	0.0138 (16)	0.0144 (17)	0.038 (2)
O13	0.0447 (19)	0.150 (4)	0.084 (3)	0.013 (2)	0.0219 (18)	0.039 (3)
O21	0.088 (3)	0.0756 (14)	0.067 (2)	0.042 (2)	0.017 (2)	−0.005 (2)
O23	0.068 (2)	0.084 (2)	0.0419 (16)	0.002 (2)	0.0066 (14)	−0.0105 (19)
S11	0.0329 (5)	0.0667 (8)	0.0409 (6)	0.0069 (5)	0.0075 (4)	0.0087 (6)
S13	0.0647 (7)	0.0846 (11)	0.0581 (7)	0.0277 (8)	0.0285 (6)	0.0153 (8)
S21	0.0375 (5)	0.0755 (8)	0.0490 (6)	0.0137 (7)	0.0123 (4)	0.0022 (7)
S23	0.0454 (6)	0.0521 (7)	0.0412 (6)	0.0039 (5)	0.0088 (5)	0.0021 (5)

Geometric parameters (Å, º)

C10—C11	1.409 (6)	C20—S21	1.775 (4)
C10—C14	1.426 (7)	C20—Fe2	2.021 (4)
C10—S11	1.783 (4)	C21—C22	1.429 (6)
C10—Fe1	2.022 (4)	C21—Fe2	2.029 (4)
C11—C12	1.430 (6)	C21—H21	0.9300
C11—Fe1	2.015 (4)	C22—C23	1.434 (7)
C11—H11	0.9300	C22—S23	1.774 (4)
C12—C13	1.409 (7)	C22—Fe2	2.027 (4)
C12—S13	1.764 (4)	C23—C24	1.421 (6)
C12—Fe1	2.020 (4)	C23—Fe2	2.048 (4)
C13—C14	1.421 (7)	C23—H23	0.9300
C13—Fe1	2.045 (5)	C24—Fe2	2.045 (5)
C13—H13	0.9300	C24—H24	0.9300
C14—Fe1	2.053 (5)	C25A—C29A	1.396 (4)
C14—H14	0.9300	C25A—C26A	1.396 (4)
C15A—C16A	1.382 (4)	C25A—Fe2	2.015 (6)
C15A—C19A	1.382 (4)	C25A—H25A	0.9300
C15A—Fe1	2.068 (7)	C26A—C27A	1.396 (4)
C15A—H15A	0.9300	C26A—Fe2	2.029 (6)
C16A—C17A	1.382 (4)	C26A—H26A	0.9300
C16A—Fe1	2.018 (5)	C27A—C28A	1.396 (4)
C16A—H16A	0.9300	C27A—Fe2	2.031 (6)
C17A—C18A	1.382 (4)	C27A—H27A	0.9300
C17A—Fe1	1.992 (6)	C28A—C29A	1.396 (4)
C17A—H17A	0.9300	C28A—Fe2	2.018 (5)
C18A—C19A	1.382 (4)	C28A—H28A	0.9300
C18A—Fe1	2.026 (5)	C29A—Fe2	2.008 (5)
C18A—H18A	0.9300	C29A—H29A	0.9300
C19A—Fe1	2.073 (7)	C25B—C26B	1.415 (4)

C19A—H19A	0.9300	C25B—C29B	1.415 (4)
C15B—C19B	1.430 (4)	C25B—Fe2	2.082 (6)
C15B—C16B	1.430 (4)	C25B—H25B	0.9300
C15B—Fe1	2.022 (7)	C26B—C27B	1.415 (4)
C15B—H15B	0.9300	C26B—Fe2	2.041 (6)
C16B—C17B	1.430 (4)	C26B—H26B	0.9300
C16B—Fe1	2.024 (6)	C27B—C28B	1.415 (4)
C16B—H16B	0.9300	C27B—Fe2	2.028 (5)
C17B—C18B	1.430 (4)	C27B—H27B	0.9300
C17B—Fe1	2.050 (7)	C28B—C29B	1.415 (4)
C17B—H17B	0.9300	C28B—Fe2	2.061 (5)
C18B—C19B	1.430 (4)	C28B—H28B	0.9300
C18B—Fe1	2.064 (6)	C29B—Fe2	2.094 (6)
C18B—H18B	0.9300	C29B—H29B	0.9300
C19B—Fe1	2.046 (6)	C211—C212	1.375 (7)
C19B—H19B	0.9300	C211—C216	1.392 (6)
C111—C116	1.363 (6)	C211—S21	1.794 (5)
C111—C112	1.386 (7)	C212—C213	1.385 (7)
C111—S11	1.803 (4)	C212—H212	0.9300
C112—C113	1.380 (6)	C213—C214	1.375 (7)
C112—H112	0.9300	C213—H213	0.9300
C113—C114	1.391 (7)	C214—C215	1.372 (8)
C113—H113	0.9300	C214—C217	1.510 (7)
C114—C115	1.373 (7)	C215—C216	1.376 (7)
C114—C117	1.494 (6)	C215—H215	0.9300
C115—C116	1.396 (6)	C216—H216	0.9300
C115—H115	0.9300	C217—H21A	0.9600
C116—H116	0.9300	C217—H21B	0.9600
C117—H11A	0.9600	C217—H21C	0.9600
C117—H11B	0.9600	C231—C236	1.360 (7)
C117—H11C	0.9600	C231—C232	1.377 (7)
C131—C132	1.368 (8)	C231—S23	1.799 (5)
C131—C136	1.375 (7)	C232—C233	1.399 (8)
C131—S13	1.797 (6)	C232—H232	0.9300
C132—C133	1.392 (7)	C233—C234	1.367 (9)
C132—H132	0.9300	C233—H233	0.9300
C133—C134	1.382 (7)	C234—C235	1.369 (8)
C133—H133	0.9300	C234—C237	1.511 (6)
C134—C135	1.384 (9)	C235—C236	1.387 (7)
C134—C137	1.498 (8)	C235—H235	0.9300
C135—C136	1.366 (8)	C236—H236	0.9300
C135—H135	0.9300	C237—H23A	0.9600
C136—H136	0.9300	C237—H23B	0.9600
C137—H13A	0.9600	C237—H23C	0.9600
C137—H13B	0.9600	O11—S11	1.488 (4)
C137—H13C	0.9600	O13—S13	1.477 (4)
C20—C21	1.426 (6)	O21—S21	1.477 (4)
C20—C24	1.430 (6)	O23—S23	1.490 (3)

C11—C10—C14	109.3 (4)	C26B—C25B—Fe2	68.4 (2)
C11—C10—S11	125.4 (4)	C29B—C25B—Fe2	70.7 (3)
C14—C10—S11	125.3 (4)	C26B—C25B—H25B	126.0
C11—C10—Fe1	69.3 (2)	C29B—C25B—H25B	126.0
C14—C10—Fe1	70.7 (2)	Fe2—C25B—H25B	126.5
S11—C10—Fe1	124.3 (2)	C27B—C26B—C25B	108.0
C10—C11—C12	107.0 (4)	C27B—C26B—Fe2	69.2 (2)
C10—C11—Fe1	69.8 (2)	C25B—C26B—Fe2	71.5 (2)
C12—C11—Fe1	69.4 (3)	C27B—C26B—H26B	126.0
C10—C11—H11	126.5	C25B—C26B—H26B	126.0
C12—C11—H11	126.5	Fe2—C26B—H26B	124.9
Fe1—C11—H11	125.8	C28B—C27B—C26B	108.0
C13—C12—C11	108.3 (4)	C28B—C27B—Fe2	71.0 (3)
C13—C12—S13	126.4 (4)	C26B—C27B—Fe2	70.1 (2)
C11—C12—S13	125.1 (4)	C28B—C27B—H27B	126.0
C13—C12—Fe1	70.7 (3)	C26B—C27B—H27B	126.0
C11—C12—Fe1	69.1 (2)	Fe2—C27B—H27B	124.4
S13—C12—Fe1	123.4 (2)	C27B—C28B—C29B	108.0
C12—C13—C14	108.6 (4)	C27B—C28B—Fe2	68.5 (2)
C12—C13—Fe1	68.8 (3)	C29B—C28B—Fe2	71.3 (2)
C14—C13—Fe1	70.0 (3)	C27B—C28B—H28B	126.0
C12—C13—H13	125.7	C29B—C28B—H28B	126.0
C14—C13—H13	125.7	Fe2—C28B—H28B	125.7
Fe1—C13—H13	127.1	C28B—C29B—C25B	108.0
C13—C14—C10	106.7 (4)	C28B—C29B—Fe2	68.8 (2)
C13—C14—Fe1	69.4 (3)	C25B—C29B—Fe2	69.7 (2)
C10—C14—Fe1	68.4 (2)	C28B—C29B—H29B	126.0
C13—C14—H14	126.6	C25B—C29B—H29B	126.0
C10—C14—H14	126.6	Fe2—C29B—H29B	127.0
Fe1—C14—H14	127.1	C212—C211—C216	120.2 (4)
C16A—C15A—C19A	108.0	C212—C211—S21	119.8 (4)
C16A—C15A—Fe1	68.3 (3)	C216—C211—S21	119.9 (4)
C19A—C15A—Fe1	70.7 (2)	C211—C212—C213	119.2 (5)
C16A—C15A—H15A	126.0	C211—C212—H212	120.4
C19A—C15A—H15A	126.0	C213—C212—H212	120.4
Fe1—C15A—H15A	126.6	C214—C213—C212	121.4 (5)
C15A—C16A—C17A	108.0	C214—C213—H213	119.3
C15A—C16A—Fe1	72.2 (3)	C212—C213—H213	119.3
C17A—C16A—Fe1	68.8 (3)	C215—C214—C213	118.4 (5)
C15A—C16A—H16A	126.0	C215—C214—C217	120.1 (5)
C17A—C16A—H16A	126.0	C213—C214—C217	121.5 (5)
Fe1—C16A—H16A	124.6	C214—C215—C216	121.8 (5)
C18A—C17A—C16A	108.0	C214—C215—H215	119.1
C18A—C17A—Fe1	71.2 (2)	C216—C215—H215	119.1
C16A—C17A—Fe1	70.9 (2)	C215—C216—C211	119.0 (5)
C18A—C17A—H17A	126.0	C215—C216—H216	120.5
C16A—C17A—H17A	126.0	C211—C216—H216	120.5

Fe1—C17A—H17A	123.5	C214—C217—H21A	109.5
C17A—C18A—C19A	108.0	C214—C217—H21B	109.5
C17A—C18A—Fe1	68.5 (3)	H21A—C217—H21B	109.5
C19A—C18A—Fe1	72.1 (3)	C214—C217—H21C	109.5
C17A—C18A—H18A	126.0	H21A—C217—H21C	109.5
C19A—C18A—H18A	126.0	H21B—C217—H21C	109.5
Fe1—C18A—H18A	124.9	C236—C231—C232	119.8 (5)
C18A—C19A—C15A	108.0	C236—C231—S23	121.4 (4)
C18A—C19A—Fe1	68.5 (3)	C232—C231—S23	118.8 (4)
C15A—C19A—Fe1	70.3 (2)	C231—C232—C233	118.8 (5)
C18A—C19A—H19A	126.0	C231—C232—H232	120.6
C15A—C19A—H19A	126.0	C233—C232—H232	120.6
Fe1—C19A—H19A	126.8	C234—C233—C232	121.9 (5)
C19B—C15B—C16B	108.0	C234—C233—H233	119.1
C19B—C15B—Fe1	70.3 (2)	C232—C233—H233	119.1
C16B—C15B—Fe1	69.4 (2)	C233—C234—C235	117.9 (5)
C19B—C15B—H15B	126.0	C233—C234—C237	121.4 (6)
C16B—C15B—H15B	126.0	C235—C234—C237	120.7 (6)
Fe1—C15B—H15B	125.9	C234—C235—C236	121.2 (5)
C15B—C16B—C17B	108.0	C234—C235—H235	119.4
C15B—C16B—Fe1	69.2 (3)	C236—C235—H235	119.4
C17B—C16B—Fe1	70.4 (3)	C231—C236—C235	120.4 (5)
C15B—C16B—H16B	126.0	C231—C236—H236	119.8
C17B—C16B—H16B	126.0	C235—C236—H236	119.8
Fe1—C16B—H16B	125.9	C234—C237—H23A	109.5
C18B—C17B—C16B	108.0	C234—C237—H23B	109.5
C18B—C17B—Fe1	70.2 (2)	H23A—C237—H23B	109.5
C16B—C17B—Fe1	68.5 (3)	C234—C237—H23C	109.5
C18B—C17B—H17B	126.0	H23A—C237—H23C	109.5
C16B—C17B—H17B	126.0	H23B—C237—H23C	109.5
Fe1—C17B—H17B	126.9	C17A—Fe1—C11	176.2 (3)
C19B—C18B—C17B	108.0	C11—Fe1—C15B	108.8 (2)
C19B—C18B—Fe1	69.0 (3)	C17A—Fe1—C16A	40.31 (13)
C17B—C18B—Fe1	69.1 (2)	C11—Fe1—C16A	135.9 (3)
C19B—C18B—H18B	126.0	C17A—Fe1—C12	142.3 (3)
C17B—C18B—H18B	126.0	C11—Fe1—C12	41.50 (17)
Fe1—C18B—H18B	127.4	C15B—Fe1—C12	124.5 (3)
C15B—C19B—C18B	108.0	C16A—Fe1—C12	175.6 (4)
C15B—C19B—Fe1	68.5 (3)	C17A—Fe1—C18A	40.21 (13)
C18B—C19B—Fe1	70.3 (3)	C11—Fe1—C18A	141.1 (4)
C15B—C19B—H19B	126.0	C16A—Fe1—C18A	67.12 (19)
C18B—C19B—H19B	126.0	C12—Fe1—C18A	112.8 (2)
Fe1—C19B—H19B	126.8	C17A—Fe1—C10	137.8 (4)
C116—C111—C112	120.4 (4)	C11—Fe1—C10	40.86 (17)
C116—C111—S11	119.0 (4)	C15B—Fe1—C10	124.1 (3)
C112—C111—S11	120.5 (3)	C16A—Fe1—C10	111.4 (2)
C113—C112—C111	119.1 (4)	C12—Fe1—C10	68.74 (16)
C113—C112—H112	120.4	C18A—Fe1—C10	178.0 (4)

C111—C112—H112	120.4	C11—Fe1—C16B	124.1 (3)
C112—C113—C114	121.8 (5)	C15B—Fe1—C16B	41.41 (14)
C112—C113—H113	119.1	C12—Fe1—C16B	161.6 (4)
C114—C113—H113	119.1	C10—Fe1—C16B	107.7 (2)
C115—C114—C113	117.2 (4)	C11—Fe1—C19B	124.0 (3)
C115—C114—C117	121.9 (4)	C15B—Fe1—C19B	41.16 (15)
C113—C114—C117	120.9 (4)	C12—Fe1—C19B	107.7 (2)
C114—C115—C116	122.0 (4)	C10—Fe1—C19B	160.7 (4)
C114—C115—H115	119.0	C16B—Fe1—C19B	69.3 (2)
C116—C115—H115	119.0	C17A—Fe1—C13	114.3 (3)
C111—C116—C115	119.2 (4)	C11—Fe1—C13	69.05 (19)
C111—C116—H116	120.4	C15B—Fe1—C13	159.7 (4)
C115—C116—H116	120.4	C16A—Fe1—C13	143.8 (4)
C114—C117—H11A	109.5	C12—Fe1—C13	40.5 (2)
C114—C117—H11B	109.5	C18A—Fe1—C13	111.9 (3)
H11A—C117—H11B	109.5	C10—Fe1—C13	68.36 (17)
C114—C117—H11C	109.5	C16B—Fe1—C13	156.6 (4)
H11A—C117—H11C	109.5	C19B—Fe1—C13	122.1 (3)
H11B—C117—H11C	109.5	C11—Fe1—C17B	159.6 (4)
C132—C131—C136	119.9 (5)	C15B—Fe1—C17B	69.27 (19)
C132—C131—S13	119.9 (4)	C12—Fe1—C17B	156.3 (4)
C136—C131—S13	120.1 (5)	C10—Fe1—C17B	122.3 (3)
C131—C132—C133	119.1 (5)	C16B—Fe1—C17B	41.10 (13)
C131—C132—H132	120.5	C19B—Fe1—C17B	68.80 (19)
C133—C132—H132	120.5	C13—Fe1—C17B	120.0 (3)
C134—C133—C132	122.2 (6)	C17A—Fe1—C14	111.9 (3)
C134—C133—H133	118.9	C11—Fe1—C14	69.27 (19)
C132—C133—H133	118.9	C15B—Fe1—C14	159.1 (4)
C133—C134—C135	116.5 (5)	C16A—Fe1—C14	114.5 (3)
C133—C134—C137	121.3 (6)	C12—Fe1—C14	68.70 (18)
C135—C134—C137	122.1 (6)	C18A—Fe1—C14	138.0 (4)
C136—C135—C134	122.2 (6)	C10—Fe1—C14	40.96 (19)
C136—C135—H135	118.9	C16B—Fe1—C14	121.3 (3)
C134—C135—H135	118.9	C19B—Fe1—C14	157.2 (4)
C135—C136—C131	120.1 (6)	C13—Fe1—C14	40.59 (19)
C135—C136—H136	120.0	C17B—Fe1—C14	105.0 (2)
C131—C136—H136	120.0	C29A—Fe2—C28A	40.56 (15)
C134—C137—H13A	109.5	C29A—Fe2—C25A	40.59 (14)
C134—C137—H13B	109.5	C28A—Fe2—C25A	68.1 (2)
H13A—C137—H13B	109.5	C29A—Fe2—C20	111.4 (2)
C134—C137—H13C	109.5	C28A—Fe2—C20	120.2 (3)
H13A—C137—H13C	109.5	C25A—Fe2—C20	131.4 (3)
H13B—C137—H13C	109.5	C29A—Fe2—C22	151.9 (3)
C21—C20—C24	109.2 (4)	C28A—Fe2—C22	164.4 (4)
C21—C20—S21	123.2 (4)	C25A—Fe2—C22	116.8 (3)
C24—C20—S21	127.5 (3)	C20—Fe2—C22	68.84 (16)
C21—C20—Fe2	69.7 (2)	C20—Fe2—C27B	170.2 (4)
C24—C20—Fe2	70.3 (2)	C22—Fe2—C27B	117.6 (3)

S21—C20—Fe2	123.2 (2)	C29A—Fe2—C27A	68.0 (2)
C20—C21—C22	106.5 (4)	C28A—Fe2—C27A	40.33 (13)
C20—C21—Fe2	69.1 (2)	C25A—Fe2—C27A	67.86 (18)
C22—C21—Fe2	69.3 (2)	C20—Fe2—C27A	151.7 (4)
C20—C21—H21	126.7	C22—Fe2—C27A	125.8 (3)
C22—C21—H21	126.7	C29A—Fe2—C21	119.8 (3)
Fe2—C21—H21	126.4	C28A—Fe2—C21	153.7 (4)
C21—C22—C23	109.0 (4)	C25A—Fe2—C21	108.7 (2)
C21—C22—S23	123.8 (4)	C20—Fe2—C21	41.23 (17)
C23—C22—S23	127.0 (4)	C22—Fe2—C21	41.26 (16)
C21—C22—Fe2	69.4 (2)	C27B—Fe2—C21	148.4 (4)
C23—C22—Fe2	70.2 (2)	C27A—Fe2—C21	164.8 (4)
S23—C22—Fe2	123.2 (2)	C29A—Fe2—C26A	68.02 (19)
C24—C23—C22	107.5 (4)	C28A—Fe2—C26A	67.84 (19)
C24—C23—Fe2	69.6 (2)	C25A—Fe2—C26A	40.38 (13)
C22—C23—Fe2	68.6 (2)	C20—Fe2—C26A	167.9 (4)
C24—C23—H23	126.2	C22—Fe2—C26A	105.7 (3)
C22—C23—H23	126.2	C27A—Fe2—C26A	40.22 (12)
Fe2—C23—H23	127.1	C21—Fe2—C26A	127.7 (3)
C23—C24—C20	107.7 (4)	C20—Fe2—C26B	146.5 (4)
C23—C24—Fe2	69.8 (3)	C22—Fe2—C26B	110.2 (3)
C20—C24—Fe2	68.5 (2)	C27B—Fe2—C26B	40.70 (12)
C23—C24—H24	126.2	C21—Fe2—C26B	115.2 (3)
C20—C24—H24	126.2	C29A—Fe2—C24	131.0 (3)
Fe2—C24—H24	127.1	C28A—Fe2—C24	108.7 (2)
C29A—C25A—C26A	108.0	C25A—Fe2—C24	170.0 (4)
C29A—C25A—Fe2	69.4 (3)	C20—Fe2—C24	41.18 (18)
C26A—C25A—Fe2	70.3 (2)	C22—Fe2—C24	68.87 (18)
C29A—C25A—H25A	126.0	C27B—Fe2—C24	132.1 (4)
C26A—C25A—H25A	126.0	C27A—Fe2—C24	116.3 (3)
Fe2—C25A—H25A	125.8	C21—Fe2—C24	69.70 (18)
C27A—C26A—C25A	108.0	C26A—Fe2—C24	148.3 (4)
C27A—C26A—Fe2	70.0 (2)	C26B—Fe2—C24	172.1 (4)
C25A—C26A—Fe2	69.3 (2)	C29A—Fe2—C23	166.8 (3)
C27A—C26A—H26A	126.0	C28A—Fe2—C23	127.1 (3)
C25A—C26A—H26A	126.0	C25A—Fe2—C23	148.9 (4)
Fe2—C26A—H26A	126.3	C20—Fe2—C23	68.91 (17)
C26A—C27A—C28A	108.0	C22—Fe2—C23	41.19 (19)
C26A—C27A—Fe2	69.8 (2)	C27B—Fe2—C23	110.5 (3)
C28A—C27A—Fe2	69.4 (3)	C27A—Fe2—C23	105.2 (3)
C26A—C27A—H27A	126.0	C21—Fe2—C23	69.75 (18)
C28A—C27A—H27A	126.0	C26A—Fe2—C23	114.6 (4)
Fe2—C27A—H27A	126.4	C26B—Fe2—C23	133.7 (4)
C29A—C28A—C27A	108.0	C24—Fe2—C23	40.63 (17)
C29A—C28A—Fe2	69.3 (2)	O11—S11—C10	107.1 (2)
C27A—C28A—Fe2	70.3 (2)	O11—S11—C111	105.5 (2)
C29A—C28A—H28A	126.0	C10—S11—C111	96.34 (18)
C27A—C28A—H28A	126.0	O13—S13—C12	107.4 (3)

Fe2—C28A—H28A	125.9	O13—S13—C131	106.8 (3)
C28A—C29A—C25A	108.0	C12—S13—C131	96.4 (2)
C28A—C29A—Fe2	70.1 (2)	O21—S21—C20	106.1 (2)
C25A—C29A—Fe2	70.0 (3)	O21—S21—C211	107.3 (2)
C28A—C29A—H29A	126.0	C20—S21—C211	97.51 (18)
C25A—C29A—H29A	126.0	O23—S23—C22	107.1 (2)
Fe2—C29A—H29A	125.5	O23—S23—C231	106.6 (2)
C26B—C25B—C29B	108.0	C22—S23—C231	96.41 (19)
C14—C10—C11—C12	0.2 (5)	Fe2—C20—C24—C23	−59.0 (3)
S11—C10—C11—C12	177.8 (3)	C21—C20—C24—Fe2	59.0 (3)
Fe1—C10—C11—C12	59.8 (3)	S21—C20—C24—Fe2	−117.3 (3)
C14—C10—C11—Fe1	−59.5 (3)	C29A—C25A—C26A—C27A	0.0
S11—C10—C11—Fe1	118.0 (3)	Fe2—C25A—C26A—C27A	−59.5 (3)
C10—C11—C12—C13	0.0 (5)	C29A—C25A—C26A—Fe2	59.5 (3)
Fe1—C11—C12—C13	60.0 (3)	C25A—C26A—C27A—C28A	0.0
C10—C11—C12—S13	−176.9 (3)	Fe2—C26A—C27A—C28A	−59.0 (3)
Fe1—C11—C12—S13	−116.9 (3)	C25A—C26A—C27A—Fe2	59.0 (3)
C10—C11—C12—Fe1	−60.0 (3)	C26A—C27A—C28A—C29A	0.0
C11—C12—C13—C14	−0.2 (5)	Fe2—C27A—C28A—C29A	−59.3 (2)
S13—C12—C13—C14	176.6 (3)	C26A—C27A—C28A—Fe2	59.3 (2)
Fe1—C12—C13—C14	58.8 (3)	C27A—C28A—C29A—C25A	0.0
C11—C12—C13—Fe1	−59.0 (3)	Fe2—C28A—C29A—C25A	−59.9 (2)
S13—C12—C13—Fe1	117.8 (3)	C27A—C28A—C29A—Fe2	59.9 (2)
C12—C13—C14—C10	0.3 (5)	C26A—C25A—C29A—C28A	0.0
Fe1—C13—C14—C10	58.4 (3)	Fe2—C25A—C29A—C28A	60.0 (2)
C12—C13—C14—Fe1	−58.1 (3)	C26A—C25A—C29A—Fe2	−60.0 (2)
C11—C10—C14—C13	−0.3 (5)	C29B—C25B—C26B—C27B	0.0
S11—C10—C14—C13	−177.9 (3)	Fe2—C25B—C26B—C27B	−59.8 (2)
Fe1—C10—C14—C13	−59.0 (3)	C29B—C25B—C26B—Fe2	59.8 (2)
C11—C10—C14—Fe1	58.7 (3)	C25B—C26B—C27B—C28B	0.0
S11—C10—C14—Fe1	−118.9 (3)	Fe2—C26B—C27B—C28B	−61.2 (3)
C19A—C15A—C16A—C17A	0.0	C25B—C26B—C27B—Fe2	61.2 (3)
Fe1—C15A—C16A—C17A	59.8 (2)	C26B—C27B—C28B—C29B	0.0
C19A—C15A—C16A—Fe1	−59.8 (2)	Fe2—C27B—C28B—C29B	−60.7 (2)
C15A—C16A—C17A—C18A	0.0	C26B—C27B—C28B—Fe2	60.7 (2)
Fe1—C16A—C17A—C18A	61.9 (3)	C27B—C28B—C29B—C25B	0.0
C15A—C16A—C17A—Fe1	−61.9 (3)	Fe2—C28B—C29B—C25B	−58.9 (2)
C16A—C17A—C18A—C19A	0.0	C27B—C28B—C29B—Fe2	58.9 (2)
Fe1—C17A—C18A—C19A	61.7 (3)	C26B—C25B—C29B—C28B	0.0
C16A—C17A—C18A—Fe1	−61.7 (3)	Fe2—C25B—C29B—C28B	58.4 (2)
C17A—C18A—C19A—C15A	0.0	C26B—C25B—C29B—Fe2	−58.4 (2)
Fe1—C18A—C19A—C15A	59.4 (2)	C216—C211—C212—C213	0.0 (7)
C17A—C18A—C19A—Fe1	−59.4 (2)	S21—C211—C212—C213	−178.9 (3)
C16A—C15A—C19A—C18A	0.0	C211—C212—C213—C214	1.1 (7)
Fe1—C15A—C19A—C18A	−58.3 (3)	C212—C213—C214—C215	−1.9 (7)
C16A—C15A—C19A—Fe1	58.3 (3)	C212—C213—C214—C217	178.8 (5)
C19B—C15B—C16B—C17B	0.0	C213—C214—C215—C216	1.5 (7)

Fe1—C15B—C16B—C17B	60.0 (3)
C19B—C15B—C16B—Fe1	−60.0 (3)
C15B—C16B—C17B—C18B	0.0
Fe1—C16B—C17B—C18B	59.2 (2)
C15B—C16B—C17B—Fe1	−59.2 (2)
C16B—C17B—C18B—C19B	0.0
Fe1—C17B—C18B—C19B	58.2 (3)
C16B—C17B—C18B—Fe1	−58.2 (3)
C16B—C15B—C19B—C18B	0.0
Fe1—C15B—C19B—C18B	−59.4 (3)
C16B—C15B—C19B—Fe1	59.4 (3)
C17B—C18B—C19B—C15B	0.0
Fe1—C18B—C19B—C15B	58.3 (2)
C17B—C18B—C19B—Fe1	−58.3 (2)
C116—C111—C112—C113	4.4 (7)
S11—C111—C112—C113	−178.9 (4)
C111—C112—C113—C114	−1.1 (8)
C112—C113—C114—C115	−2.5 (7)
C112—C113—C114—C117	178.1 (5)
C113—C114—C115—C116	2.9 (8)
C117—C114—C115—C116	−177.7 (5)
C112—C111—C116—C115	−4.1 (7)
S11—C111—C116—C115	179.2 (4)
C114—C115—C116—C111	0.3 (8)
C136—C131—C132—C133	−2.2 (7)
S13—C131—C132—C133	−179.6 (4)
C131—C132—C133—C134	1.0 (8)
C132—C133—C134—C135	0.7 (8)
C132—C133—C134—C137	−179.1 (5)
C133—C134—C135—C136	−1.4 (8)
C137—C134—C135—C136	178.5 (6)
C134—C135—C136—C131	0.2 (9)
C132—C131—C136—C135	1.6 (8)
S13—C131—C136—C135	179.0 (4)
C24—C20—C21—C22	0.1 (5)
S21—C20—C21—C22	176.5 (3)
Fe2—C20—C21—C22	59.5 (3)
C24—C20—C21—Fe2	−59.4 (3)
S21—C20—C21—Fe2	117.1 (3)
C20—C21—C22—C23	−0.1 (5)
Fe2—C21—C22—C23	59.2 (3)
C20—C21—C22—S23	−176.2 (3)
Fe2—C21—C22—S23	−116.9 (3)
C20—C21—C22—Fe2	−59.3 (3)
C21—C22—C23—C24	0.2 (5)
S23—C22—C23—C24	176.0 (3)
Fe2—C22—C23—C24	58.9 (3)
C21—C22—C23—Fe2	−58.7 (3)
C217—C214—C215—C216	−179.1 (5)
C214—C215—C216—C211	−0.5 (7)
C212—C211—C216—C215	−0.3 (7)
S21—C211—C216—C215	178.6 (3)
C236—C231—C232—C233	1.2 (8)
S23—C231—C232—C233	−179.4 (4)
C231—C232—C233—C234	−0.8 (9)
C232—C233—C234—C235	0.4 (8)
C232—C233—C234—C237	179.4 (5)
C233—C234—C235—C236	−0.6 (8)
C237—C234—C235—C236	−179.5 (5)
C232—C231—C236—C235	−1.3 (8)
S23—C231—C236—C235	179.3 (4)
C234—C235—C236—C231	1.0 (8)
C11—C10—S11—O11	−20.2 (4)
C14—C10—S11—O11	157.0 (4)
Fe1—C10—S11—O11	67.5 (3)
C11—C10—S11—C111	88.2 (4)
C14—C10—S11—C111	−94.6 (4)
Fe1—C10—S11—C111	175.9 (3)
C116—C111—S11—O11	−14.2 (4)
C112—C111—S11—O11	169.0 (4)
C116—C111—S11—C10	−123.9 (4)
C112—C111—S11—C10	59.3 (4)
C13—C12—S13—O13	−28.1 (5)
C11—C12—S13—O13	148.2 (4)
Fe1—C12—S13—O13	61.6 (4)
C13—C12—S13—C131	81.8 (4)
C11—C12—S13—C131	−101.9 (4)
Fe1—C12—S13—C131	171.5 (3)
C132—C131—S13—O13	12.6 (5)
C136—C131—S13—O13	−164.8 (4)
C132—C131—S13—C12	−97.8 (4)
C136—C131—S13—C12	84.8 (4)
C21—C20—S21—O21	−13.9 (4)
C24—C20—S21—O21	161.8 (4)
Fe2—C20—S21—O21	72.2 (3)
C21—C20—S21—C211	96.5 (4)
C24—C20—S21—C211	−87.7 (4)
Fe2—C20—S21—C211	−177.4 (3)
C212—C211—S21—O21	−154.4 (4)
C216—C211—S21—O21	26.8 (4)
C212—C211—S21—C20	96.1 (4)
C216—C211—S21—C20	−82.7 (4)
C21—C22—S23—O23	160.2 (3)
C23—C22—S23—O23	−15.1 (4)
Fe2—C22—S23—O23	74.1 (3)
C21—C22—S23—C231	−90.2 (4)

S23—C22—C23—Fe2	117.2 (3)	C23—C22—S23—C231	94.5 (4)
C22—C23—C24—C20	−0.1 (5)	Fe2—C22—S23—C231	−176.3 (3)
Fe2—C23—C24—C20	58.2 (3)	C236—C231—S23—O23	32.5 (5)
C22—C23—C24—Fe2	−58.3 (3)	C232—C231—S23—O23	−146.9 (4)
C21—C20—C24—C23	0.0 (5)	C236—C231—S23—C22	−77.6 (4)
S21—C20—C24—C23	−176.2 (3)	C232—C231—S23—C22	103.0 (4)

1,2,3-Tris[(4-methylbenzene)sulfinyl]ferrocene (comp_3a)

Crystal data

$[Fe(C_5H_5)(C_{26}H_{23}O_3S_3)]$
M_r = 600.56
Triclinic, $P\overline{1}$
a = 7.8298 (5) Å
b = 9.8573 (6) Å
c = 17.4937 (11) Å
α = 93.379 (2)°
β = 91.120 (2)°
γ = 98.051 (2)°
V = 1334.02 (14) Å^3
Z = 2
$F(000)$ = 624
D_x = 1.495 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9984 reflections
θ = 2.6–26.8°
μ = 0.83 mm^{-1}
T = 110 K
Rod, yellow
0.10 × 0.03 × 0.02 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.3910 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.809, T_{max} = 0.862
21012 measured reflections
10957 independent reflections
9889 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.8°, θ_{min} = 3.2°
h = −9→9
k = −12→12
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.073
S = 1.02
10957 reflections
691 parameters
6 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack x determined using 4237 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.014 (8)

Special details

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. All crystal structure determinations were performed on a Bruker D8 VENTURE system. Structures were solved by SHELXT (Sheldrick, 2015a) and refined by SHELXL (Sheldrick, 2015b). Structure evaluation was performed with PLATON (Spek, 2020) structure plots were made with ORTEP-3 for Windows and Mercury (Macrae *et al.*, 2020), all as part of the WinGX program suite. CCDC 2330910–2330913 contain the supplementary crystallographic data for **2a**, **2b**, **3a**, **4**.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C10	0.1204 (5)	0.4872 (4)	0.7716 (2)	0.0146 (9)
C11	0.1901 (5)	0.6032 (4)	0.7304 (3)	0.0152 (9)
C12	0.1459 (5)	0.5703 (4)	0.6503 (2)	0.0144 (9)
C13	0.0483 (5)	0.4365 (4)	0.6435 (2)	0.0163 (9)
H13	0.001425	0.389403	0.597194	0.020*
C14	0.0331 (5)	0.3861 (4)	0.7171 (2)	0.0177 (9)
H14	−0.025542	0.298998	0.728642	0.021*
C15	0.5100 (6)	0.4451 (5)	0.6326 (3)	0.0320 (12)
H15	0.541880	0.506754	0.593906	0.038*
C16	0.4148 (6)	0.3109 (5)	0.6210 (3)	0.0280 (11)
H16	0.372661	0.266574	0.573278	0.034*
C17	0.3944 (6)	0.2554 (5)	0.6946 (3)	0.0249 (11)
H17	0.335265	0.167463	0.704134	0.030*
C18	0.4765 (6)	0.3526 (5)	0.7502 (3)	0.0281 (11)
H18	0.483000	0.342191	0.803815	0.034*
C19	0.5482 (6)	0.4698 (5)	0.7115 (3)	0.0330 (13)
H19	0.611472	0.551262	0.735189	0.040*
C20	0.7945 (5)	0.4645 (4)	0.2338 (2)	0.0165 (9)
C21	0.7460 (5)	0.3562 (4)	0.2845 (2)	0.0145 (9)
C22	0.8068 (5)	0.4057 (4)	0.3598 (2)	0.0158 (9)
C23	0.8958 (5)	0.5417 (4)	0.3558 (2)	0.0164 (9)
H23	0.950781	0.598275	0.397587	0.020*
C24	0.8879 (6)	0.5773 (4)	0.2788 (2)	0.0181 (9)
H24	0.936670	0.662280	0.260123	0.022*
C25	0.3816 (7)	0.4812 (6)	0.3168 (5)	0.0571 (17)
H25	0.317397	0.393668	0.303382	0.068*
C26	0.4406 (7)	0.5310 (6)	0.3900 (4)	0.0381 (13)
H26	0.422934	0.483655	0.435529	0.046*
C27	0.5288 (7)	0.6604 (5)	0.3850 (3)	0.0306 (12)
H27	0.582699	0.717074	0.426966	0.037*
C28	0.5274 (7)	0.6962 (6)	0.3099 (3)	0.0400 (13)
H28	0.579445	0.780481	0.291466	0.048*
C29	0.4348 (7)	0.5850 (7)	0.2655 (3)	0.0535 (15)
H29	0.412260	0.580170	0.211748	0.064*
C111	0.0024 (6)	0.5737 (5)	0.9060 (3)	0.0184 (9)
C112	−0.1765 (6)	0.5364 (5)	0.8954 (3)	0.0259 (10)
H112	−0.222008	0.451152	0.869561	0.031*
C113	−0.2851 (6)	0.6252 (5)	0.9230 (3)	0.0297 (11)
H113	−0.406197	0.601295	0.914841	0.036*

C114	−0.2217 (6)	0.7484 (5)	0.9622 (3)	0.0278 (11)
C115	−0.0447 (6)	0.7834 (5)	0.9735 (3)	0.0266 (11)
H115	0.000007	0.868071	1.000154	0.032*
C116	0.0679 (6)	0.6957 (5)	0.9460 (3)	0.0227 (10)
H116	0.188800	0.719395	0.954675	0.027*
C117	−0.3443 (7)	0.8412 (5)	0.9942 (3)	0.0403 (13)
H11A	−0.393215	0.805248	1.041329	0.060*
H11B	−0.437518	0.844847	0.956498	0.060*
H11C	−0.281841	0.933714	1.005557	0.060*
C121	0.1312 (6)	0.8543 (5)	0.7852 (3)	0.0161 (9)
C122	0.1768 (6)	0.9842 (5)	0.8205 (3)	0.0215 (10)
H122	0.294303	1.016717	0.833711	0.026*
C123	0.0517 (6)	1.0664 (4)	0.8365 (3)	0.0216 (10)
H123	0.084048	1.156089	0.859705	0.026*
C124	−0.1218 (6)	1.0194 (4)	0.8190 (3)	0.0218 (10)
C125	−0.1664 (6)	0.8879 (4)	0.7839 (2)	0.0208 (10)
H125	−0.283838	0.854543	0.771129	0.025*
C126	−0.0403 (6)	0.8060 (4)	0.7676 (2)	0.0185 (9)
H126	−0.071630	0.716239	0.744269	0.022*
C127	−0.2595 (6)	1.1085 (5)	0.8382 (3)	0.0322 (11)
H12A	−0.286268	1.156969	0.793104	0.048*
H12B	−0.217551	1.175416	0.880374	0.048*
H12C	−0.363921	1.050725	0.853528	0.048*
C131	0.0492 (5)	0.7820 (4)	0.5786 (2)	0.0146 (9)
C132	0.1070 (6)	0.9201 (4)	0.5943 (2)	0.0179 (9)
H132	0.227092	0.952500	0.598314	0.021*
C133	−0.0130 (6)	1.0112 (5)	0.6042 (3)	0.0201 (10)
H133	0.026110	1.106158	0.614836	0.024*
C134	−0.1887 (6)	0.9650 (5)	0.5986 (3)	0.0195 (10)
C135	−0.2436 (6)	0.8235 (5)	0.5816 (3)	0.0193 (10)
H135	−0.363480	0.790117	0.577211	0.023*
C136	−0.1258 (6)	0.7338 (5)	0.5712 (3)	0.0187 (9)
H136	−0.163946	0.639081	0.559089	0.022*
C137	−0.3196 (6)	1.0621 (5)	0.6108 (3)	0.0258 (11)
H13A	−0.261851	1.150494	0.633210	0.039*
H13B	−0.407527	1.023268	0.645534	0.039*
H13C	−0.374450	1.075608	0.561503	0.039*
C211	0.9168 (6)	0.4012 (5)	0.0960 (3)	0.0225 (11)
C212	0.8883 (7)	0.2692 (5)	0.0613 (3)	0.0254 (11)
H212	0.776015	0.217958	0.057818	0.030*
C213	1.0294 (6)	0.2147 (5)	0.0319 (3)	0.0271 (11)
H213	1.012196	0.124716	0.007820	0.033*
C214	1.1936 (6)	0.2872 (5)	0.0365 (3)	0.0312 (11)
C215	1.2172 (6)	0.4208 (5)	0.0703 (3)	0.0323 (11)
H215	1.328823	0.473267	0.072361	0.039*
C216	1.0792 (6)	0.4771 (5)	0.1006 (3)	0.0297 (11)
H216	1.096071	0.567256	0.124478	0.036*
C217	1.3488 (7)	0.2247 (6)	0.0065 (3)	0.0419 (13)

H21A	1.432511	0.222550	0.048626	0.063*
H21B	1.402815	0.280489	−0.033420	0.063*
H21C	1.310670	0.131074	−0.014994	0.063*
C221	0.8352 (5)	0.1160 (4)	0.2279 (3)	0.0166 (9)
C222	0.8029 (6)	−0.0183 (4)	0.1950 (3)	0.0200 (10)
H222	0.688134	−0.064583	0.189163	0.024*
C223	0.9408 (6)	−0.0830 (4)	0.1712 (3)	0.0221 (10)
H223	0.918562	−0.173452	0.147848	0.026*
C224	1.1094 (6)	−0.0198 (4)	0.1803 (2)	0.0205 (9)
C225	1.1391 (6)	0.1146 (4)	0.2142 (2)	0.0208 (9)
H225	1.253951	0.160407	0.220799	0.025*
C226	1.0032 (5)	0.1811 (4)	0.2381 (2)	0.0174 (9)
H226	1.025335	0.271439	0.261548	0.021*
C227	1.2580 (6)	−0.0914 (5)	0.1553 (3)	0.0310 (11)
H22A	1.301832	−0.136168	0.198653	0.046*
H22B	1.350057	−0.024143	0.137092	0.046*
H22C	1.218962	−0.160574	0.113757	0.046*
C231	0.9079 (6)	0.1957 (4)	0.4319 (2)	0.0157 (9)
C232	0.8353 (6)	0.0601 (5)	0.4143 (3)	0.0196 (10)
H232	0.713672	0.034660	0.411910	0.023*
C233	0.9446 (6)	−0.0366 (5)	0.4003 (3)	0.0222 (10)
H233	0.896784	−0.129568	0.388207	0.027*
C234	1.1222 (6)	−0.0012 (5)	0.4036 (3)	0.0197 (10)
C235	1.1914 (6)	0.1349 (5)	0.4228 (3)	0.0215 (10)
H235	1.313049	0.160346	0.425582	0.026*
C236	1.0845 (6)	0.2333 (5)	0.4378 (3)	0.0201 (10)
H236	1.132080	0.325546	0.452057	0.024*
C237	1.2399 (7)	−0.1067 (5)	0.3873 (3)	0.0336 (13)
H23A	1.181428	−0.197458	0.398811	0.050*
H23B	1.345357	−0.083894	0.419275	0.050*
H23C	1.269744	−0.107678	0.333131	0.050*
O11	0.3203 (4)	0.5191 (3)	0.89684 (17)	0.0292 (7)
O12	0.4075 (4)	0.8210 (3)	0.70414 (17)	0.0241 (7)
O13	0.1400 (4)	0.5650 (3)	0.50279 (15)	0.0198 (6)
O21	0.7628 (4)	0.6220 (3)	0.12303 (17)	0.0290 (8)
O22	0.5511 (4)	0.2025 (3)	0.18061 (16)	0.0245 (7)
O23	0.5909 (4)	0.2519 (3)	0.44638 (17)	0.0236 (7)
S11	0.14271 (14)	0.45895 (11)	0.87060 (6)	0.0206 (2)
S12	0.30955 (13)	0.75906 (10)	0.76915 (6)	0.0165 (2)
S13	0.20447 (13)	0.66475 (10)	0.56810 (6)	0.0157 (2)
S21	0.73480 (15)	0.47210 (11)	0.13514 (6)	0.0212 (2)
S22	0.64492 (13)	0.18842 (10)	0.25434 (6)	0.0177 (2)
S23	0.77031 (13)	0.32518 (11)	0.44833 (6)	0.0174 (2)
Fe1	0.28755 (6)	0.43306 (5)	0.69293 (3)	0.01587 (14)
Fe2	0.64410 (7)	0.52532 (5)	0.31808 (3)	0.01766 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C10	0.016 (2)	0.017 (2)	0.012 (2)	0.0072 (17)	−0.0007 (16)	−0.0022 (16)
C11	0.016 (2)	0.012 (2)	0.018 (2)	0.0044 (18)	−0.0003 (18)	−0.0008 (18)
C12	0.013 (2)	0.0150 (19)	0.016 (2)	0.0069 (17)	−0.0006 (16)	0.0004 (17)
C13	0.016 (2)	0.017 (2)	0.016 (2)	0.0037 (17)	−0.0009 (17)	−0.0019 (17)
C14	0.018 (2)	0.016 (2)	0.019 (2)	0.0029 (18)	0.0005 (17)	−0.0020 (17)
C15	0.021 (2)	0.033 (3)	0.047 (3)	0.014 (2)	0.013 (2)	0.015 (3)
C16	0.027 (3)	0.034 (3)	0.027 (3)	0.019 (2)	0.002 (2)	−0.001 (2)
C17	0.030 (3)	0.019 (2)	0.029 (3)	0.013 (2)	0.002 (2)	0.001 (2)
C18	0.027 (2)	0.037 (3)	0.026 (3)	0.022 (2)	−0.003 (2)	0.004 (2)
C19	0.016 (2)	0.024 (3)	0.058 (4)	0.008 (2)	−0.010 (2)	−0.007 (2)
C20	0.015 (2)	0.016 (2)	0.019 (2)	0.0024 (18)	0.0009 (17)	0.0018 (17)
C21	0.010 (2)	0.016 (2)	0.017 (2)	0.0022 (18)	0.0005 (17)	0.0007 (18)
C22	0.018 (2)	0.017 (2)	0.014 (2)	0.0073 (18)	0.0024 (17)	0.0018 (17)
C23	0.015 (2)	0.015 (2)	0.019 (2)	0.0022 (17)	−0.0027 (17)	−0.0008 (17)
C24	0.021 (2)	0.016 (2)	0.018 (2)	0.0009 (18)	0.0012 (18)	0.0055 (17)
C25	0.016 (3)	0.043 (3)	0.109 (5)	0.009 (2)	−0.004 (3)	−0.029 (3)
C26	0.029 (3)	0.042 (3)	0.048 (4)	0.017 (3)	0.019 (3)	0.008 (3)
C27	0.031 (3)	0.034 (3)	0.030 (3)	0.019 (2)	0.005 (2)	−0.005 (2)
C28	0.041 (3)	0.038 (3)	0.049 (4)	0.028 (2)	0.011 (3)	0.014 (2)
C29	0.040 (3)	0.095 (4)	0.034 (3)	0.052 (3)	−0.018 (2)	−0.020 (2)
C111	0.020 (2)	0.021 (2)	0.013 (2)	0.0006 (19)	0.0020 (18)	0.0004 (17)
C112	0.022 (2)	0.030 (2)	0.022 (2)	−0.004 (2)	−0.0031 (19)	−0.004 (2)
C113	0.020 (2)	0.041 (3)	0.028 (3)	0.003 (2)	0.0022 (19)	0.002 (2)
C114	0.034 (3)	0.037 (3)	0.015 (2)	0.011 (2)	0.003 (2)	0.008 (2)
C115	0.037 (3)	0.020 (2)	0.022 (2)	0.001 (2)	−0.001 (2)	0.0010 (19)
C116	0.025 (2)	0.024 (2)	0.017 (2)	−0.002 (2)	−0.0010 (19)	0.0018 (19)
C117	0.047 (3)	0.044 (3)	0.033 (3)	0.017 (3)	0.006 (3)	0.004 (2)
C121	0.019 (2)	0.018 (2)	0.012 (2)	0.0019 (17)	0.0012 (16)	0.0029 (16)
C122	0.022 (2)	0.021 (2)	0.021 (2)	−0.0010 (19)	0.0000 (19)	0.0027 (19)
C123	0.030 (3)	0.012 (2)	0.022 (2)	0.0006 (19)	0.003 (2)	0.0035 (18)
C124	0.026 (2)	0.022 (2)	0.020 (2)	0.008 (2)	0.0048 (19)	0.0062 (18)
C125	0.017 (2)	0.025 (2)	0.021 (2)	0.0034 (19)	0.0013 (17)	0.0063 (19)
C126	0.025 (2)	0.015 (2)	0.015 (2)	0.0019 (19)	0.0003 (18)	0.0017 (17)
C127	0.035 (3)	0.029 (3)	0.035 (3)	0.014 (2)	0.010 (2)	0.004 (2)
C131	0.015 (2)	0.018 (2)	0.012 (2)	0.0054 (18)	0.0000 (16)	0.0022 (17)
C132	0.020 (2)	0.018 (2)	0.015 (2)	−0.0003 (19)	0.0014 (18)	0.0021 (18)
C133	0.028 (3)	0.015 (2)	0.018 (2)	0.0052 (19)	0.0023 (19)	0.0030 (18)
C134	0.023 (2)	0.022 (2)	0.015 (2)	0.009 (2)	−0.0007 (18)	0.0030 (18)
C135	0.014 (2)	0.024 (2)	0.020 (2)	0.0028 (19)	−0.0023 (18)	0.0029 (19)
C136	0.022 (2)	0.017 (2)	0.017 (2)	0.0026 (19)	−0.0020 (18)	−0.0007 (18)
C137	0.028 (3)	0.022 (2)	0.030 (3)	0.011 (2)	0.005 (2)	0.005 (2)
C211	0.029 (3)	0.027 (2)	0.010 (2)	−0.004 (2)	−0.0018 (19)	0.0034 (18)
C212	0.031 (3)	0.027 (2)	0.017 (2)	−0.001 (2)	−0.002 (2)	0.000 (2)
C213	0.039 (3)	0.024 (2)	0.018 (2)	0.004 (2)	0.001 (2)	0.0002 (19)
C214	0.035 (3)	0.046 (3)	0.015 (2)	0.014 (2)	0.000 (2)	0.004 (2)

C215	0.027 (3)	0.045 (3)	0.022 (2)	−0.005 (2)	−0.004 (2)	−0.002 (2)
C216	0.033 (3)	0.033 (3)	0.021 (2)	−0.002 (2)	0.001 (2)	−0.001 (2)
C217	0.035 (3)	0.064 (4)	0.029 (3)	0.018 (3)	0.001 (2)	0.001 (3)
C221	0.020 (2)	0.015 (2)	0.015 (2)	0.0024 (18)	0.0032 (18)	0.0031 (17)
C222	0.022 (2)	0.016 (2)	0.020 (2)	−0.0020 (19)	0.0007 (19)	−0.0017 (18)
C223	0.032 (3)	0.012 (2)	0.022 (2)	0.0021 (19)	0.003 (2)	−0.0020 (17)
C224	0.025 (2)	0.023 (2)	0.014 (2)	0.0077 (19)	0.0003 (17)	−0.0023 (18)
C225	0.020 (2)	0.021 (2)	0.022 (2)	0.0024 (18)	−0.0006 (18)	−0.0019 (18)
C226	0.018 (2)	0.014 (2)	0.019 (2)	−0.0009 (18)	−0.0029 (18)	−0.0030 (17)
C227	0.030 (3)	0.024 (2)	0.041 (3)	0.012 (2)	−0.001 (2)	−0.005 (2)
C231	0.020 (2)	0.015 (2)	0.013 (2)	0.0048 (18)	−0.0002 (17)	0.0029 (17)
C232	0.017 (2)	0.023 (2)	0.019 (2)	0.0035 (19)	0.0024 (18)	0.0020 (19)
C233	0.031 (3)	0.016 (2)	0.020 (2)	0.002 (2)	0.001 (2)	0.0026 (18)
C234	0.024 (2)	0.021 (2)	0.016 (2)	0.008 (2)	0.0032 (18)	0.0026 (18)
C235	0.018 (2)	0.025 (2)	0.022 (2)	0.003 (2)	−0.0005 (19)	0.0019 (19)
C236	0.020 (2)	0.017 (2)	0.023 (2)	−0.0027 (19)	0.0003 (19)	0.0018 (19)
C237	0.039 (3)	0.028 (3)	0.037 (3)	0.016 (2)	0.007 (2)	0.005 (2)
O11	0.0201 (16)	0.045 (2)	0.0213 (16)	0.0033 (15)	−0.0059 (13)	−0.0007 (14)
O12	0.0193 (15)	0.0202 (15)	0.0320 (17)	−0.0004 (13)	0.0076 (13)	0.0005 (13)
O13	0.0262 (16)	0.0209 (15)	0.0124 (14)	0.0063 (13)	0.0003 (12)	−0.0043 (12)
O21	0.046 (2)	0.0176 (15)	0.0228 (17)	0.0024 (15)	−0.0072 (15)	0.0057 (13)
O22	0.0220 (15)	0.0243 (15)	0.0258 (16)	0.0014 (13)	−0.0083 (13)	−0.0015 (13)
O23	0.0133 (15)	0.0303 (17)	0.0280 (17)	0.0023 (13)	0.0063 (13)	0.0088 (14)
S11	0.0227 (6)	0.0239 (6)	0.0156 (5)	0.0034 (5)	−0.0008 (4)	0.0037 (4)
S12	0.0144 (5)	0.0158 (5)	0.0187 (5)	0.0022 (4)	−0.0018 (4)	−0.0028 (4)
S13	0.0172 (5)	0.0163 (5)	0.0145 (5)	0.0052 (4)	0.0017 (4)	0.0007 (4)
S21	0.0286 (6)	0.0178 (5)	0.0166 (5)	0.0015 (5)	−0.0043 (5)	0.0019 (4)
S22	0.0154 (5)	0.0163 (5)	0.0204 (6)	−0.0007 (4)	−0.0004 (4)	−0.0003 (4)
S23	0.0167 (5)	0.0206 (5)	0.0161 (5)	0.0052 (4)	0.0019 (4)	0.0032 (4)
Fe1	0.0171 (3)	0.0149 (3)	0.0166 (3)	0.0060 (3)	−0.0003 (3)	0.0003 (3)
Fe2	0.0164 (3)	0.0178 (3)	0.0196 (3)	0.0063 (3)	−0.0009 (3)	−0.0008 (3)

Geometric parameters (Å, º)

C10—C14	1.428 (6)	C122—C123	1.378 (6)
C10—C11	1.436 (6)	C122—H122	0.9500
C10—S11	1.780 (4)	C123—C124	1.395 (6)
C10—Fe1	2.017 (4)	C123—H123	0.9500
C11—C12	1.444 (6)	C124—C125	1.396 (6)
C11—S12	1.773 (4)	C124—C127	1.514 (6)
C11—Fe1	2.019 (4)	C125—C126	1.384 (6)
C12—C13	1.426 (6)	C125—H125	0.9500
C12—S13	1.792 (4)	C126—H126	0.9500
C12—Fe1	2.030 (4)	C127—H12A	0.9800
C13—C14	1.409 (6)	C127—H12B	0.9800
C13—Fe1	2.054 (4)	C127—H12C	0.9800
C13—H13	0.9500	C131—C132	1.382 (6)
C14—Fe1	2.039 (4)	C131—C136	1.387 (6)

C14—H14	0.9500	C131—S13	1.796 (4)
C15—C19	1.408 (8)	C132—C133	1.394 (6)
C15—C16	1.425 (7)	C132—H132	0.9500
C15—Fe1	2.047 (5)	C133—C134	1.387 (6)
C15—H15	0.9500	C133—H133	0.9500
C16—C17	1.431 (7)	C134—C135	1.413 (6)
C16—Fe1	2.057 (5)	C134—C137	1.507 (6)
C16—H16	0.9500	C135—C136	1.371 (6)
C17—C18	1.404 (7)	C135—H135	0.9500
C17—Fe1	2.045 (5)	C136—H136	0.9500
C17—H17	0.9500	C137—H13A	0.9800
C18—C19	1.426 (7)	C137—H13B	0.9800
C18—Fe1	2.046 (4)	C137—H13C	0.9800
C18—H18	0.9500	C211—C216	1.381 (6)
C19—Fe1	2.039 (5)	C211—C212	1.389 (7)
C19—H19	0.9500	C211—S21	1.803 (5)
C20—C24	1.427 (6)	C212—C213	1.389 (7)
C20—C21	1.443 (6)	C212—H212	0.9500
C20—S21	1.788 (4)	C213—C214	1.379 (7)
C20—Fe2	2.020 (4)	C213—H213	0.9500
C21—C22	1.426 (6)	C214—C215	1.397 (7)
C21—S22	1.776 (4)	C214—C217	1.525 (7)
C21—Fe2	2.009 (4)	C215—C216	1.383 (7)
C22—C23	1.428 (6)	C215—H215	0.9500
C22—S23	1.791 (4)	C216—H216	0.9500
C22—Fe2	2.008 (4)	C217—H21A	0.9800
C23—C24	1.415 (6)	C217—H21B	0.9800
C23—Fe2	2.048 (4)	C217—H21C	0.9800
C23—H23	0.9500	C221—C226	1.384 (6)
C24—Fe2	2.049 (4)	C221—C222	1.399 (6)
C24—H24	0.9500	C221—S22	1.797 (5)
C25—C26	1.391 (9)	C222—C223	1.388 (6)
C25—C29	1.424 (10)	C222—H222	0.9500
C25—Fe2	2.039 (5)	C223—C224	1.380 (6)
C25—H25	0.9500	C223—H223	0.9500
C26—C27	1.371 (7)	C224—C225	1.406 (6)
C26—Fe2	2.054 (5)	C224—C227	1.502 (6)
C26—H26	0.9500	C225—C226	1.384 (6)
C27—C28	1.381 (7)	C225—H225	0.9500
C27—Fe2	2.038 (5)	C226—H226	0.9500
C27—H27	0.9500	C227—H22A	0.9800
C28—C29	1.409 (8)	C227—H22B	0.9800
C28—Fe2	2.036 (5)	C227—H22C	0.9800
C28—H28	0.9500	C231—C236	1.381 (6)
C29—Fe2	2.038 (5)	C231—C232	1.392 (6)
C29—H29	0.9500	C231—S23	1.796 (4)
C111—C116	1.383 (6)	C232—C233	1.382 (6)
C111—C112	1.403 (6)	C232—H232	0.9500

C111—S11	1.778 (5)	C233—C234	1.385 (6)
C112—C113	1.377 (7)	C233—H233	0.9500
C112—H112	0.9500	C234—C235	1.393 (6)
C113—C114	1.383 (7)	C234—C237	1.502 (7)
C113—H113	0.9500	C235—C236	1.385 (7)
C114—C115	1.387 (7)	C235—H235	0.9500
C114—C117	1.509 (7)	C236—H236	0.9500
C115—C116	1.392 (7)	C237—H23A	0.9800
C115—H115	0.9500	C237—H23B	0.9800
C116—H116	0.9500	C237—H23C	0.9800
C117—H11A	0.9800	O11—S11	1.486 (3)
C117—H11B	0.9800	O12—S12	1.496 (3)
C117—H11C	0.9800	O13—S13	1.494 (3)
C121—C126	1.383 (6)	O21—S21	1.492 (3)
C121—C122	1.385 (6)	O22—S22	1.495 (3)
C121—S12	1.806 (5)	O23—S23	1.486 (3)

C14—C10—C11	107.6 (4)	C134—C137—H13A	109.5
C14—C10—S11	122.9 (3)	C134—C137—H13B	109.5
C11—C10—S11	129.4 (3)	H13A—C137—H13B	109.5
C14—C10—Fe1	70.2 (3)	C134—C137—H13C	109.5
C11—C10—Fe1	69.2 (2)	H13A—C137—H13C	109.5
S11—C10—Fe1	122.9 (2)	H13B—C137—H13C	109.5
C10—C11—C12	107.4 (3)	C216—C211—C212	121.5 (5)
C10—C11—S12	127.2 (3)	C216—C211—S21	120.3 (4)
C12—C11—S12	125.5 (3)	C212—C211—S21	118.2 (4)
C10—C11—Fe1	69.1 (2)	C213—C212—C211	117.9 (4)
C12—C11—Fe1	69.5 (2)	C213—C212—H212	121.1
S12—C11—Fe1	126.4 (2)	C211—C212—H212	121.1
C13—C12—C11	107.8 (4)	C214—C213—C212	122.0 (5)
C13—C12—S13	121.8 (3)	C214—C213—H213	119.0
C11—C12—S13	130.3 (3)	C212—C213—H213	119.0
C13—C12—Fe1	70.4 (2)	C213—C214—C215	118.7 (5)
C11—C12—Fe1	68.7 (2)	C213—C214—C217	121.7 (5)
S13—C12—Fe1	123.6 (2)	C215—C214—C217	119.6 (5)
C14—C13—C12	108.3 (4)	C216—C215—C214	120.5 (5)
C14—C13—Fe1	69.3 (2)	C216—C215—H215	119.8
C12—C13—Fe1	68.7 (2)	C214—C215—H215	119.8
C14—C13—H13	125.8	C211—C216—C215	119.4 (5)
C12—C13—H13	125.8	C211—C216—H216	120.3
Fe1—C13—H13	127.7	C215—C216—H216	120.3
C13—C14—C10	108.9 (4)	C214—C217—H21A	109.5
C13—C14—Fe1	70.4 (3)	C214—C217—H21B	109.5
C10—C14—Fe1	68.6 (2)	H21A—C217—H21B	109.5
C13—C14—H14	125.5	C214—C217—H21C	109.5
C10—C14—H14	125.5	H21A—C217—H21C	109.5
Fe1—C14—H14	127.1	H21B—C217—H21C	109.5
C19—C15—C16	107.8 (4)	C226—C221—C222	119.9 (4)

C19—C15—Fe1	69.5 (3)	C226—C221—S22	125.6 (3)
C16—C15—Fe1	70.1 (3)	C222—C221—S22	114.4 (3)
C19—C15—H15	126.1	C223—C222—C221	119.1 (4)
C16—C15—H15	126.1	C223—C222—H222	120.4
Fe1—C15—H15	125.9	C221—C222—H222	120.4
C15—C16—C17	107.3 (5)	C224—C223—C222	121.9 (4)
C15—C16—Fe1	69.3 (3)	C224—C223—H223	119.0
C17—C16—Fe1	69.1 (3)	C222—C223—H223	119.0
C15—C16—H16	126.4	C223—C224—C225	118.0 (4)
C17—C16—H16	126.4	C223—C224—C227	121.6 (4)
Fe1—C16—H16	126.8	C225—C224—C227	120.4 (4)
C18—C17—C16	108.7 (4)	C226—C225—C224	120.9 (4)
C18—C17—Fe1	70.0 (3)	C226—C225—H225	119.5
C16—C17—Fe1	70.0 (3)	C224—C225—H225	119.5
C18—C17—H17	125.7	C225—C226—C221	120.0 (4)
C16—C17—H17	125.7	C225—C226—H226	120.0
Fe1—C17—H17	125.9	C221—C226—H226	120.0
C17—C18—C19	107.4 (4)	C224—C227—H22A	109.5
C17—C18—Fe1	69.9 (3)	C224—C227—H22B	109.5
C19—C18—Fe1	69.3 (3)	H22A—C227—H22B	109.5
C17—C18—H18	126.3	C224—C227—H22C	109.5
C19—C18—H18	126.3	H22A—C227—H22C	109.5
Fe1—C18—H18	126.1	H22B—C227—H22C	109.5
C15—C19—C18	108.8 (4)	C236—C231—C232	121.3 (4)
C15—C19—Fe1	70.2 (3)	C236—C231—S23	118.9 (3)
C18—C19—Fe1	69.9 (3)	C232—C231—S23	119.8 (3)
C15—C19—H19	125.6	C233—C232—C231	118.4 (4)
C18—C19—H19	125.6	C233—C232—H232	120.8
Fe1—C19—H19	126.0	C231—C232—H232	120.8
C24—C20—C21	107.3 (4)	C232—C233—C234	121.5 (4)
C24—C20—S21	123.6 (3)	C232—C233—H233	119.2
C21—C20—S21	128.8 (3)	C234—C233—H233	119.2
C24—C20—Fe2	70.5 (3)	C233—C234—C235	118.9 (4)
C21—C20—Fe2	68.6 (2)	C233—C234—C237	121.1 (4)
S21—C20—Fe2	121.2 (2)	C235—C234—C237	120.0 (4)
C22—C21—C20	107.6 (3)	C236—C235—C234	120.6 (4)
C22—C21—S22	127.6 (3)	C236—C235—H235	119.7
C20—C21—S22	124.6 (3)	C234—C235—H235	119.7
C22—C21—Fe2	69.2 (2)	C231—C236—C235	119.2 (4)
C20—C21—Fe2	69.4 (2)	C231—C236—H236	120.4
S22—C21—Fe2	130.7 (2)	C235—C236—H236	120.4
C21—C22—C23	108.3 (4)	C234—C237—H23A	109.5
C21—C22—S23	128.7 (3)	C234—C237—H23B	109.5
C23—C22—S23	122.8 (3)	H23A—C237—H23B	109.5
C21—C22—Fe2	69.3 (2)	C234—C237—H23C	109.5
C23—C22—Fe2	70.9 (2)	H23A—C237—H23C	109.5
S23—C22—Fe2	122.0 (2)	H23B—C237—H23C	109.5
C24—C23—C22	108.0 (4)	O11—S11—C111	106.7 (2)

C24—C23—Fe2	69.8 (2)	O11—S11—C10	107.87 (19)
C22—C23—Fe2	67.9 (2)	C111—S11—C10	97.7 (2)
C24—C23—H23	126.0	O12—S12—C11	105.94 (19)
C22—C23—H23	126.0	O12—S12—C121	106.82 (19)
Fe2—C23—H23	127.9	C11—S12—C121	98.2 (2)
C23—C24—C20	108.8 (4)	O13—S13—C12	102.97 (18)
C23—C24—Fe2	69.8 (2)	O13—S13—C131	106.36 (18)
C20—C24—Fe2	68.4 (2)	C12—S13—C131	96.96 (19)
C23—C24—H24	125.6	O21—S21—C20	103.54 (18)
C20—C24—H24	125.6	O21—S21—C211	107.1 (2)
Fe2—C24—H24	127.8	C20—S21—C211	96.7 (2)
C26—C25—C29	107.7 (5)	O22—S22—C21	105.92 (18)
C26—C25—Fe2	70.7 (3)	O22—S22—C221	105.50 (19)
C29—C25—Fe2	69.5 (3)	C21—S22—C221	98.2 (2)
C26—C25—H25	126.1	O23—S23—C22	108.47 (18)
C29—C25—H25	126.1	O23—S23—C231	106.25 (19)
Fe2—C25—H25	125.3	C22—S23—C231	97.1 (2)
C27—C26—C25	108.1 (5)	C10—Fe1—C11	41.69 (17)
C27—C26—Fe2	69.8 (3)	C10—Fe1—C12	69.95 (17)
C25—C26—Fe2	69.6 (3)	C11—Fe1—C12	41.78 (17)
C27—C26—H26	125.9	C10—Fe1—C19	122.4 (2)
C25—C26—H26	125.9	C11—Fe1—C19	107.60 (19)
Fe2—C26—H26	126.2	C12—Fe1—C19	124.09 (19)
C26—C27—C28	109.8 (5)	C10—Fe1—C14	41.22 (16)
C26—C27—Fe2	71.0 (3)	C11—Fe1—C14	69.42 (17)
C28—C27—Fe2	70.1 (3)	C12—Fe1—C14	68.76 (17)
C26—C27—H27	125.1	C19—Fe1—C14	158.4 (2)
C28—C27—H27	125.1	C10—Fe1—C17	123.14 (19)
Fe2—C27—H27	125.4	C11—Fe1—C17	160.29 (19)
C27—C28—C29	107.6 (5)	C12—Fe1—C17	156.74 (18)
C27—C28—Fe2	70.3 (3)	C19—Fe1—C17	67.9 (2)
C29—C28—Fe2	69.8 (3)	C14—Fe1—C17	107.30 (19)
C27—C28—H28	126.2	C10—Fe1—C18	107.16 (18)
C29—C28—H28	126.2	C11—Fe1—C18	123.95 (19)
Fe2—C28—H28	125.3	C12—Fe1—C18	161.33 (18)
C28—C29—C25	106.7 (5)	C19—Fe1—C18	40.9 (2)
C28—C29—Fe2	69.7 (3)	C14—Fe1—C18	121.94 (19)
C25—C29—Fe2	69.6 (3)	C17—Fe1—C18	40.15 (19)
C28—C29—H29	126.7	C10—Fe1—C15	157.9 (2)
C25—C29—H29	126.7	C11—Fe1—C15	121.47 (19)
Fe2—C29—H29	125.6	C12—Fe1—C15	106.85 (19)
C116—C111—C112	120.3 (4)	C19—Fe1—C15	40.3 (2)
C116—C111—S11	120.6 (4)	C14—Fe1—C15	159.6 (2)
C112—C111—S11	119.1 (3)	C17—Fe1—C15	68.4 (2)
C113—C112—C111	119.0 (4)	C18—Fe1—C15	68.5 (2)
C113—C112—H112	120.5	C10—Fe1—C13	69.07 (17)
C111—C112—H112	120.5	C11—Fe1—C13	69.40 (17)
C112—C113—C114	121.4 (4)	C12—Fe1—C13	40.86 (16)

C112—C113—H113	119.3	C19—Fe1—C13	160.4 (2)
C114—C113—H113	119.3	C14—Fe1—C13	40.26 (17)
C113—C114—C115	119.1 (5)	C17—Fe1—C13	121.42 (18)
C113—C114—C117	120.1 (4)	C18—Fe1—C13	156.78 (18)
C115—C114—C117	120.7 (5)	C15—Fe1—C13	123.56 (19)
C114—C115—C116	120.6 (4)	C10—Fe1—C16	159.79 (18)
C114—C115—H115	119.7	C11—Fe1—C16	157.20 (19)
C116—C115—H115	119.7	C12—Fe1—C16	120.77 (18)
C111—C116—C115	119.5 (4)	C19—Fe1—C16	67.9 (2)
C111—C116—H116	120.2	C14—Fe1—C16	123.12 (19)
C115—C116—H116	120.2	C17—Fe1—C16	40.82 (19)
C114—C117—H11A	109.5	C18—Fe1—C16	68.3 (2)
C114—C117—H11B	109.5	C15—Fe1—C16	40.6 (2)
H11A—C117—H11B	109.5	C13—Fe1—C16	106.89 (19)
C114—C117—H11C	109.5	C22—Fe2—C21	41.59 (17)
H11A—C117—H11C	109.5	C22—Fe2—C20	70.18 (17)
H11B—C117—H11C	109.5	C21—Fe2—C20	41.98 (16)
C126—C121—C122	120.0 (4)	C22—Fe2—C28	157.3 (2)
C126—C121—S12	125.4 (4)	C21—Fe2—C28	159.0 (2)
C122—C121—S12	114.6 (3)	C20—Fe2—C28	120.9 (2)
C123—C122—C121	120.0 (4)	C22—Fe2—C29	161.1 (2)
C123—C122—H122	120.0	C21—Fe2—C29	123.7 (2)
C121—C122—H122	120.0	C20—Fe2—C29	106.5 (2)
C122—C123—C124	120.8 (4)	C28—Fe2—C29	40.5 (2)
C122—C123—H123	119.6	C22—Fe2—C27	123.3 (2)
C124—C123—H123	119.6	C21—Fe2—C27	160.3 (2)
C123—C124—C125	118.7 (4)	C20—Fe2—C27	156.59 (19)
C123—C124—C127	120.8 (4)	C28—Fe2—C27	39.6 (2)
C125—C124—C127	120.6 (4)	C29—Fe2—C27	67.1 (2)
C126—C125—C124	120.3 (4)	C22—Fe2—C25	124.8 (2)
C126—C125—H125	119.8	C21—Fe2—C25	109.6 (2)
C124—C125—H125	119.8	C20—Fe2—C25	124.3 (2)
C121—C126—C125	120.2 (4)	C28—Fe2—C25	67.8 (2)
C121—C126—H126	119.9	C29—Fe2—C25	40.9 (3)
C125—C126—H126	119.9	C27—Fe2—C25	66.5 (2)
C124—C127—H12A	109.5	C22—Fe2—C23	41.20 (16)
C124—C127—H12B	109.5	C21—Fe2—C23	69.49 (17)
H12A—C127—H12B	109.5	C20—Fe2—C23	69.21 (17)
C124—C127—H12C	109.5	C28—Fe2—C23	120.5 (2)
H12A—C127—H12C	109.5	C29—Fe2—C23	156.4 (2)
H12B—C127—H12C	109.5	C27—Fe2—C23	107.2 (2)
C132—C131—C136	120.9 (4)	C25—Fe2—C23	160.0 (3)
C132—C131—S13	119.0 (3)	C22—Fe2—C24	69.06 (17)
C136—C131—S13	120.1 (3)	C21—Fe2—C24	69.46 (17)
C131—C132—C133	119.2 (4)	C20—Fe2—C24	41.05 (16)
C131—C132—H132	120.4	C28—Fe2—C24	105.3 (2)
C133—C132—H132	120.4	C29—Fe2—C24	121.3 (2)
C134—C133—C132	120.9 (4)	C27—Fe2—C24	121.4 (2)

C134—C133—H133	119.6	C25—Fe2—C24	159.3 (3)
C132—C133—H133	119.6	C23—Fe2—C24	40.40 (16)
C133—C134—C135	118.5 (4)	C22—Fe2—C26	109.5 (2)
C133—C134—C137	121.4 (4)	C21—Fe2—C26	125.5 (2)
C135—C134—C137	120.2 (4)	C20—Fe2—C26	161.4 (2)
C136—C135—C134	120.7 (4)	C28—Fe2—C26	66.8 (2)
C136—C135—H135	119.6	C29—Fe2—C26	67.5 (2)
C134—C135—H135	119.6	C27—Fe2—C26	39.1 (2)
C135—C136—C131	119.7 (4)	C25—Fe2—C26	39.7 (3)
C135—C136—H136	120.1	C23—Fe2—C26	123.5 (2)
C131—C136—H136	120.1	C24—Fe2—C26	157.3 (2)
C14—C10—C11—C12	−0.8 (5)	C127—C124—C125—C126	−178.9 (4)
S11—C10—C11—C12	175.3 (3)	C122—C121—C126—C125	1.1 (6)
Fe1—C10—C11—C12	59.2 (3)	S12—C121—C126—C125	178.9 (3)
C14—C10—C11—S12	179.5 (3)	C124—C125—C126—C121	−0.7 (6)
S11—C10—C11—S12	−4.4 (6)	C136—C131—C132—C133	1.2 (6)
Fe1—C10—C11—S12	−120.5 (4)	S13—C131—C132—C133	−178.6 (3)
C14—C10—C11—Fe1	−60.0 (3)	C131—C132—C133—C134	0.1 (6)
S11—C10—C11—Fe1	116.1 (4)	C132—C133—C134—C135	−0.9 (7)
C10—C11—C12—C13	0.9 (5)	C132—C133—C134—C137	178.7 (4)
S12—C11—C12—C13	−179.4 (3)	C133—C134—C135—C136	0.4 (7)
Fe1—C11—C12—C13	59.8 (3)	C137—C134—C135—C136	−179.2 (4)
C10—C11—C12—S13	−175.5 (3)	C134—C135—C136—C131	0.9 (7)
S12—C11—C12—S13	4.2 (6)	C132—C131—C136—C135	−1.7 (7)
Fe1—C11—C12—S13	−116.6 (4)	S13—C131—C136—C135	178.1 (3)
C10—C11—C12—Fe1	−59.0 (3)	C216—C211—C212—C213	0.7 (7)
S12—C11—C12—Fe1	120.8 (4)	S21—C211—C212—C213	−179.4 (3)
C11—C12—C13—C14	−0.6 (5)	C211—C212—C213—C214	0.2 (7)
S13—C12—C13—C14	176.1 (3)	C212—C213—C214—C215	−1.6 (7)
Fe1—C12—C13—C14	58.1 (3)	C212—C213—C214—C217	177.9 (5)
C11—C12—C13—Fe1	−58.7 (3)	C213—C214—C215—C216	2.1 (7)
S13—C12—C13—Fe1	118.0 (3)	C217—C214—C215—C216	−177.4 (4)
C12—C13—C14—C10	0.2 (5)	C212—C211—C216—C215	−0.1 (7)
Fe1—C13—C14—C10	57.9 (3)	S21—C211—C216—C215	180.0 (4)
C12—C13—C14—Fe1	−57.7 (3)	C214—C215—C216—C211	−1.3 (7)
C11—C10—C14—C13	0.4 (5)	C226—C221—C222—C223	−1.8 (6)
S11—C10—C14—C13	−176.0 (3)	S22—C221—C222—C223	178.8 (3)
Fe1—C10—C14—C13	−59.0 (3)	C221—C222—C223—C224	1.4 (7)
C11—C10—C14—Fe1	59.4 (3)	C222—C223—C224—C225	−0.7 (7)
S11—C10—C14—Fe1	−117.0 (3)	C222—C223—C224—C227	179.1 (4)
C19—C15—C16—C17	0.6 (5)	C223—C224—C225—C226	0.4 (6)
Fe1—C15—C16—C17	−58.9 (3)	C227—C224—C225—C226	−179.4 (4)
C19—C15—C16—Fe1	59.5 (3)	C224—C225—C226—C221	−0.8 (6)
C15—C16—C17—C18	−0.5 (5)	C222—C221—C226—C225	1.5 (6)
Fe1—C16—C17—C18	−59.5 (3)	S22—C221—C226—C225	−179.1 (3)
C15—C16—C17—Fe1	59.0 (3)	C236—C231—C232—C233	−2.0 (7)
C16—C17—C18—C19	0.2 (5)	S23—C231—C232—C233	178.7 (3)

Fe1—C17—C18—C19	−59.4 (3)	C231—C232—C233—C234	0.1 (7)
C16—C17—C18—Fe1	59.6 (3)	C232—C233—C234—C235	1.2 (7)
C16—C15—C19—C18	−0.5 (6)	C232—C233—C234—C237	−179.1 (4)
Fe1—C15—C19—C18	59.3 (3)	C233—C234—C235—C236	−0.4 (7)
C16—C15—C19—Fe1	−59.9 (3)	C237—C234—C235—C236	179.9 (4)
C17—C18—C19—C15	0.2 (6)	C232—C231—C236—C235	2.8 (7)
Fe1—C18—C19—C15	−59.5 (4)	S23—C231—C236—C235	−177.9 (3)
C17—C18—C19—Fe1	59.8 (3)	C234—C235—C236—C231	−1.5 (7)
C24—C20—C21—C22	1.4 (5)	C116—C111—S11—O11	3.1 (4)
S21—C20—C21—C22	−172.3 (3)	C112—C111—S11—O11	−174.5 (3)
Fe2—C20—C21—C22	−58.8 (3)	C116—C111—S11—C10	−108.3 (4)
C24—C20—C21—S22	−173.9 (3)	C112—C111—S11—C10	74.1 (4)
S21—C20—C21—S22	12.5 (6)	C14—C10—S11—O11	139.1 (4)
Fe2—C20—C21—S22	125.9 (3)	C11—C10—S11—O11	−36.5 (5)
C24—C20—C21—Fe2	60.2 (3)	Fe1—C10—S11—O11	52.6 (3)
S21—C20—C21—Fe2	−113.5 (4)	C14—C10—S11—C111	−110.5 (4)
C20—C21—C22—C23	−1.5 (5)	C11—C10—S11—C111	74.0 (4)
S22—C21—C22—C23	173.6 (3)	Fe1—C10—S11—C111	163.0 (2)
Fe2—C21—C22—C23	−60.4 (3)	C10—C11—S12—O12	158.8 (4)
C20—C21—C22—S23	173.9 (3)	C12—C11—S12—O12	−20.9 (4)
S22—C21—C22—S23	−11.0 (7)	Fe1—C11—S12—O12	68.6 (3)
Fe2—C21—C22—S23	115.0 (4)	C10—C11—S12—C121	−91.0 (4)
C20—C21—C22—Fe2	59.0 (3)	C12—C11—S12—C121	89.3 (4)
S22—C21—C22—Fe2	−126.0 (4)	Fe1—C11—S12—C121	178.8 (3)
C21—C22—C23—C24	1.0 (5)	C126—C121—S12—O12	108.2 (4)
S23—C22—C23—C24	−174.8 (3)	C122—C121—S12—O12	−74.0 (4)
Fe2—C22—C23—C24	−58.4 (3)	C126—C121—S12—C11	−1.3 (4)
C21—C22—C23—Fe2	59.4 (3)	C122—C121—S12—C11	176.5 (3)
S23—C22—C23—Fe2	−116.3 (3)	C13—C12—S13—O13	−4.4 (4)
C22—C23—C24—C20	−0.1 (5)	C11—C12—S13—O13	171.6 (4)
Fe2—C23—C24—C20	−57.3 (3)	Fe1—C12—S13—O13	82.2 (3)
C22—C23—C24—Fe2	57.2 (3)	C13—C12—S13—C131	104.3 (4)
C21—C20—C24—C23	−0.8 (5)	C11—C12—S13—C131	−79.8 (4)
S21—C20—C24—C23	173.3 (3)	Fe1—C12—S13—C131	−169.2 (2)
Fe2—C20—C24—C23	58.2 (3)	C132—C131—S13—O13	−139.5 (3)
C21—C20—C24—Fe2	−59.0 (3)	C136—C131—S13—O13	40.6 (4)
S21—C20—C24—Fe2	115.1 (3)	C132—C131—S13—C12	114.7 (4)
C29—C25—C26—C27	−0.5 (6)	C136—C131—S13—C12	−65.1 (4)
Fe2—C25—C26—C27	59.4 (4)	C24—C20—S21—O21	−14.2 (4)
C29—C25—C26—Fe2	−59.9 (4)	C21—C20—S21—O21	158.5 (4)
C25—C26—C27—C28	0.3 (6)	Fe2—C20—S21—O21	72.0 (3)
Fe2—C26—C27—C28	59.6 (4)	C24—C20—S21—C211	95.2 (4)
C25—C26—C27—Fe2	−59.2 (4)	C21—C20—S21—C211	−92.0 (4)
C26—C27—C28—C29	0.0 (6)	Fe2—C20—S21—C211	−178.5 (2)
Fe2—C27—C28—C29	60.1 (4)	C216—C211—S21—O21	34.9 (4)
C26—C27—C28—Fe2	−60.1 (4)	C212—C211—S21—O21	−145.0 (4)
C27—C28—C29—C25	−0.3 (6)	C216—C211—S21—C20	−71.5 (4)
Fe2—C28—C29—C25	60.1 (4)	C212—C211—S21—C20	108.5 (4)

C27—C28—C29—Fe2	−60.4 (4)	C22—C21—S22—O22	159.9 (4)
C26—C25—C29—C28	0.5 (6)	C20—C21—S22—O22	−25.8 (4)
Fe2—C25—C29—C28	−60.2 (4)	Fe2—C21—S22—O22	65.9 (3)
C26—C25—C29—Fe2	60.7 (4)	C22—C21—S22—C221	−91.3 (4)
C116—C111—C112—C113	2.3 (7)	C20—C21—S22—C221	83.0 (4)
S11—C111—C112—C113	179.9 (4)	Fe2—C21—S22—C221	174.7 (3)
C111—C112—C113—C114	−1.5 (7)	C226—C221—S22—O22	114.1 (4)
C112—C113—C114—C115	0.5 (7)	C222—C221—S22—O22	−66.5 (3)
C112—C113—C114—C117	−177.8 (4)	C226—C221—S22—C21	5.0 (4)
C113—C114—C115—C116	−0.3 (7)	C222—C221—S22—C21	−175.6 (3)
C117—C114—C115—C116	178.0 (4)	C21—C22—S23—O23	−37.2 (5)
C112—C111—C116—C115	−2.1 (7)	C23—C22—S23—O23	137.6 (4)
S11—C111—C116—C115	−179.7 (4)	Fe2—C22—S23—O23	50.8 (3)
C114—C115—C116—C111	1.1 (7)	C21—C22—S23—C231	72.6 (4)
C126—C121—C122—C123	−1.4 (7)	C23—C22—S23—C231	−112.6 (4)
S12—C121—C122—C123	−179.4 (3)	Fe2—C22—S23—C231	160.6 (2)
C121—C122—C123—C124	1.3 (7)	C236—C231—S23—O23	−173.9 (3)
C122—C123—C124—C125	−0.9 (6)	C232—C231—S23—O23	5.4 (4)
C122—C123—C124—C127	178.6 (4)	C236—C231—S23—C22	74.4 (4)
C123—C124—C125—C126	0.6 (6)	C232—C231—S23—C22	−106.2 (4)

1,2,3,4-Tetrakis[(4-methylbenzene)sulfinyl]ferrocene ethyl acetate 0.75-solvate (comp_4)

Crystal data

$[Fe(C_5H_5)(C_{33}H_{29}O_4S_4)]\cdot 0.75C_4H_8O_2$
M_r = 804.82
Monoclinic, $P2_1$
a = 12.8893 (7) Å
b = 8.2225 (4) Å
c = 36.500 (2) Å
β = 97.106 (2)°
V = 3838.6 (4) Å^3
Z = 4
$F(000)$ = 1680
D_x = 1.393 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9909 reflections
θ = 2.7–26.2°
μ = 0.66 mm^{-1}
T = 107 K
Rod, brown
0.07 × 0.02 × 0.02 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.3910 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.811, T_{max} = 0.862
59999 measured reflections
15634 independent reflections
13598 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 26.4°, θ_{min} = 2.2°
h = −16→16
k = −10→10
l = −45→45

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.141
S = 1.12
15634 reflections
936 parameters
77 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 8.7247P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Absolute structure: Flack *x* determined using 4943 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.053 (8)

Special details

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. All crystal structure determinations were performed on a Bruker D8 VENTURE system. Structures were solved by SHELXT (Sheldrick, 2015a) and refined by SHELXL (Sheldrick, 2015b). Structure evaluation was performed with PLATON (Spek, 2020) structure plots were made with ORTEP-3 for Windows and Mercury (Macrae *et al.*, 2020), all as part of the WinGX program suite. CCDC 2330910–2330913 contain the supplementary crystallographic data for **2a**, **2b**, **3a**, **4**.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O302	0.2019 (5)	0.8800 (9)	0.06724 (16)	0.0404 (16)	
O301	0.3328 (8)	1.0441 (10)	0.0871 (3)	0.082 (3)	
C302	0.2893 (7)	0.9172 (12)	0.0894 (3)	0.039 (2)	
C301	0.3220 (7)	0.7888 (12)	0.1170 (3)	0.042 (2)	
H31A	0.394050	0.809118	0.128069	0.063*	
H31B	0.318020	0.682261	0.104850	0.063*	
H31C	0.275572	0.790119	0.136324	0.063*	
C303	0.1616 (9)	1.0037 (15)	0.0410 (3)	0.053 (3)	
H33A	0.218106	1.043681	0.027269	0.064*	
H33B	0.134494	1.096791	0.054169	0.064*	
C304	0.0751 (8)	0.9301 (18)	0.0146 (3)	0.070 (4)	
H34A	0.103034	0.840200	0.001197	0.104*	
H34B	0.045733	1.013067	−0.002940	0.104*	
H34C	0.020113	0.889019	0.028512	0.104*	
C401	0.019 (4)	0.620 (5)	0.4610 (11)	0.122 (14)*	0.5
H41A	0.073944	0.678074	0.450308	0.184*	0.5
H41B	0.044979	0.513789	0.470248	0.184*	0.5
H41C	−0.041286	0.603631	0.442006	0.184*	0.5
C402	−0.014 (4)	0.715 (5)	0.4916 (12)	0.132 (15)*	0.5
C403	−0.030 (3)	0.938 (4)	0.5289 (9)	0.101 (11)*	0.5
H43A	−0.007999	0.870434	0.550955	0.121*	0.5
H43B	−0.106811	0.945374	0.525171	0.121*	0.5
C404	0.019 (11)	1.108 (8)	0.533 (3)	0.48 (11)*	0.5
H44A	−0.003684	1.161578	0.554988	0.716*	0.5
H44B	0.095859	1.098378	0.536910	0.716*	0.5
H44C	−0.002382	1.172886	0.511276	0.716*	0.5
O401	−0.080 (4)	0.619 (7)	0.4992 (17)	0.30 (3)*	0.5
O402	0.009 (3)	0.869 (5)	0.4964 (10)	0.195 (14)*	0.5
C101	0.6785 (6)	0.7154 (8)	0.15101 (19)	0.0170 (15)	
C102	0.7860 (5)	0.7386 (8)	0.14467 (18)	0.0147 (14)	

C103	0.7917 (5)	0.7065 (8)	0.10642 (19)	0.0137 (14)
C104	0.6898 (6)	0.6617 (8)	0.0894 (2)	0.0164 (15)
C105	0.6191 (6)	0.6691 (9)	0.11706 (19)	0.0169 (15)
H105	0.546178	0.647098	0.113320	0.020*
C106	0.6740 (9)	1.1116 (10)	0.1363 (3)	0.048 (2)
H106	0.676195	1.130635	0.162033	0.058*
C107	0.7578 (8)	1.1165 (10)	0.1166 (2)	0.0357 (18)
H107	0.827240	1.141860	0.126978	0.043*
C108	0.7284 (8)	1.0796 (10)	0.0797 (2)	0.036 (2)
H108	0.772492	1.075304	0.060682	0.043*
C109	0.6193 (9)	1.0497 (11)	0.0760 (3)	0.052 (2)
H109	0.576682	1.019493	0.053953	0.062*
C110	0.5843 (9)	1.0736 (12)	0.1119 (4)	0.060 (3)
H110	0.514688	1.065122	0.117771	0.073*
C111	0.5623 (6)	0.5692 (9)	0.19891 (18)	0.0184 (16)
C112	0.4568 (6)	0.5759 (10)	0.2025 (2)	0.0255 (18)
H112	0.420108	0.676118	0.199333	0.031*
C113	0.4053 (6)	0.4366 (10)	0.2105 (2)	0.030 (2)
H113	0.332850	0.441734	0.212936	0.036*
C114	0.4566 (6)	0.2891 (10)	0.2153 (2)	0.0277 (18)
C115	0.5640 (6)	0.2842 (10)	0.2127 (2)	0.0270 (18)
H115	0.601207	0.184750	0.216704	0.032*
C116	0.6164 (6)	0.4242 (9)	0.2042 (2)	0.0237 (17)
H116	0.689038	0.420314	0.202045	0.028*
C117	0.4005 (7)	0.1389 (11)	0.2242 (3)	0.038 (2)
H11A	0.324963	0.159234	0.220905	0.057*
H11B	0.422818	0.107744	0.249918	0.057*
H11C	0.416613	0.050714	0.207783	0.057*
C121	0.8877 (5)	0.6139 (9)	0.20564 (19)	0.0175 (14)
C122	0.9002 (6)	0.4589 (10)	0.1911 (2)	0.0227 (17)
H122	0.908717	0.446872	0.165782	0.027*
C123	0.9003 (6)	0.3230 (9)	0.2134 (2)	0.0208 (16)
H123	0.908866	0.217976	0.203387	0.025*
C124	0.8880 (6)	0.3398 (9)	0.2505 (2)	0.0229 (17)
C125	0.8758 (7)	0.4941 (10)	0.2647 (2)	0.0269 (19)
H125	0.866093	0.506131	0.289974	0.032*
C126	0.8777 (6)	0.6324 (11)	0.2425 (2)	0.0245 (17)
H126	0.872088	0.737845	0.252668	0.029*
C127	0.8859 (8)	0.1917 (11)	0.2746 (3)	0.039 (2)
H12A	0.850430	0.102623	0.260276	0.058*
H12B	0.848268	0.217017	0.295646	0.058*
H12C	0.957674	0.159130	0.283617	0.058*
C131	0.9776 (6)	0.5641 (9)	0.0996 (2)	0.0197 (16)
C132	0.9466 (6)	0.4070 (10)	0.0901 (2)	0.0241 (17)
H132	0.885212	0.387619	0.073402	0.029*
C133	1.0065 (7)	0.2791 (10)	0.1052 (2)	0.0304 (19)
H133	0.986432	0.171149	0.098372	0.036*
C134	1.0954 (7)	0.3038 (10)	0.1303 (3)	0.034 (2)

C135	1.1247 (7)	0.4620 (11)	0.1387 (3)	0.036 (2)
H135	1.185795	0.481630	0.155551	0.043*
C136	1.0668 (6)	0.5942 (10)	0.1232 (2)	0.0251 (17)
H136	1.088703	0.702586	0.128963	0.030*
C137	1.1523 (8)	0.1629 (12)	0.1493 (3)	0.055 (3)
H13A	1.118087	0.061268	0.140591	0.082*
H13B	1.151337	0.172696	0.176051	0.082*
H13C	1.224881	0.162491	0.143867	0.082*
C141	0.5258 (6)	0.5780 (9)	0.03975 (19)	0.0201 (16)
C142	0.4546 (6)	0.6859 (10)	0.0215 (2)	0.0278 (18)
H142	0.478353	0.782038	0.010764	0.033*
C143	0.3488 (7)	0.6527 (12)	0.0191 (2)	0.033 (2)
H143	0.300445	0.728624	0.007112	0.039*
C144	0.3112 (7)	0.5114 (11)	0.0337 (2)	0.0298 (19)
C145	0.3859 (6)	0.4020 (10)	0.0516 (2)	0.0291 (18)
H145	0.362839	0.304189	0.061867	0.035*
C146	0.4922 (6)	0.4354 (9)	0.0545 (2)	0.0224 (17)
H146	0.541403	0.360830	0.066588	0.027*
C147	0.1990 (8)	0.4707 (14)	0.0302 (3)	0.053 (3)
H14A	0.157576	0.570024	0.025253	0.079*
H14B	0.182573	0.421036	0.053162	0.079*
H14C	0.182263	0.394032	0.009727	0.079*
O101	0.5471 (4)	0.8825 (7)	0.18655 (16)	0.0320 (13)
O102	0.8646 (5)	0.9309 (6)	0.19989 (15)	0.0297 (13)
O103	0.9574 (4)	0.8810 (7)	0.09473 (16)	0.0276 (12)
O104	0.7156 (5)	0.4602 (8)	0.03656 (16)	0.0355 (15)
S101	0.63028 (15)	0.7577 (2)	0.19392 (5)	0.0228 (4)
S102	0.89479 (15)	0.7922 (2)	0.17760 (5)	0.0206 (4)
S103	0.90017 (14)	0.7324 (2)	0.08063 (5)	0.0190 (4)
S104	0.66225 (15)	0.6178 (3)	0.04131 (5)	0.0231 (4)
Fe1	0.69263 (8)	0.88908 (13)	0.11238 (3)	0.0196 (2)
C201	0.3745 (6)	0.3500 (8)	0.4237 (2)	0.0182 (15)
C202	0.4148 (6)	0.2993 (8)	0.3905 (2)	0.0175 (15)
C203	0.3270 (6)	0.2731 (9)	0.36286 (19)	0.0191 (15)
C204	0.2339 (6)	0.3009 (9)	0.3793 (2)	0.0229 (17)
C205	0.2620 (6)	0.3500 (8)	0.4165 (2)	0.0170 (15)
H205	0.215040	0.377873	0.433633	0.020*
C206	0.3394 (8)	−0.1137 (11)	0.3920 (3)	0.042 (2)
H206	0.355231	−0.152206	0.368798	0.050*
C207	0.2399 (8)	−0.0883 (10)	0.4019 (3)	0.043 (2)
H207	0.175703	−0.105685	0.386607	0.052*
C208	0.2511 (8)	−0.0320 (11)	0.4388 (3)	0.037 (2)
H208	0.195430	−0.004158	0.452395	0.045*
C209	0.3570 (8)	−0.0240 (10)	0.4519 (2)	0.034 (2)
H209	0.387117	0.007772	0.475917	0.041*
C210	0.4114 (7)	−0.0731 (10)	0.4219 (2)	0.033 (2)
H210	0.485183	−0.077261	0.422473	0.039*
C211	0.3660 (6)	0.4463 (9)	0.4945 (2)	0.0226 (17)

C212	0.3400 (7)	0.3503 (11)	0.5225 (2)	0.038 (2)
H212	0.363088	0.240605	0.524826	0.045*
C213	0.2789 (8)	0.4169 (15)	0.5477 (3)	0.053 (3)
H213	0.259883	0.350910	0.567165	0.064*
C214	0.2449 (8)	0.5790 (14)	0.5450 (3)	0.044 (3)
C215	0.2722 (8)	0.6676 (11)	0.5163 (3)	0.043 (2)
H215	0.248836	0.777076	0.513905	0.051*
C216	0.3316 (7)	0.6080 (10)	0.4906 (2)	0.0322 (19)
H216	0.348872	0.673973	0.470908	0.039*
C217	0.1813 (9)	0.6507 (19)	0.5726 (3)	0.072 (4)
H21A	0.164808	0.764253	0.566084	0.108*
H21B	0.221131	0.645999	0.597236	0.108*
H21C	0.116247	0.588928	0.572498	0.108*
C221	0.5747 (5)	0.4392 (9)	0.3607 (2)	0.0174 (15)
C222	0.5648 (6)	0.5958 (9)	0.3742 (2)	0.0184 (16)
H222	0.549024	0.612267	0.398659	0.022*
C223	0.5781 (6)	0.7284 (9)	0.3515 (2)	0.0238 (17)
H223	0.570910	0.835536	0.360606	0.029*
C224	0.6020 (6)	0.7056 (10)	0.3156 (2)	0.0217 (16)
C225	0.6153 (7)	0.5481 (11)	0.3034 (2)	0.0301 (19)
H225	0.634158	0.531351	0.279364	0.036*
C226	0.6018 (6)	0.4150 (10)	0.3255 (2)	0.0245 (17)
H226	0.610885	0.308029	0.316567	0.029*
C227	0.6101 (8)	0.8468 (11)	0.2903 (2)	0.035 (2)
H22A	0.550007	0.846661	0.270979	0.052*
H22B	0.674810	0.837783	0.278828	0.052*
H22C	0.610914	0.948323	0.304338	0.052*
C231	0.2836 (6)	0.3862 (10)	0.29424 (19)	0.0213 (15)
C232	0.3325 (6)	0.5376 (9)	0.3003 (2)	0.0210 (16)
H232	0.393805	0.546765	0.317552	0.025*
C233	0.2921 (6)	0.6729 (9)	0.2816 (2)	0.0241 (17)
H233	0.326192	0.774844	0.285798	0.029*
C234	0.2023 (6)	0.6621 (9)	0.2566 (2)	0.0223 (17)
C235	0.1552 (6)	0.5128 (9)	0.2506 (2)	0.0213 (16)
H235	0.094025	0.504442	0.233252	0.026*
C236	0.1943 (6)	0.3741 (10)	0.2690 (2)	0.0238 (16)
H236	0.160336	0.272239	0.264440	0.029*
C237	0.1561 (7)	0.8133 (10)	0.2355 (3)	0.035 (2)
H23A	0.139064	0.786503	0.209259	0.053*
H23B	0.207381	0.901845	0.238207	0.053*
H23C	0.092486	0.847602	0.245520	0.053*
C241	0.0439 (6)	0.4509 (9)	0.3576 (2)	0.0245 (17)
C242	0.0849 (6)	0.5880 (9)	0.3426 (2)	0.0233 (17)
H242	0.152781	0.584398	0.335017	0.028*
C243	0.0276 (6)	0.7291 (10)	0.3387 (2)	0.0265 (17)
H243	0.055685	0.822251	0.328084	0.032*
C244	−0.0712 (6)	0.7366 (10)	0.3501 (2)	0.0261 (17)
C245	−0.1111 (6)	0.6008 (10)	0.3655 (2)	0.0296 (19)

H245	−0.178254	0.605451	0.373562	0.035*
C246	−0.0541 (7)	0.4571 (10)	0.3692 (2)	0.0295 (19)
H246	−0.082224	0.363761	0.379709	0.035*
C247	−0.1350 (7)	0.8923 (12)	0.3456 (3)	0.041 (2)
H24A	−0.155199	0.913946	0.319305	0.061*
H24B	−0.092931	0.983100	0.356717	0.061*
H24C	−0.197887	0.880348	0.357953	0.061*
O201	0.5249 (5)	0.5209 (7)	0.45890 (15)	0.0303 (14)
O202	0.5658 (4)	0.1217 (7)	0.36649 (15)	0.0286 (13)
O203	0.2665 (5)	0.0724 (7)	0.30660 (16)	0.0333 (14)
O204	0.0520 (5)	0.1572 (7)	0.3851 (2)	0.0505 (19)
S201	0.45882 (14)	0.3781 (2)	0.46578 (5)	0.0211 (4)
S202	0.55233 (14)	0.2685 (2)	0.38916 (5)	0.0209 (4)
S203	0.34028 (16)	0.2077 (2)	0.31656 (5)	0.0240 (4)
S204	0.10400 (16)	0.2534 (3)	0.35781 (6)	0.0308 (5)
Fe2	0.32104 (9)	0.12531 (13)	0.40688 (3)	0.0220 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O302	0.032 (3)	0.058 (4)	0.031 (3)	0.011 (3)	0.006 (3)	0.018 (3)
O301	0.114 (8)	0.043 (5)	0.083 (6)	−0.027 (5)	−0.015 (6)	0.028 (5)
C302	0.031 (5)	0.045 (6)	0.043 (5)	−0.001 (4)	0.009 (4)	0.007 (5)
C301	0.038 (5)	0.041 (6)	0.048 (6)	0.002 (4)	0.004 (4)	0.010 (5)
C303	0.059 (7)	0.068 (7)	0.035 (6)	0.025 (6)	0.017 (5)	0.020 (5)
C304	0.030 (5)	0.133 (13)	0.047 (6)	0.005 (7)	0.006 (5)	0.045 (7)
C101	0.020 (4)	0.013 (4)	0.017 (4)	0.001 (3)	0.000 (3)	−0.003 (3)
C102	0.015 (3)	0.010 (3)	0.019 (3)	−0.004 (3)	0.004 (3)	−0.005 (3)
C103	0.018 (3)	0.007 (3)	0.018 (4)	0.000 (3)	0.007 (3)	0.003 (3)
C104	0.022 (4)	0.009 (3)	0.019 (4)	0.002 (3)	0.006 (3)	0.001 (3)
C105	0.012 (3)	0.022 (4)	0.017 (4)	−0.002 (3)	0.002 (3)	−0.002 (3)
C106	0.087 (6)	0.009 (4)	0.057 (5)	0.006 (5)	0.043 (4)	0.000 (4)
C107	0.056 (5)	0.010 (4)	0.043 (4)	−0.012 (4)	0.011 (4)	0.005 (4)
C108	0.058 (5)	0.018 (4)	0.034 (4)	0.001 (4)	0.019 (4)	0.011 (4)
C109	0.060 (5)	0.016 (4)	0.073 (6)	0.007 (4)	−0.021 (5)	0.019 (5)
C110	0.043 (5)	0.023 (5)	0.123 (8)	0.014 (4)	0.041 (5)	0.035 (6)
C111	0.022 (4)	0.028 (4)	0.006 (3)	−0.001 (3)	0.007 (3)	0.000 (3)
C112	0.027 (4)	0.024 (4)	0.026 (4)	0.009 (3)	0.005 (3)	0.012 (3)
C113	0.021 (4)	0.034 (5)	0.037 (5)	0.006 (3)	0.013 (4)	0.009 (4)
C114	0.031 (4)	0.029 (4)	0.025 (4)	−0.003 (4)	0.013 (3)	0.001 (4)
C115	0.028 (4)	0.027 (4)	0.028 (4)	0.004 (4)	0.012 (3)	−0.002 (4)
C116	0.021 (4)	0.024 (4)	0.028 (4)	0.001 (3)	0.010 (3)	−0.002 (3)
C117	0.047 (5)	0.020 (4)	0.052 (6)	−0.008 (4)	0.033 (5)	−0.003 (4)
C121	0.019 (4)	0.012 (3)	0.021 (4)	−0.005 (3)	0.001 (3)	0.002 (3)
C122	0.018 (4)	0.028 (4)	0.023 (4)	−0.010 (3)	0.005 (3)	−0.008 (3)
C123	0.016 (4)	0.021 (4)	0.025 (4)	−0.003 (3)	0.000 (3)	−0.005 (3)
C124	0.018 (4)	0.019 (4)	0.030 (4)	−0.003 (3)	−0.001 (3)	0.002 (3)
C125	0.034 (5)	0.031 (5)	0.015 (4)	−0.004 (4)	0.000 (3)	−0.008 (3)

C126	0.021 (4)	0.025 (4)	0.028 (4)	−0.002 (3)	0.006 (3)	−0.006 (4)
C127	0.052 (6)	0.033 (5)	0.031 (5)	−0.001 (4)	0.005 (4)	0.005 (4)
C131	0.015 (4)	0.018 (4)	0.029 (4)	−0.007 (3)	0.012 (3)	−0.004 (3)
C132	0.025 (4)	0.019 (4)	0.029 (4)	−0.002 (3)	0.006 (3)	−0.005 (3)
C133	0.035 (5)	0.015 (4)	0.043 (5)	−0.003 (4)	0.011 (4)	−0.002 (4)
C134	0.033 (5)	0.026 (5)	0.045 (5)	0.012 (4)	0.015 (4)	0.006 (4)
C135	0.017 (4)	0.036 (5)	0.052 (6)	−0.005 (4)	−0.001 (4)	0.004 (4)
C136	0.018 (4)	0.020 (4)	0.039 (5)	−0.002 (3)	0.010 (3)	−0.002 (3)
C137	0.044 (6)	0.035 (6)	0.083 (9)	0.016 (5)	0.002 (6)	0.009 (6)
C141	0.024 (4)	0.024 (4)	0.011 (3)	−0.007 (3)	−0.001 (3)	−0.006 (3)
C142	0.030 (4)	0.032 (5)	0.022 (4)	−0.002 (4)	0.004 (3)	0.003 (3)
C143	0.027 (4)	0.046 (6)	0.023 (4)	0.003 (4)	−0.006 (3)	0.009 (4)
C144	0.028 (5)	0.037 (5)	0.023 (4)	0.000 (4)	0.001 (4)	−0.004 (4)
C145	0.034 (4)	0.021 (4)	0.034 (4)	−0.006 (4)	0.009 (4)	0.000 (4)
C146	0.030 (4)	0.018 (4)	0.018 (4)	0.002 (3)	0.000 (3)	0.000 (3)
C147	0.036 (6)	0.055 (7)	0.068 (8)	−0.013 (5)	0.004 (5)	−0.007 (6)
O101	0.039 (3)	0.021 (3)	0.041 (3)	0.003 (3)	0.024 (3)	−0.004 (3)
O102	0.044 (4)	0.018 (3)	0.027 (3)	−0.004 (2)	0.001 (3)	−0.007 (2)
O103	0.032 (3)	0.010 (2)	0.043 (3)	−0.007 (2)	0.012 (3)	−0.001 (3)
O104	0.035 (3)	0.046 (4)	0.027 (3)	0.006 (3)	0.007 (3)	−0.019 (3)
S101	0.0270 (10)	0.0240 (10)	0.0192 (9)	−0.0033 (8)	0.0100 (8)	−0.0061 (8)
S102	0.0235 (10)	0.0153 (9)	0.0226 (9)	−0.0061 (7)	0.0012 (8)	−0.0026 (8)
S103	0.0193 (9)	0.0150 (9)	0.0246 (9)	−0.0006 (7)	0.0103 (7)	0.0003 (7)
S104	0.0245 (10)	0.0300 (10)	0.0153 (9)	−0.0031 (9)	0.0048 (7)	−0.0017 (8)
Fe1	0.0217 (5)	0.0145 (5)	0.0234 (6)	0.0014 (5)	0.0063 (4)	0.0003 (5)
C201	0.021 (4)	0.007 (3)	0.025 (4)	0.001 (3)	−0.001 (3)	0.001 (3)
C202	0.025 (4)	0.007 (3)	0.021 (4)	−0.005 (3)	0.002 (3)	0.000 (3)
C203	0.029 (4)	0.009 (3)	0.019 (4)	0.002 (3)	−0.003 (3)	0.001 (3)
C204	0.031 (4)	0.016 (4)	0.019 (4)	0.004 (3)	−0.006 (3)	0.006 (3)
C205	0.022 (4)	0.011 (3)	0.017 (4)	0.001 (3)	0.002 (3)	−0.002 (3)
C206	0.071 (7)	0.011 (4)	0.042 (5)	0.003 (5)	0.002 (5)	−0.001 (4)
C207	0.053 (6)	0.012 (4)	0.059 (7)	−0.008 (4)	−0.013 (5)	0.011 (4)
C208	0.046 (6)	0.025 (5)	0.043 (6)	0.002 (4)	0.012 (5)	0.017 (4)
C209	0.060 (6)	0.013 (4)	0.027 (5)	−0.003 (4)	−0.003 (4)	0.012 (3)
C210	0.042 (5)	0.016 (4)	0.038 (5)	0.002 (4)	−0.001 (4)	0.009 (4)
C211	0.031 (4)	0.020 (4)	0.016 (4)	−0.003 (3)	0.000 (3)	0.000 (3)
C212	0.044 (5)	0.033 (5)	0.037 (5)	0.009 (4)	0.008 (4)	0.013 (4)
C213	0.055 (6)	0.079 (8)	0.030 (5)	0.027 (6)	0.023 (5)	0.027 (5)
C214	0.038 (5)	0.068 (8)	0.028 (5)	0.012 (5)	0.010 (4)	−0.002 (5)
C215	0.048 (6)	0.032 (5)	0.049 (6)	0.014 (4)	0.014 (5)	−0.004 (4)
C216	0.053 (6)	0.021 (4)	0.023 (4)	0.007 (4)	0.008 (4)	−0.002 (4)
C217	0.064 (8)	0.114 (11)	0.043 (6)	0.043 (8)	0.026 (6)	0.014 (7)
C221	0.012 (3)	0.017 (4)	0.022 (4)	0.006 (3)	0.001 (3)	0.002 (3)
C222	0.022 (4)	0.017 (4)	0.016 (3)	−0.001 (3)	0.001 (3)	−0.002 (3)
C223	0.027 (4)	0.016 (4)	0.029 (4)	−0.001 (3)	0.006 (3)	−0.001 (3)
C224	0.021 (4)	0.026 (4)	0.018 (4)	0.002 (3)	0.001 (3)	−0.001 (3)
C225	0.032 (5)	0.034 (5)	0.026 (4)	0.006 (4)	0.009 (4)	−0.003 (4)
C226	0.027 (4)	0.023 (4)	0.024 (4)	0.009 (3)	0.007 (3)	−0.003 (3)

C227	0.052 (6)	0.028 (5)	0.025 (4)	−0.003 (4)	0.006 (4)	0.007 (4)
C231	0.032 (4)	0.016 (4)	0.014 (3)	0.003 (3)	−0.001 (3)	−0.002 (3)
C232	0.024 (4)	0.022 (4)	0.017 (4)	−0.003 (3)	0.003 (3)	−0.002 (3)
C233	0.024 (4)	0.019 (4)	0.029 (4)	−0.002 (3)	0.003 (3)	0.001 (3)
C234	0.020 (4)	0.021 (4)	0.025 (4)	0.003 (3)	0.002 (3)	0.005 (3)
C235	0.014 (4)	0.022 (4)	0.027 (4)	0.001 (3)	−0.002 (3)	0.006 (3)
C236	0.029 (4)	0.022 (4)	0.020 (4)	−0.003 (4)	0.005 (3)	−0.003 (3)
C237	0.035 (5)	0.025 (5)	0.043 (5)	−0.004 (4)	−0.008 (4)	0.010 (4)
C241	0.031 (4)	0.019 (4)	0.023 (4)	−0.001 (3)	0.000 (3)	−0.001 (3)
C242	0.019 (4)	0.024 (4)	0.026 (4)	0.002 (3)	0.002 (3)	0.001 (3)
C243	0.036 (5)	0.023 (4)	0.021 (4)	−0.007 (3)	0.003 (3)	−0.002 (3)
C244	0.023 (4)	0.029 (4)	0.025 (4)	−0.004 (3)	−0.004 (3)	−0.007 (4)
C245	0.028 (4)	0.032 (5)	0.030 (4)	−0.005 (4)	0.009 (3)	−0.003 (4)
C246	0.036 (5)	0.030 (5)	0.021 (4)	−0.008 (4)	0.001 (4)	0.007 (4)
C247	0.035 (5)	0.032 (5)	0.054 (6)	0.002 (4)	0.005 (4)	−0.003 (5)
O201	0.032 (3)	0.036 (3)	0.022 (3)	−0.011 (3)	0.001 (2)	−0.009 (3)
O202	0.040 (3)	0.016 (3)	0.031 (3)	0.010 (3)	0.008 (3)	−0.006 (3)
O203	0.053 (4)	0.016 (3)	0.027 (3)	−0.006 (3)	−0.008 (3)	−0.002 (2)
O204	0.029 (3)	0.023 (3)	0.097 (6)	−0.008 (3)	−0.004 (4)	0.021 (4)
S201	0.0252 (10)	0.0204 (9)	0.0170 (9)	0.0001 (8)	−0.0010 (7)	−0.0017 (8)
S202	0.0230 (9)	0.0148 (9)	0.0237 (9)	0.0038 (7)	−0.0015 (7)	−0.0009 (8)
S203	0.0346 (11)	0.0166 (9)	0.0191 (9)	0.0029 (8)	−0.0038 (8)	−0.0023 (8)
S204	0.0273 (11)	0.0228 (10)	0.0386 (12)	−0.0024 (9)	−0.0102 (9)	−0.0015 (9)
Fe2	0.0293 (6)	0.0141 (5)	0.0213 (5)	−0.0021 (5)	−0.0022 (5)	0.0004 (5)

Geometric parameters (Å, º)

O302—C302	1.338 (11)	C143—H143	0.9500
O302—C303	1.448 (11)	C144—C145	1.417 (12)
O301—C302	1.192 (12)	C144—C147	1.475 (12)
C302—C301	1.485 (13)	C145—C146	1.388 (11)
C301—H31A	0.9800	C145—H145	0.9500
C301—H31B	0.9800	C146—H146	0.9500
C301—H31C	0.9800	C147—H14A	0.9800
C303—C304	1.508 (16)	C147—H14B	0.9800
C303—H33A	0.9900	C147—H14C	0.9800
C303—H33B	0.9900	O101—S101	1.485 (6)
C304—H34A	0.9800	O102—S102	1.481 (6)
C304—H34B	0.9800	O103—S103	1.486 (6)
C304—H34C	0.9800	O104—S104	1.487 (6)
C401—C402	1.47 (3)	C201—C202	1.438 (10)
C401—H41A	0.9800	C201—C205	1.441 (10)
C401—H41B	0.9800	C201—S201	1.784 (8)
C401—H41C	0.9800	C201—Fe2	2.039 (7)
C402—O401	1.21 (3)	C202—C203	1.435 (10)
C402—O402	1.30 (3)	C202—S202	1.797 (8)
C403—O402	1.46 (3)	C202—Fe2	2.011 (7)
C403—C404	1.54 (3)	C203—C204	1.426 (11)

C403—H43A	0.9900	C203—S203	1.802 (7)
C403—H43B	0.9900	C203—Fe2	2.023 (7)
C404—H44A	0.9800	C204—C205	1.421 (10)
C404—H44B	0.9800	C204—S204	1.801 (8)
C404—H44C	0.9800	C204—Fe2	2.020 (7)
C101—C105	1.426 (10)	C205—Fe2	2.045 (7)
C101—C102	1.445 (9)	C205—H205	0.9500
C101—S101	1.789 (7)	C206—C210	1.383 (13)
C101—Fe1	2.031 (7)	C206—C207	1.391 (14)
C102—C103	1.432 (9)	C206—Fe2	2.060 (9)
C102—S102	1.786 (7)	C206—H206	0.9500
C102—Fe1	2.004 (7)	C207—C208	1.414 (14)
C103—C104	1.429 (10)	C207—Fe2	2.041 (9)
C103—S103	1.792 (7)	C207—H207	0.9500
C103—Fe1	2.000 (7)	C208—C209	1.391 (13)
C104—C105	1.441 (9)	C208—Fe2	2.025 (8)
C104—S104	1.786 (7)	C208—H208	0.9500
C104—Fe1	2.047 (7)	C209—C210	1.428 (13)
C105—Fe1	2.059 (7)	C209—Fe2	2.058 (8)
C105—H105	0.9500	C209—H209	0.9500
C106—C107	1.369 (13)	C210—Fe2	2.040 (8)
C106—C110	1.404 (17)	C210—H210	0.9500
C106—Fe1	2.054 (9)	C211—C212	1.366 (11)
C106—H106	0.9500	C211—C216	1.403 (11)
C107—C108	1.389 (13)	C211—S201	1.777 (8)
C107—Fe1	2.048 (8)	C212—C213	1.394 (13)
C107—H107	0.9500	C212—H212	0.9500
C108—C109	1.417 (14)	C213—C214	1.402 (15)
C108—Fe1	2.056 (8)	C213—H213	0.9500
C108—H108	0.9500	C214—C215	1.357 (13)
C109—C110	1.452 (17)	C214—C217	1.496 (13)
C109—Fe1	2.022 (9)	C215—C216	1.372 (12)
C109—H109	0.9500	C215—H215	0.9500
C110—Fe1	2.060 (9)	C216—H216	0.9500
C110—H110	0.9500	C217—H21A	0.9800
C111—C116	1.382 (11)	C217—H21B	0.9800
C111—C112	1.384 (11)	C217—H21C	0.9800
C111—S101	1.801 (8)	C221—C226	1.389 (10)
C112—C113	1.374 (11)	C221—C222	1.390 (10)
C112—H112	0.9500	C221—S202	1.790 (7)
C113—C114	1.381 (11)	C222—C223	1.392 (10)
C113—H113	0.9500	C222—H222	0.9500
C114—C115	1.400 (11)	C223—C224	1.396 (10)
C114—C117	1.488 (11)	C223—H223	0.9500
C115—C116	1.388 (11)	C224—C225	1.387 (11)
C115—H115	0.9500	C224—C227	1.496 (11)
C116—H116	0.9500	C225—C226	1.382 (12)
C117—H11A	0.9800	C225—H225	0.9500

C117—H11B	0.9800	C226—H226	0.9500
C117—H11C	0.9800	C227—H22A	0.9800
C121—C126	1.374 (10)	C227—H22B	0.9800
C121—C122	1.397 (11)	C227—H22C	0.9800
C121—S102	1.796 (7)	C231—C236	1.386 (10)
C122—C123	1.383 (11)	C231—C232	1.400 (11)
C122—H122	0.9500	C231—S203	1.790 (8)
C123—C124	1.388 (11)	C232—C233	1.374 (11)
C123—H123	0.9500	C232—H232	0.9500
C124—C125	1.388 (11)	C233—C234	1.384 (11)
C124—C127	1.504 (11)	C233—H233	0.9500
C125—C126	1.400 (12)	C234—C235	1.376 (11)
C125—H125	0.9500	C234—C237	1.544 (11)
C126—H126	0.9500	C235—C236	1.387 (11)
C127—H12A	0.9800	C235—H235	0.9500
C127—H12B	0.9800	C236—H236	0.9500
C127—H12C	0.9800	C237—H23A	0.9800
C131—C136	1.372 (11)	C237—H23B	0.9800
C131—C132	1.383 (10)	C237—H23C	0.9800
C131—S103	1.795 (8)	C241—C246	1.382 (12)
C132—C133	1.380 (11)	C241—C242	1.386 (11)
C132—H132	0.9500	C241—S204	1.799 (8)
C133—C134	1.389 (13)	C242—C243	1.373 (11)
C133—H133	0.9500	C242—H242	0.9500
C134—C135	1.379 (12)	C243—C244	1.389 (11)
C134—C137	1.496 (12)	C243—H243	0.9500
C135—C136	1.398 (12)	C244—C245	1.377 (11)
C135—H135	0.9500	C244—C247	1.519 (12)
C136—H136	0.9500	C245—C246	1.389 (12)
C137—H13A	0.9800	C245—H245	0.9500
C137—H13B	0.9800	C246—H246	0.9500
C137—H13C	0.9800	C247—H24A	0.9800
C141—C146	1.383 (10)	C247—H24B	0.9800
C141—C142	1.386 (11)	C247—H24C	0.9800
C141—S104	1.783 (8)	O201—S201	1.489 (6)
C142—C143	1.383 (11)	O202—S202	1.486 (6)
C142—H142	0.9500	O203—S203	1.480 (6)
C143—C144	1.390 (12)	O204—S204	1.493 (7)

C302—O302—C303	116.4 (8)	C109—Fe1—C108	40.7 (4)
O301—C302—O302	121.7 (10)	C101—Fe1—C108	169.9 (4)
O301—C302—C301	125.0 (10)	C104—Fe1—C108	116.9 (3)
O302—C302—C301	113.2 (8)	C107—Fe1—C108	39.6 (4)
C302—C301—H31A	109.5	C106—Fe1—C108	67.3 (4)
C302—C301—H31B	109.5	C103—Fe1—C105	69.9 (3)
H31A—C301—H31B	109.5	C102—Fe1—C105	70.0 (3)
C302—C301—H31C	109.5	C109—Fe1—C105	116.5 (4)
H31A—C301—H31C	109.5	C101—Fe1—C105	40.8 (3)

H31B—C301—H31C	109.5	C104—Fe1—C105	41.1 (3)
O302—C303—C304	108.5 (10)	C107—Fe1—C105	169.9 (3)
O302—C303—H33A	110.0	C106—Fe1—C105	131.9 (3)
C304—C303—H33A	110.0	C108—Fe1—C105	148.9 (3)
O302—C303—H33B	110.0	C103—Fe1—C110	173.2 (5)
C304—C303—H33B	110.0	C102—Fe1—C110	144.7 (4)
H33A—C303—H33B	108.4	C109—Fe1—C110	41.6 (5)
C303—C304—H34A	109.5	C101—Fe1—C110	113.9 (4)
C303—C304—H34B	109.5	C104—Fe1—C110	133.7 (4)
H34A—C304—H34B	109.5	C107—Fe1—C110	66.4 (4)
C303—C304—H34C	109.5	C106—Fe1—C110	39.9 (5)
H34A—C304—H34C	109.5	C108—Fe1—C110	68.6 (4)
H34B—C304—H34C	109.5	C105—Fe1—C110	109.2 (4)
C402—C401—H41A	109.5	C202—C201—C205	107.9 (6)
C402—C401—H41B	109.5	C202—C201—S201	121.3 (5)
H41A—C401—H41B	109.5	C205—C201—S201	130.4 (6)
C402—C401—H41C	109.5	C202—C201—Fe2	68.1 (4)
H41A—C401—H41C	109.5	C205—C201—Fe2	69.6 (4)
H41B—C401—H41C	109.5	S201—C201—Fe2	121.6 (4)
O401—C402—O402	139 (5)	C203—C202—C201	107.5 (6)
O401—C402—C401	96 (5)	C203—C202—S202	130.9 (6)
O402—C402—C401	122 (4)	C201—C202—S202	121.5 (5)
O402—C403—C404	105 (3)	C203—C202—Fe2	69.6 (4)
O402—C403—H43A	110.6	C201—C202—Fe2	70.3 (4)
C404—C403—H43A	110.6	S202—C202—Fe2	122.6 (4)
O402—C403—H43B	110.6	C204—C203—C202	108.2 (6)
C404—C403—H43B	110.6	C204—C203—S203	128.7 (6)
H43A—C403—H43B	108.8	C202—C203—S203	123.1 (6)
C403—C404—H44A	109.5	C204—C203—Fe2	69.2 (4)
C403—C404—H44B	109.5	C202—C203—Fe2	68.7 (4)
H44A—C404—H44B	109.5	S203—C203—Fe2	125.7 (4)
C403—C404—H44C	109.5	C205—C204—C203	108.6 (7)
H44A—C404—H44C	109.5	C205—C204—S204	126.2 (6)
H44B—C404—H44C	109.5	C203—C204—S204	124.6 (6)
C402—O402—C403	113 (4)	C205—C204—Fe2	70.5 (4)
C105—C101—C102	108.6 (6)	C203—C204—Fe2	69.5 (4)
C105—C101—S101	127.2 (5)	S204—C204—Fe2	119.4 (4)
C102—C101—S101	123.9 (5)	C204—C205—C201	107.8 (6)
C105—C101—Fe1	70.7 (4)	C204—C205—Fe2	68.6 (4)
C102—C101—Fe1	68.0 (4)	C201—C205—Fe2	69.1 (4)
S101—C101—Fe1	122.8 (4)	C204—C205—H205	126.1
C103—C102—C101	107.4 (6)	C201—C205—H205	126.1
C103—C102—S102	124.8 (5)	Fe2—C205—H205	127.7
C101—C102—S102	127.8 (5)	C210—C206—C207	108.0 (9)
C103—C102—Fe1	68.9 (4)	C210—C206—Fe2	69.5 (5)
C101—C102—Fe1	70.0 (4)	C207—C206—Fe2	69.4 (5)
S102—C102—Fe1	127.4 (4)	C210—C206—H206	126.0
C104—C103—C102	108.3 (6)	C207—C206—H206	126.0

C104—C103—S103	122.5 (5)	Fe2—C206—H206	126.6
C102—C103—S103	128.9 (5)	C206—C207—C208	107.9 (9)
C104—C103—Fe1	71.1 (4)	C206—C207—Fe2	70.9 (5)
C102—C103—Fe1	69.2 (4)	C208—C207—Fe2	69.1 (5)
S103—C103—Fe1	121.2 (3)	C206—C207—H207	126.1
C103—C104—C105	108.2 (6)	C208—C207—H207	126.1
C103—C104—S104	122.6 (5)	Fe2—C207—H207	125.5
C105—C104—S104	129.1 (6)	C209—C208—C207	108.9 (9)
C103—C104—Fe1	67.6 (4)	C209—C208—Fe2	71.3 (5)
C105—C104—Fe1	69.9 (4)	C207—C208—Fe2	70.3 (5)
S104—C104—Fe1	125.3 (4)	C209—C208—H208	125.6
C101—C105—C104	107.5 (6)	C207—C208—H208	125.6
C101—C105—Fe1	68.5 (4)	Fe2—C208—H208	124.4
C104—C105—Fe1	69.0 (4)	C208—C209—C210	106.0 (8)
C101—C105—H105	126.2	C208—C209—Fe2	68.8 (5)
C104—C105—H105	126.2	C210—C209—Fe2	68.9 (5)
Fe1—C105—H105	127.8	C208—C209—H209	127.0
C107—C106—C110	108.5 (9)	C210—C209—H209	127.0
C107—C106—Fe1	70.3 (5)	Fe2—C209—H209	126.8
C110—C106—Fe1	70.3 (6)	C206—C210—C209	109.2 (9)
C107—C106—H106	125.8	C206—C210—Fe2	71.1 (5)
C110—C106—H106	125.8	C209—C210—Fe2	70.3 (5)
Fe1—C106—H106	125.2	C206—C210—H210	125.4
C106—C107—C108	111.3 (9)	C209—C210—H210	125.4
C106—C107—Fe1	70.7 (5)	Fe2—C210—H210	124.8
C108—C107—Fe1	70.5 (5)	C212—C211—C216	121.3 (8)
C106—C107—H107	124.3	C212—C211—S201	120.3 (6)
C108—C107—H107	124.3	C216—C211—S201	117.8 (6)
Fe1—C107—H107	126.0	C211—C212—C213	118.5 (9)
C107—C108—C109	106.2 (9)	C211—C212—H212	120.8
C107—C108—Fe1	69.9 (5)	C213—C212—H212	120.8
C109—C108—Fe1	68.4 (5)	C212—C213—C214	121.6 (9)
C107—C108—H108	126.9	C212—C213—H213	119.2
C109—C108—H108	126.9	C214—C213—H213	119.2
Fe1—C108—H108	126.3	C215—C214—C213	117.1 (8)
C108—C109—C110	107.9 (10)	C215—C214—C217	121.5 (10)
C108—C109—Fe1	71.0 (5)	C213—C214—C217	121.4 (10)
C110—C109—Fe1	70.6 (6)	C214—C215—C216	123.7 (9)
C108—C109—H109	126.1	C214—C215—H215	118.1
C110—C109—H109	126.1	C216—C215—H215	118.1
Fe1—C109—H109	124.0	C215—C216—C211	117.7 (8)
C106—C110—C109	106.1 (9)	C215—C216—H216	121.1
C106—C110—Fe1	69.8 (5)	C211—C216—H216	121.1
C109—C110—Fe1	67.8 (5)	C214—C217—H21A	109.5
C106—C110—H110	126.9	C214—C217—H21B	109.5
C109—C110—H110	126.9	H21A—C217—H21B	109.5
Fe1—C110—H110	127.0	C214—C217—H21C	109.5
C116—C111—C112	120.4 (7)	H21A—C217—H21C	109.5

C116—C111—S101	120.9 (6)	H21B—C217—H21C	109.5
C112—C111—S101	118.1 (6)	C226—C221—C222	120.3 (7)
C113—C112—C111	119.5 (7)	C226—C221—S202	120.1 (6)
C113—C112—H112	120.2	C222—C221—S202	119.5 (6)
C111—C112—H112	120.2	C221—C222—C223	119.5 (7)
C112—C113—C114	121.5 (7)	C221—C222—H222	120.3
C112—C113—H113	119.2	C223—C222—H222	120.3
C114—C113—H113	119.2	C222—C223—C224	120.7 (7)
C113—C114—C115	118.6 (7)	C222—C223—H223	119.6
C113—C114—C117	121.2 (7)	C224—C223—H223	119.6
C115—C114—C117	120.2 (8)	C225—C224—C223	118.5 (7)
C116—C115—C114	120.2 (7)	C225—C224—C227	120.3 (7)
C116—C115—H115	119.9	C223—C224—C227	121.2 (7)
C114—C115—H115	119.9	C226—C225—C224	121.6 (7)
C111—C116—C115	119.7 (7)	C226—C225—H225	119.2
C111—C116—H116	120.1	C224—C225—H225	119.2
C115—C116—H116	120.1	C225—C226—C221	119.3 (7)
C114—C117—H11A	109.5	C225—C226—H226	120.3
C114—C117—H11B	109.5	C221—C226—H226	120.3
H11A—C117—H11B	109.5	C224—C227—H22A	109.5
C114—C117—H11C	109.5	C224—C227—H22B	109.5
H11A—C117—H11C	109.5	H22A—C227—H22B	109.5
H11B—C117—H11C	109.5	C224—C227—H22C	109.5
C126—C121—C122	120.1 (7)	H22A—C227—H22C	109.5
C126—C121—S102	119.0 (6)	H22B—C227—H22C	109.5
C122—C121—S102	120.8 (6)	C236—C231—C232	119.4 (7)
C123—C122—C121	120.4 (7)	C236—C231—S203	120.1 (6)
C123—C122—H122	119.8	C232—C231—S203	120.4 (6)
C121—C122—H122	119.8	C233—C232—C231	120.3 (7)
C122—C123—C124	120.1 (7)	C233—C232—H232	119.8
C122—C123—H123	119.9	C231—C232—H232	119.8
C124—C123—H123	119.9	C232—C233—C234	120.7 (7)
C123—C124—C125	119.2 (7)	C232—C233—H233	119.7
C123—C124—C127	120.2 (7)	C234—C233—H233	119.7
C125—C124—C127	120.6 (7)	C235—C234—C233	118.7 (7)
C124—C125—C126	120.9 (7)	C235—C234—C237	120.2 (7)
C124—C125—H125	119.5	C233—C234—C237	121.1 (7)
C126—C125—H125	119.5	C234—C235—C236	121.9 (7)
C121—C126—C125	119.3 (7)	C234—C235—H235	119.0
C121—C126—H126	120.4	C236—C235—H235	119.0
C125—C126—H126	120.4	C231—C236—C235	119.0 (7)
C124—C127—H12A	109.5	C231—C236—H236	120.5
C124—C127—H12B	109.5	C235—C236—H236	120.5
H12A—C127—H12B	109.5	C234—C237—H23A	109.5
C124—C127—H12C	109.5	C234—C237—H23B	109.5
H12A—C127—H12C	109.5	H23A—C237—H23B	109.5
H12B—C127—H12C	109.5	C234—C237—H23C	109.5
C136—C131—C132	121.4 (8)	H23A—C237—H23C	109.5

C136—C131—S103	119.1 (6)	H23B—C237—H23C	109.5
C132—C131—S103	119.6 (6)	C246—C241—C242	119.9 (7)
C133—C132—C131	118.7 (8)	C246—C241—S204	116.2 (6)
C133—C132—H132	120.6	C242—C241—S204	123.5 (6)
C131—C132—H132	120.6	C243—C242—C241	120.1 (7)
C132—C133—C134	121.9 (8)	C243—C242—H242	120.0
C132—C133—H133	119.1	C241—C242—H242	120.0
C134—C133—H133	119.1	C242—C243—C244	120.5 (7)
C135—C134—C133	117.8 (8)	C242—C243—H243	119.7
C135—C134—C137	121.4 (9)	C244—C243—H243	119.7
C133—C134—C137	120.7 (8)	C245—C244—C243	119.2 (8)
C134—C135—C136	121.7 (8)	C245—C244—C247	120.2 (7)
C134—C135—H135	119.2	C243—C244—C247	120.6 (8)
C136—C135—H135	119.2	C244—C245—C246	120.7 (8)
C131—C136—C135	118.5 (8)	C244—C245—H245	119.7
C131—C136—H136	120.7	C246—C245—H245	119.7
C135—C136—H136	120.7	C241—C246—C245	119.6 (7)
C134—C137—H13A	109.5	C241—C246—H246	120.2
C134—C137—H13B	109.5	C245—C246—H246	120.2
H13A—C137—H13B	109.5	C244—C247—H24A	109.5
C134—C137—H13C	109.5	C244—C247—H24B	109.5
H13A—C137—H13C	109.5	H24A—C247—H24B	109.5
H13B—C137—H13C	109.5	C244—C247—H24C	109.5
C146—C141—C142	120.6 (7)	H24A—C247—H24C	109.5
C146—C141—S104	119.9 (6)	H24B—C247—H24C	109.5
C142—C141—S104	119.4 (6)	O201—S201—C211	107.0 (3)
C143—C142—C141	119.6 (8)	O201—S201—C201	104.9 (3)
C143—C142—H142	120.2	C211—S201—C201	99.6 (4)
C141—C142—H142	120.2	O202—S202—C221	106.0 (3)
C142—C143—C144	121.9 (8)	O202—S202—C202	108.2 (3)
C142—C143—H143	119.1	C221—S202—C202	97.8 (3)
C144—C143—H143	119.1	O203—S203—C231	106.9 (3)
C143—C144—C145	117.3 (8)	O203—S203—C203	108.8 (4)
C143—C144—C147	122.7 (9)	C231—S203—C203	95.8 (3)
C145—C144—C147	120.0 (8)	O204—S204—C241	104.7 (4)
C146—C145—C144	121.2 (8)	O204—S204—C204	107.1 (4)
C146—C145—H145	119.4	C241—S204—C204	100.5 (4)
C144—C145—H145	119.4	C202—Fe2—C204	70.2 (3)
C141—C146—C145	119.5 (7)	C202—Fe2—C203	41.7 (3)
C141—C146—H146	120.3	C204—Fe2—C203	41.3 (3)
C145—C146—H146	120.3	C202—Fe2—C208	162.2 (4)
C144—C147—H14A	109.5	C204—Fe2—C208	118.9 (4)
C144—C147—H14B	109.5	C203—Fe2—C208	154.6 (4)
H14A—C147—H14B	109.5	C202—Fe2—C201	41.6 (3)
C144—C147—H14C	109.5	C204—Fe2—C201	69.4 (3)
H14A—C147—H14C	109.5	C203—Fe2—C201	69.5 (3)
H14B—C147—H14C	109.5	C208—Fe2—C201	124.3 (4)
O101—S101—C101	107.3 (3)	C202—Fe2—C210	107.8 (3)

O101—S101—C111	105.3 (3)	C204—Fe2—C210	165.9 (3)
C101—S101—C111	98.4 (3)	C203—Fe2—C210	128.1 (3)
O102—S102—C102	108.8 (3)	C208—Fe2—C210	67.3 (4)
O102—S102—C121	106.3 (3)	C201—Fe2—C210	118.9 (3)
C102—S102—C121	95.2 (3)	C202—Fe2—C207	155.0 (4)
O103—S103—C103	107.6 (3)	C204—Fe2—C207	108.9 (4)
O103—S103—C131	105.8 (3)	C203—Fe2—C207	121.1 (4)
C103—S103—C131	98.0 (3)	C208—Fe2—C207	40.7 (4)
O104—S104—C141	107.8 (4)	C201—Fe2—C207	163.1 (4)
O104—S104—C104	104.6 (3)	C210—Fe2—C207	66.7 (4)
C141—S104—C104	98.3 (3)	C202—Fe2—C205	70.1 (3)
C103—Fe1—C102	41.9 (3)	C204—Fe2—C205	40.9 (3)
C103—Fe1—C109	132.2 (4)	C203—Fe2—C205	69.3 (3)
C102—Fe1—C109	170.8 (4)	C208—Fe2—C205	106.0 (3)
C103—Fe1—C101	70.2 (3)	C201—Fe2—C205	41.3 (3)
C102—Fe1—C101	42.0 (3)	C210—Fe2—C205	152.7 (3)
C109—Fe1—C101	147.2 (4)	C207—Fe2—C205	126.5 (4)
C103—Fe1—C104	41.3 (3)	C202—Fe2—C209	125.3 (3)
C102—Fe1—C104	69.8 (3)	C204—Fe2—C209	151.8 (4)
C109—Fe1—C104	110.2 (4)	C203—Fe2—C209	164.9 (4)
C101—Fe1—C104	69.1 (3)	C208—Fe2—C209	39.8 (4)
C103—Fe1—C107	115.6 (3)	C201—Fe2—C209	105.4 (3)
C102—Fe1—C107	108.0 (3)	C210—Fe2—C209	40.8 (4)
C109—Fe1—C107	66.9 (4)	C207—Fe2—C209	67.7 (4)
C101—Fe1—C107	131.3 (3)	C205—Fe2—C209	117.0 (3)
C104—Fe1—C107	148.4 (3)	C202—Fe2—C206	120.5 (4)
C103—Fe1—C106	145.5 (4)	C204—Fe2—C206	128.7 (4)
C102—Fe1—C106	113.2 (4)	C203—Fe2—C206	110.3 (3)
C109—Fe1—C106	68.1 (5)	C208—Fe2—C206	67.4 (4)
C101—Fe1—C106	107.8 (3)	C201—Fe2—C206	153.8 (4)
C104—Fe1—C106	172.0 (4)	C210—Fe2—C206	39.4 (4)
C107—Fe1—C106	39.0 (4)	C207—Fe2—C206	39.7 (4)
C103—Fe1—C108	108.5 (3)	C205—Fe2—C206	164.7 (4)
C102—Fe1—C108	130.6 (3)	C209—Fe2—C206	67.6 (4)

C303—O302—C302—O301	−1.5 (14)	C103—C104—S104—C141	−178.8 (6)
C303—O302—C302—C301	176.4 (8)	C105—C104—S104—C141	−2.7 (7)
C302—O302—C303—C304	170.5 (8)	Fe1—C104—S104—C141	−94.6 (5)
O401—C402—O402—C403	25 (11)	C205—C201—C202—C203	1.6 (8)
C401—C402—O402—C403	−179 (4)	S201—C201—C202—C203	174.6 (5)
C404—C403—O402—C402	171 (8)	Fe2—C201—C202—C203	60.0 (5)
C105—C101—C102—C103	0.2 (8)	C205—C201—C202—S202	−175.2 (5)
S101—C101—C102—C103	−174.6 (5)	S201—C201—C202—S202	−2.2 (8)
Fe1—C101—C102—C103	−59.0 (5)	Fe2—C201—C202—S202	−116.8 (5)
C105—C101—C102—S102	−178.4 (5)	C205—C201—C202—Fe2	−58.3 (5)
S101—C101—C102—S102	6.8 (10)	S201—C201—C202—Fe2	114.6 (5)
Fe1—C101—C102—S102	122.4 (6)	C201—C202—C203—C204	−2.3 (8)
C105—C101—C102—Fe1	59.2 (5)	S202—C202—C203—C204	174.1 (6)

S101—C101—C102—Fe1	−115.6 (5)
C101—C102—C103—C104	−0.9 (8)
S102—C102—C103—C104	177.7 (5)
Fe1—C102—C103—C104	−60.6 (5)
C101—C102—C103—S103	173.6 (5)
S102—C102—C103—S103	−7.8 (10)
Fe1—C102—C103—S103	113.9 (6)
C101—C102—C103—Fe1	59.7 (5)
S102—C102—C103—Fe1	−121.7 (5)
C102—C103—C104—C105	1.2 (8)
S103—C103—C104—C105	−173.7 (5)
Fe1—C103—C104—C105	−58.2 (5)
C102—C103—C104—S104	178.0 (5)
S103—C103—C104—S104	3.1 (8)
Fe1—C103—C104—S104	118.6 (5)
C102—C103—C104—Fe1	59.4 (5)
S103—C103—C104—Fe1	−115.5 (5)
C102—C101—C105—C104	0.6 (8)
S101—C101—C105—C104	175.2 (5)
Fe1—C101—C105—C104	58.1 (5)
C102—C101—C105—Fe1	−57.6 (5)
S101—C101—C105—Fe1	117.0 (6)
C103—C104—C105—C101	−1.1 (8)
S104—C104—C105—C101	−177.6 (5)
Fe1—C104—C105—C101	−57.9 (5)
C103—C104—C105—Fe1	56.8 (5)
S104—C104—C105—Fe1	−119.7 (6)
C110—C106—C107—C108	−1.2 (11)
Fe1—C106—C107—C108	59.0 (6)
C110—C106—C107—Fe1	−60.2 (6)
C106—C107—C108—C109	0.0 (10)
Fe1—C107—C108—C109	59.1 (6)
C106—C107—C108—Fe1	−59.1 (6)
C107—C108—C109—C110	1.2 (9)
Fe1—C108—C109—C110	61.3 (6)
C107—C108—C109—Fe1	−60.0 (6)
C107—C106—C110—C109	1.9 (10)
Fe1—C106—C110—C109	−58.2 (6)
C107—C106—C110—Fe1	60.2 (6)
C108—C109—C110—C106	−2.0 (10)
Fe1—C109—C110—C106	59.5 (6)
C108—C109—C110—Fe1	−61.5 (6)
C116—C111—C112—C113	−1.3 (12)
S101—C111—C112—C113	−172.6 (6)
C111—C112—C113—C114	0.1 (13)
C112—C113—C114—C115	1.7 (13)
C112—C113—C114—C117	179.7 (8)
C113—C114—C115—C116	−2.2 (12)
Fe2—C202—C203—C204	58.1 (5)
C201—C202—C203—S203	−179.9 (5)
S202—C202—C203—S203	−3.5 (10)
Fe2—C202—C203—S203	−119.6 (6)
C201—C202—C203—Fe2	−60.4 (5)
S202—C202—C203—Fe2	116.0 (6)
C202—C203—C204—C205	2.1 (8)
S203—C203—C204—C205	179.5 (6)
Fe2—C203—C204—C205	59.8 (5)
C202—C203—C204—S204	−170.0 (5)
S203—C203—C204—S204	7.4 (10)
Fe2—C203—C204—S204	−112.3 (6)
C202—C203—C204—Fe2	−57.8 (5)
S203—C203—C204—Fe2	119.7 (6)
C203—C204—C205—C201	−1.1 (8)
S204—C204—C205—C201	170.9 (5)
Fe2—C204—C205—C201	58.1 (5)
C203—C204—C205—Fe2	−59.2 (5)
S204—C204—C205—Fe2	112.7 (6)
C202—C201—C205—C204	−0.4 (8)
S201—C201—C205—C204	−172.5 (6)
Fe2—C201—C205—C204	−57.8 (5)
C202—C201—C205—Fe2	57.5 (5)
S201—C201—C205—Fe2	−114.6 (6)
C210—C206—C207—C208	−0.4 (10)
Fe2—C206—C207—C208	−59.4 (6)
C210—C206—C207—Fe2	59.0 (6)
C206—C207—C208—C209	−0.6 (10)
Fe2—C207—C208—C209	−61.2 (6)
C206—C207—C208—Fe2	60.6 (6)
C207—C208—C209—C210	1.3 (9)
Fe2—C208—C209—C210	−59.2 (5)
C207—C208—C209—Fe2	60.5 (6)
C207—C206—C210—C209	1.3 (10)
Fe2—C206—C210—C209	60.2 (6)
C207—C206—C210—Fe2	−58.9 (6)
C208—C209—C210—C206	−1.6 (9)
Fe2—C209—C210—C206	−60.7 (6)
C208—C209—C210—Fe2	59.1 (6)
C216—C211—C212—C213	−0.6 (14)
S201—C211—C212—C213	170.8 (8)
C211—C212—C213—C214	−0.6 (16)
C212—C213—C214—C215	1.4 (16)
C212—C213—C214—C217	−178.7 (11)
C213—C214—C215—C216	−1.0 (16)
C217—C214—C215—C216	179.1 (11)
C214—C215—C216—C211	−0.2 (15)
C212—C211—C216—C215	1.0 (13)

C117—C114—C115—C116	179.8 (8)
C112—C111—C116—C115	0.8 (11)
S101—C111—C116—C115	171.8 (6)
C114—C115—C116—C111	1.0 (12)
C126—C121—C122—C123	1.4 (11)
S102—C121—C122—C123	176.5 (6)
C121—C122—C123—C124	0.0 (11)
C122—C123—C124—C125	−0.1 (11)
C122—C123—C124—C127	178.8 (8)
C123—C124—C125—C126	−1.1 (12)
C127—C124—C125—C126	180.0 (8)
C122—C121—C126—C125	−2.6 (11)
S102—C121—C126—C125	−177.8 (6)
C124—C125—C126—C121	2.5 (12)
C136—C131—C132—C133	0.9 (11)
S103—C131—C132—C133	−179.3 (6)
C131—C132—C133—C134	1.4 (12)
C132—C133—C134—C135	−2.2 (13)
C132—C133—C134—C137	173.4 (8)
C133—C134—C135—C136	0.8 (14)
C137—C134—C135—C136	−174.7 (9)
C132—C131—C136—C135	−2.1 (12)
S103—C131—C136—C135	178.0 (6)
C134—C135—C136—C131	1.3 (13)
C146—C141—C142—C143	1.9 (12)
S104—C141—C142—C143	177.7 (6)
C141—C142—C143—C144	−1.6 (13)
C142—C143—C144—C145	0.6 (12)
C142—C143—C144—C147	−177.6 (9)
C143—C144—C145—C146	0.1 (12)
C147—C144—C145—C146	178.4 (8)
C142—C141—C146—C145	−1.2 (11)
S104—C141—C146—C145	−177.0 (6)
C144—C145—C146—C141	0.2 (12)
C105—C101—S101—O101	−53.6 (7)
C102—C101—S101—O101	120.3 (6)
Fe1—C101—S101—O101	36.2 (5)
C105—C101—S101—C111	55.4 (7)
C102—C101—S101—C111	−130.7 (6)
Fe1—C101—S101—C111	145.2 (4)
C116—C111—S101—O101	176.7 (6)
C112—C111—S101—O101	−12.2 (7)
C116—C111—S101—C101	66.0 (6)
C112—C111—S101—C101	−122.8 (6)
C103—C102—S102—O102	134.3 (6)
C101—C102—S102—O102	−47.4 (7)
Fe1—C102—S102—O102	45.4 (5)
C103—C102—S102—C121	−116.5 (6)
S201—C211—C216—C215	−170.6 (7)
C226—C221—C222—C223	2.5 (11)
S202—C221—C222—C223	−177.4 (6)
C221—C222—C223—C224	−0.4 (11)
C222—C223—C224—C225	−2.0 (12)
C222—C223—C224—C227	176.3 (7)
C223—C224—C225—C226	2.4 (13)
C227—C224—C225—C226	−175.9 (8)
C224—C225—C226—C221	−0.3 (13)
C222—C221—C226—C225	−2.1 (11)
S202—C221—C226—C225	177.8 (6)
C236—C231—C232—C233	0.1 (11)
S203—C231—C232—C233	176.3 (6)
C231—C232—C233—C234	0.5 (12)
C232—C233—C234—C235	−1.0 (12)
C232—C233—C234—C237	179.8 (7)
C233—C234—C235—C236	0.8 (12)
C237—C234—C235—C236	180.0 (8)
C232—C231—C236—C235	−0.3 (11)
S203—C231—C236—C235	−176.5 (6)
C234—C235—C236—C231	−0.1 (12)
C246—C241—C242—C243	−1.2 (12)
S204—C241—C242—C243	170.8 (6)
C241—C242—C243—C244	0.9 (12)
C242—C243—C244—C245	0.1 (12)
C242—C243—C244—C247	−179.7 (8)
C243—C244—C245—C246	−0.7 (12)
C247—C244—C245—C246	179.1 (8)
C242—C241—C246—C245	0.6 (12)
S204—C241—C246—C245	−172.0 (6)
C244—C245—C246—C241	0.3 (13)
C212—C211—S201—O201	−140.0 (7)
C216—C211—S201—O201	31.7 (7)
C212—C211—S201—C201	111.1 (7)
C216—C211—S201—C201	−77.2 (7)
C202—C201—S201—O201	67.2 (6)
C205—C201—S201—O201	−121.6 (7)
Fe2—C201—S201—O201	149.2 (4)
C202—C201—S201—C211	177.7 (6)
C205—C201—S201—C211	−11.1 (7)
Fe2—C201—S201—C211	−100.2 (5)
C226—C221—S202—O202	−1.7 (7)
C222—C221—S202—O202	178.3 (6)
C226—C221—S202—C202	−113.2 (6)
C222—C221—S202—C202	66.7 (6)
C203—C202—S202—O202	−35.9 (8)
C201—C202—S202—O202	140.0 (6)
Fe2—C202—S202—O202	54.5 (5)

C101—C102—S102—C121	61.8 (7)	C203—C202—S202—C221	73.8 (7)
Fe1—C102—S102—C121	154.6 (4)	C201—C202—S202—C221	−110.2 (6)
C126—C121—S102—O102	−12.1 (7)	Fe2—C202—S202—C221	164.3 (4)
C122—C121—S102—O102	172.7 (6)	C236—C231—S203—O203	−8.0 (7)
C126—C121—S102—C102	−123.4 (6)	C232—C231—S203—O203	175.9 (6)
C122—C121—S102—C102	61.4 (6)	C236—C231—S203—C203	−119.7 (6)
C104—C103—S103—O103	137.2 (6)	C232—C231—S203—C203	64.2 (6)
C102—C103—S103—O103	−36.6 (7)	C204—C203—S203—O203	−44.6 (8)
Fe1—C103—S103—O103	50.9 (5)	C202—C203—S203—O203	132.6 (6)
C104—C103—S103—C131	−113.4 (6)	Fe2—C203—S203—O203	46.3 (6)
C102—C103—S103—C131	72.8 (7)	C204—C203—S203—C231	65.5 (7)
Fe1—C103—S103—C131	160.3 (4)	C202—C203—S203—C231	−117.3 (6)
C136—C131—S103—O103	2.7 (7)	Fe2—C203—S203—C231	156.5 (5)
C132—C131—S103—O103	−177.2 (6)	C246—C241—S204—O204	−23.0 (7)
C136—C131—S103—C103	−108.2 (6)	C242—C241—S204—O204	164.7 (7)
C132—C131—S103—C103	71.9 (6)	C246—C241—S204—C204	−134.0 (6)
C146—C141—S104—O104	35.3 (7)	C242—C241—S204—C204	53.7 (8)
C142—C141—S104—O104	−140.5 (6)	C205—C204—S204—O204	−41.4 (8)
C146—C141—S104—C104	−73.0 (6)	C203—C204—S204—O204	129.4 (7)
C142—C141—S104—C104	111.2 (6)	Fe2—C204—S204—O204	45.1 (6)
C103—C104—S104—O104	70.3 (6)	C205—C204—S204—C241	67.7 (7)
C105—C104—S104—O104	−113.6 (7)	C203—C204—S204—C241	−121.6 (7)
Fe1—C104—S104—O104	154.5 (4)	Fe2—C204—S204—C241	154.2 (4)

1,2-Bis(phenylsulfanyl)ferrocene (comp_5)

Crystal data

$[Fe(C_5H_5)(C_{17}H_{13}S_2)]$
M_r = 402.33
Orthorhombic, $Pmn2_1$
a = 14.0977 (11) Å
b = 7.1607 (5) Å
c = 8.8504 (5) Å
V = 893.44 (11) Å^3
Z = 2
$F(000)$ = 416
D_x = 1.496 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3015 reflections
θ = 2.9–29.6°
μ = 1.08 mm^{-1}
T = 110 K
Block, yellow
0.10 × 0.08 × 0.05 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.3910 pixels mm^{-1}
mix of ω and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.682, T_{max} = 0.746
9831 measured reflections
2561 independent reflections
2426 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 29.6°, θ_{min} = 3.7°
h = −19→19
k = −9→9
l = −11→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.060$
$S = 1.05$
2561 reflections
118 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0202P)^2 + 0.1142P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Absolute structure: Flack *x* determined using 1069 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.018 (9)

Special details

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. All crystal structure determinations were performed on a Bruker D8 VENTURE system. Structures were solved by SHELXT (Sheldrick, 2015a) and refined by SHELXL (Sheldrick, 2015b). Structure evaluation was performed with PLATON (Spek, 2020) structure plots were made with ORTEP-3 for Windows and Mercury (Macrae *et al.*, 2020), all as part of the WinGX program suite. CCDC 2330910–2330913 contain the supplementary crystallographic data for **2a**, **2b**, **3a**, **4**.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.44864 (16)	0.2970 (3)	0.5545 (2)	0.0149 (4)
C2	0.41809 (17)	0.1963 (3)	0.6855 (3)	0.0171 (4)
H2	0.354150	0.173175	0.713812	0.021*
C3	0.500000	0.1367 (4)	0.7661 (4)	0.0176 (7)
H3	0.500000	0.068589	0.858189	0.021*
C4	0.500000	0.5289 (5)	0.9562 (4)	0.0216 (7)
H4	0.499999	0.459166	1.047557	0.026*
C5	0.58196 (19)	0.5911 (3)	0.8748 (3)	0.0199 (5)
H5	0.646125	0.569846	0.902712	0.024*
C6	0.55062 (15)	0.6899 (3)	0.7451 (4)	0.0192 (4)
H6	0.590158	0.746306	0.671160	0.023*
C11	0.35275 (16)	0.2425 (3)	0.2842 (2)	0.0152 (4)
C12	0.38165 (17)	0.0571 (3)	0.2942 (3)	0.0187 (5)
H12	0.414275	0.014123	0.381404	0.022*
C13	0.36261 (17)	−0.0649 (3)	0.1761 (3)	0.0208 (5)
H13	0.383471	−0.190849	0.182213	0.025*
C14	0.31365 (17)	−0.0053 (4)	0.0496 (3)	0.0212 (5)
H14	0.300928	−0.089439	−0.030900	0.025*
C15	0.28314 (18)	0.1798 (4)	0.0413 (3)	0.0206 (5)
H15	0.248600	0.220974	−0.044617	0.025*
C16	0.30272 (17)	0.3041 (3)	0.1573 (3)	0.0190 (5)
H16	0.282293	0.430289	0.150583	0.023*
S1	0.37457 (4)	0.41313 (8)	0.42625 (7)	0.01859 (14)
Fe1	0.500000	0.42175 (6)	0.74149 (4)	0.01288 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0177 (11)	0.0118 (9)	0.0150 (10)	0.0000 (8)	−0.0006 (9)	−0.0030 (8)
C2	0.0210 (11)	0.0137 (10)	0.0167 (10)	−0.0040 (9)	0.0029 (9)	−0.0041 (9)
C3	0.0273 (16)	0.0094 (13)	0.0163 (17)	0.000	0.000	−0.0022 (12)
C4	0.0288 (18)	0.0201 (16)	0.0158 (16)	0.000	0.000	−0.0083 (13)
C5	0.0211 (11)	0.0167 (11)	0.0220 (11)	−0.0008 (9)	−0.0035 (10)	−0.0086 (9)
C6	0.0212 (11)	0.0118 (9)	0.0246 (10)	−0.0017 (8)	0.0006 (11)	−0.0034 (11)
C11	0.0151 (10)	0.0170 (11)	0.0136 (10)	−0.0005 (8)	0.0019 (8)	−0.0029 (8)
C12	0.0179 (11)	0.0198 (12)	0.0182 (11)	0.0010 (9)	−0.0019 (9)	−0.0013 (9)
C13	0.0205 (11)	0.0165 (12)	0.0252 (12)	0.0006 (9)	0.0003 (10)	−0.0054 (10)
C14	0.0202 (11)	0.0230 (12)	0.0205 (11)	−0.0018 (10)	0.0005 (9)	−0.0073 (10)
C15	0.0200 (11)	0.0270 (13)	0.0149 (10)	0.0005 (9)	−0.0032 (9)	−0.0008 (10)
C16	0.0209 (12)	0.0170 (11)	0.0191 (11)	0.0017 (9)	0.0010 (9)	−0.0014 (9)
S1	0.0221 (3)	0.0152 (3)	0.0184 (3)	0.0040 (2)	−0.0052 (2)	−0.0042 (2)
Fe1	0.0157 (2)	0.0099 (2)	0.0130 (2)	0.000	0.000	−0.00291 (19)

Geometric parameters (Å, º)

C1—C2	1.432 (3)	C6—C6^{i}	1.427 (4)
C1—C1^{i}	1.448 (5)	C6—Fe1	2.049 (2)
C1—S1	1.752 (2)	C6—H6	0.9500
C1—Fe1	2.015 (2)	C11—C12	1.392 (3)
C2—C3	1.422 (3)	C11—C16	1.398 (3)
C2—Fe1	2.046 (2)	C11—S1	1.780 (2)
C2—H2	0.9500	C12—C13	1.388 (3)
C3—Fe1	2.053 (3)	C12—H12	0.9500
C3—H3	0.9500	C13—C14	1.383 (4)
C4—C5^{i}	1.433 (3)	C13—H13	0.9500
C4—C5	1.433 (3)	C14—C15	1.395 (3)
C4—Fe1	2.050 (3)	C14—H14	0.9500
C4—H4	0.9500	C15—C16	1.387 (3)
C5—C6	1.418 (4)	C15—H15	0.9500
C5—Fe1	2.049 (2)	C16—H16	0.9500
C5—H5	0.9500		
C2—C1—C1^{i}	107.50 (13)	C14—C15—H15	119.7
C2—C1—S1	125.76 (18)	C15—C16—C11	119.5 (2)
C1^{i}—C1—S1	126.58 (7)	C15—C16—H16	120.2
C2—C1—Fe1	70.51 (12)	C11—C16—H16	120.2
C1^{i}—C1—Fe1	68.94 (6)	C1—S1—C11	103.57 (11)
S1—C1—Fe1	122.39 (11)	C1—Fe1—C1^{i}	42.11 (13)
C3—C2—C1	108.2 (2)	C1—Fe1—C2^{i}	69.77 (9)
C3—C2—Fe1	69.95 (15)	C1^{i}—Fe1—C2^{i}	41.29 (9)
C1—C2—Fe1	68.20 (12)	C1—Fe1—C2	41.29 (9)
C3—C2—H2	125.9	C1^{i}—Fe1—C2	69.77 (9)
C1—C2—H2	125.9	C2^{i}—Fe1—C2	68.72 (13)

Fe1—C2—H2	127.5	C1—Fe1—C5^{i}	122.18 (10)
C2^{i}—C3—C2	108.5 (3)	C1^{i}—Fe1—C5^{i}	159.70 (10)
C2^{i}—C3—Fe1	69.44 (15)	C2^{i}—Fe1—C5^{i}	157.64 (10)
C2—C3—Fe1	69.44 (15)	C2—Fe1—C5^{i}	106.75 (10)
C2^{i}—C3—H3	125.7	C1—Fe1—C5	159.70 (10)
C2—C3—H3	125.7	C1^{i}—Fe1—C5	122.18 (10)
Fe1—C3—H3	127.0	C2^{i}—Fe1—C5	106.75 (10)
C5^{i}—C4—C5	107.5 (3)	C2—Fe1—C5	157.65 (10)
C5^{i}—C4—Fe1	69.50 (16)	C5^{i}—Fe1—C5	68.67 (15)
C5—C4—Fe1	69.50 (16)	C1—Fe1—C6	123.61 (11)
C5^{i}—C4—H4	126.3	C1^{i}—Fe1—C6	107.65 (11)
C5—C4—H4	126.3	C2^{i}—Fe1—C6	123.16 (9)
Fe1—C4—H4	126.3	C2—Fe1—C6	160.07 (10)
C6—C5—C4	108.1 (2)	C5^{i}—Fe1—C6	68.44 (10)
C6—C5—Fe1	69.75 (13)	C5—Fe1—C6	40.51 (11)
C4—C5—Fe1	69.57 (16)	C1—Fe1—C6^{i}	107.65 (11)
C6—C5—H5	125.9	C1^{i}—Fe1—C6^{i}	123.61 (11)
C4—C5—H5	125.9	C2^{i}—Fe1—C6^{i}	160.07 (10)
Fe1—C5—H5	126.3	C2—Fe1—C6^{i}	123.16 (9)
C5—C6—C6^{i}	108.15 (14)	C5^{i}—Fe1—C6^{i}	40.51 (11)
C5—C6—Fe1	69.74 (13)	C5—Fe1—C6^{i}	68.44 (10)
C6^{i}—C6—Fe1	69.62 (6)	C6—Fe1—C6^{i}	40.77 (12)
C5—C6—H6	125.9	C1—Fe1—C4	158.04 (7)
C6^{i}—C6—H6	125.9	C1^{i}—Fe1—C4	158.04 (7)
Fe1—C6—H6	126.3	C2^{i}—Fe1—C4	121.32 (11)
C12—C11—C16	120.0 (2)	C2—Fe1—C4	121.32 (11)
C12—C11—S1	124.05 (18)	C5^{i}—Fe1—C4	40.93 (9)
C16—C11—S1	115.97 (18)	C5—Fe1—C4	40.93 (9)
C13—C12—C11	119.8 (2)	C6—Fe1—C4	68.56 (13)
C13—C12—H12	120.1	C6^{i}—Fe1—C4	68.56 (13)
C11—C12—H12	120.1	C1—Fe1—C3	69.28 (10)
C14—C13—C12	120.8 (2)	C1^{i}—Fe1—C3	69.28 (10)
C14—C13—H13	119.6	C2^{i}—Fe1—C3	40.61 (8)
C12—C13—H13	119.6	C2—Fe1—C3	40.61 (8)
C13—C14—C15	119.3 (2)	C5^{i}—Fe1—C3	121.84 (10)
C13—C14—H14	120.3	C5—Fe1—C3	121.84 (10)
C15—C14—H14	120.3	C6—Fe1—C3	158.48 (7)
C16—C15—C14	120.6 (2)	C6^{i}—Fe1—C3	158.48 (7)
C16—C15—H15	119.7	C4—Fe1—C3	105.90 (14)

C1^{i}—C1—C2—C3	0.6 (2)	C16—C11—C12—C13	1.6 (3)
S1—C1—C2—C3	−175.09 (18)	S1—C11—C12—C13	−178.91 (18)
Fe1—C1—C2—C3	−58.64 (18)	C11—C12—C13—C14	−1.2 (4)
C1^{i}—C1—C2—Fe1	59.25 (6)	C12—C13—C14—C15	−0.1 (4)
S1—C1—C2—Fe1	−116.45 (17)	C13—C14—C15—C16	1.0 (4)
C1—C2—C3—C2^{i}	−1.0 (3)	C14—C15—C16—C11	−0.6 (4)
Fe1—C2—C3—C2^{i}	−58.6 (2)	C12—C11—C16—C15	−0.7 (3)
C1—C2—C3—Fe1	57.57 (15)	S1—C11—C16—C15	179.78 (18)

C5^{i}—C4—C5—C6	0.0 (4)	C2—C1—S1—C11	−92.7 (2)
Fe1—C4—C5—C6	59.31 (17)	C1^{i}—C1—S1—C11	92.42 (10)
C5^{i}—C4—C5—Fe1	−59.4 (2)	Fe1—C1—S1—C11	179.04 (12)
C4—C5—C6—C6^{i}	0.0 (2)	C12—C11—S1—C1	6.9 (2)
Fe1—C5—C6—C6^{i}	59.22 (7)	C16—C11—S1—C1	−173.51 (17)
C4—C5—C6—Fe1	−59.20 (19)		

Symmetry code: (i) −*x*+1, *y*, *z*.

1,2,3,4-Tetrakis(phenylsulfanyl)ferrocene (comp_6)

Crystal data

[Fe(C_5H_5)($C_{29}H_{21}S_4$)]
M_r = 618.64
Triclinic, $P\overline{1}$
a = 8.4836 (4) Å
b = 10.3028 (5) Å
c = 16.7210 (8) Å
α = 90.730 (2)°
β = 103.948 (2)°
γ = 94.999 (2)°
V = 1412.15 (12) Å^3
Z = 2
F(000) = 640
D_x = 1.455 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9949 reflections
θ = 3.0–28.3°
μ = 0.85 mm^{-1}
T = 110 K
Platelet, yellow
0.06 × 0.05 × 0.02 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: rotating anode generator, Bruker TXS
Detector resolution: 7.3910 pixels mm^{-1}
mix of *ω* and phi scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.691, T_{max} = 0.746
23494 measured reflections
7023 independent reflections
5898 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 28.3°, θ_{min} = 3.0°
h = −11→11
k = −13→13
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.088
S = 1.04
7023 reflections
352 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 0.9306P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Special details

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. All crystal structure determinations were performed on a Bruker D8 VENTURE system. Structures were solved by SHELXT (Sheldrick, 2015a) and refined by SHELXL (Sheldrick, 2015b). Structure evaluation was performed with PLATON (Spek, 2020) structure plots were made with ORTEP-3 for Windows and Mercury (Macrae *et al.*, 2020), all as part of the WinGX program suite. CCDC 2330910–2330913 contain the supplementary crystallographic data for **2a**, **2b**, **3a**, **4**.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4986 (2)	0.74784 (17)	0.26133 (11)	0.0174 (4)
C2	0.3492 (2)	0.69583 (17)	0.20503 (11)	0.0158 (3)
C3	0.3869 (2)	0.58876 (17)	0.15810 (11)	0.0156 (3)
C4	0.5591 (2)	0.57642 (17)	0.18679 (11)	0.0163 (3)
C5	0.6268 (2)	0.67403 (17)	0.24958 (11)	0.0179 (4)
H5	0.738130	0.687788	0.278705	0.021*
C6	0.4470 (3)	0.9208 (2)	0.08050 (13)	0.0283 (5)
H6	0.361341	0.970040	0.087490	0.034*
C7	0.4322 (3)	0.8157 (2)	0.02457 (12)	0.0257 (4)
H7	0.334064	0.781622	−0.013019	0.031*
C8	0.5846 (3)	0.7691 (2)	0.03284 (13)	0.0287 (5)
H8	0.607552	0.698086	0.001997	0.034*
C9	0.6984 (3)	0.8449 (3)	0.09456 (15)	0.0374 (6)
H9	0.811476	0.834580	0.112812	0.045*
C10	0.6125 (3)	0.9406 (2)	0.12487 (14)	0.0378 (6)
H10	0.658041	1.005476	0.166943	0.045*
C11	0.5858 (2)	0.82071 (18)	0.42627 (11)	0.0192 (4)
C12	0.5761 (2)	0.68870 (19)	0.44207 (12)	0.0227 (4)
H12	0.529136	0.626621	0.398484	0.027*
C13	0.6349 (3)	0.6473 (2)	0.52160 (12)	0.0242 (4)
H13	0.630904	0.556685	0.531771	0.029*
C14	0.6991 (3)	0.7368 (2)	0.58610 (12)	0.0277 (4)
H14	0.738973	0.708144	0.640423	0.033*
C15	0.7047 (3)	0.8686 (2)	0.57054 (13)	0.0300 (5)
H15	0.745738	0.930687	0.614759	0.036*
C16	0.6509 (3)	0.91061 (19)	0.49121 (12)	0.0244 (4)
H16	0.658453	1.001162	0.480998	0.029*
C21	0.1021 (2)	0.71144 (18)	0.28239 (11)	0.0177 (4)
C22	0.0604 (2)	0.8070 (2)	0.33089 (13)	0.0246 (4)
H22	0.066915	0.895597	0.316034	0.030*
C23	0.0090 (3)	0.7722 (2)	0.40131 (13)	0.0326 (5)
H23	−0.020527	0.837100	0.434392	0.039*
C24	0.0010 (3)	0.6435 (3)	0.42310 (13)	0.0333 (5)
H24	−0.032187	0.620140	0.471744	0.040*
C25	0.0412 (3)	0.5484 (2)	0.37435 (13)	0.0289 (5)
H25	0.034794	0.459858	0.389407	0.035*
C26	0.0909 (2)	0.58179 (19)	0.30365 (12)	0.0227 (4)
H26	0.117077	0.516216	0.269851	0.027*
C31	0.1930 (2)	0.35543 (17)	0.10084 (11)	0.0161 (3)

C32	0.2707 (2)	0.29670 (18)	0.17192 (11)	0.0197 (4)
H32	0.356237	0.344456	0.211391	0.024*
C33	0.2234 (2)	0.16811 (19)	0.18526 (12)	0.0235 (4)
H33	0.277751	0.127746	0.233665	0.028*
C34	0.0976 (2)	0.09805 (19)	0.12854 (13)	0.0250 (4)
H34	0.065282	0.010119	0.138052	0.030*
C35	0.0192 (2)	0.15720 (19)	0.05783 (13)	0.0243 (4)
H35	−0.067380	0.109606	0.018897	0.029*
C36	0.0663 (2)	0.28528 (18)	0.04355 (12)	0.0202 (4)
H36	0.012513	0.325205	−0.005140	0.024*
C41	0.7255 (2)	0.36124 (18)	0.23461 (11)	0.0181 (4)
C42	0.6678 (2)	0.36423 (19)	0.30561 (11)	0.0202 (4)
H42	0.593540	0.425392	0.311616	0.024*
C43	0.7186 (2)	0.2779 (2)	0.36791 (12)	0.0235 (4)
H43	0.678373	0.280035	0.416206	0.028*
C44	0.8278 (3)	0.1887 (2)	0.35975 (13)	0.0257 (4)
H44	0.862551	0.129710	0.402274	0.031*
C45	0.8856 (3)	0.18637 (19)	0.28911 (13)	0.0254 (4)
H45	0.960021	0.125138	0.283371	0.030*
C46	0.8366 (2)	0.27201 (18)	0.22663 (12)	0.0210 (4)
H46	0.878152	0.270197	0.178736	0.025*
Fe1	0.51862 (3)	0.75646 (2)	0.14300 (2)	0.01529 (7)
S1	0.52213 (7)	0.88588 (5)	0.32725 (3)	0.02503 (12)
S2	0.15921 (6)	0.75891 (5)	0.19058 (3)	0.02236 (11)
S3	0.25386 (6)	0.51205 (4)	0.07023 (3)	0.01947 (10)
S4	0.67137 (6)	0.46433 (5)	0.14972 (3)	0.02090 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0238 (9)	0.0142 (8)	0.0146 (8)	0.0003 (7)	0.0059 (7)	0.0015 (6)
C2	0.0157 (8)	0.0162 (8)	0.0169 (8)	0.0022 (7)	0.0061 (7)	0.0055 (7)
C3	0.0181 (9)	0.0147 (8)	0.0141 (8)	−0.0001 (7)	0.0044 (7)	0.0035 (6)
C4	0.0198 (9)	0.0158 (8)	0.0142 (8)	0.0040 (7)	0.0048 (7)	0.0031 (6)
C5	0.0181 (9)	0.0189 (9)	0.0159 (8)	0.0004 (7)	0.0032 (7)	0.0025 (7)
C6	0.0393 (12)	0.0223 (10)	0.0307 (11)	0.0105 (9)	0.0194 (9)	0.0133 (8)
C7	0.0308 (11)	0.0279 (10)	0.0188 (9)	0.0008 (8)	0.0071 (8)	0.0089 (8)
C8	0.0410 (12)	0.0275 (11)	0.0253 (10)	0.0060 (9)	0.0218 (9)	0.0079 (8)
C9	0.0198 (10)	0.0521 (15)	0.0422 (13)	−0.0016 (10)	0.0121 (9)	0.0253 (11)
C10	0.0623 (17)	0.0222 (11)	0.0243 (11)	−0.0198 (11)	0.0095 (11)	0.0023 (8)
C11	0.0197 (9)	0.0204 (9)	0.0181 (9)	0.0007 (7)	0.0063 (7)	−0.0012 (7)
C12	0.0277 (10)	0.0202 (9)	0.0191 (9)	−0.0032 (8)	0.0056 (8)	−0.0041 (7)
C13	0.0292 (11)	0.0227 (10)	0.0207 (10)	−0.0008 (8)	0.0073 (8)	0.0012 (7)
C14	0.0269 (11)	0.0367 (12)	0.0173 (9)	0.0011 (9)	0.0020 (8)	0.0001 (8)
C15	0.0341 (12)	0.0307 (11)	0.0220 (10)	−0.0027 (9)	0.0033 (9)	−0.0106 (8)
C16	0.0283 (10)	0.0193 (9)	0.0253 (10)	0.0009 (8)	0.0069 (8)	−0.0042 (8)
C21	0.0149 (8)	0.0215 (9)	0.0172 (8)	0.0016 (7)	0.0050 (7)	0.0008 (7)
C22	0.0220 (10)	0.0230 (10)	0.0280 (10)	−0.0003 (8)	0.0055 (8)	−0.0043 (8)

C23	0.0250 (11)	0.0481 (14)	0.0245 (11)	0.0024 (10)	0.0069 (9)	−0.0125 (10)
C24	0.0240 (11)	0.0588 (15)	0.0183 (10)	0.0015 (10)	0.0079 (8)	0.0082 (10)
C25	0.0219 (10)	0.0363 (12)	0.0290 (11)	0.0021 (9)	0.0069 (8)	0.0135 (9)
C26	0.0236 (10)	0.0232 (10)	0.0229 (10)	0.0034 (8)	0.0085 (8)	0.0040 (8)
C31	0.0170 (8)	0.0158 (8)	0.0163 (8)	0.0026 (7)	0.0054 (7)	0.0003 (6)
C32	0.0194 (9)	0.0193 (9)	0.0190 (9)	0.0005 (7)	0.0019 (7)	0.0035 (7)
C33	0.0256 (10)	0.0217 (10)	0.0251 (10)	0.0059 (8)	0.0085 (8)	0.0063 (8)
C34	0.0274 (10)	0.0140 (9)	0.0370 (11)	0.0019 (8)	0.0146 (9)	−0.0006 (8)
C35	0.0192 (9)	0.0209 (10)	0.0312 (11)	0.0002 (8)	0.0041 (8)	−0.0079 (8)
C36	0.0178 (9)	0.0214 (9)	0.0205 (9)	0.0035 (7)	0.0025 (7)	−0.0014 (7)
C41	0.0168 (9)	0.0169 (9)	0.0195 (9)	0.0013 (7)	0.0023 (7)	0.0016 (7)
C42	0.0191 (9)	0.0217 (9)	0.0198 (9)	0.0024 (7)	0.0045 (7)	0.0013 (7)
C43	0.0212 (10)	0.0277 (10)	0.0215 (9)	0.0003 (8)	0.0053 (8)	0.0049 (8)
C44	0.0248 (10)	0.0238 (10)	0.0268 (10)	0.0038 (8)	0.0019 (8)	0.0097 (8)
C45	0.0251 (10)	0.0197 (10)	0.0315 (11)	0.0079 (8)	0.0051 (8)	0.0030 (8)
C46	0.0223 (9)	0.0204 (9)	0.0207 (9)	0.0053 (7)	0.0051 (7)	−0.0007 (7)
Fe1	0.01639 (13)	0.01474 (13)	0.01561 (13)	0.00073 (10)	0.00571 (10)	0.00310 (9)
S1	0.0399 (3)	0.0148 (2)	0.0198 (2)	0.0026 (2)	0.0062 (2)	−0.00044 (17)
S2	0.0219 (2)	0.0266 (2)	0.0229 (2)	0.01073 (19)	0.01018 (19)	0.01187 (19)
S3	0.0229 (2)	0.0175 (2)	0.0150 (2)	−0.00054 (18)	−0.00051 (17)	0.00358 (16)
S4	0.0258 (2)	0.0232 (2)	0.0165 (2)	0.01045 (19)	0.00754 (18)	0.00343 (17)

Geometric parameters (Å, º)

C1—C5	1.429 (3)	C15—C16	1.383 (3)
C1—C2	1.440 (3)	C15—H15	0.9500
C1—S1	1.7556 (18)	C16—H16	0.9500
C1—Fe1	2.0286 (18)	C21—C26	1.388 (3)
C2—C3	1.447 (2)	C21—C22	1.389 (3)
C2—S2	1.7545 (18)	C21—S2	1.7796 (18)
C2—Fe1	2.0272 (17)	C22—C23	1.391 (3)
C3—C4	1.441 (2)	C22—H22	0.9500
C3—S3	1.7529 (18)	C23—C24	1.380 (3)
C3—Fe1	2.0269 (17)	C23—H23	0.9500
C4—C5	1.423 (2)	C24—C25	1.383 (3)
C4—S4	1.7558 (18)	C24—H24	0.9500
C4—Fe1	2.0295 (17)	C25—C26	1.385 (3)
C5—Fe1	2.0311 (18)	C25—H25	0.9500
C5—H5	0.9500	C26—H26	0.9500
C6—C7	1.398 (3)	C31—C32	1.387 (2)
C6—C10	1.417 (3)	C31—C36	1.395 (3)
C6—Fe1	2.061 (2)	C31—S3	1.7709 (18)
C6—H6	0.9500	C32—C33	1.387 (3)
C7—C8	1.395 (3)	C32—H32	0.9500
C7—Fe1	2.0594 (19)	C33—C34	1.386 (3)
C7—H7	0.9500	C33—H33	0.9500
C8—C9	1.405 (3)	C34—C35	1.386 (3)
C8—Fe1	2.053 (2)	C34—H34	0.9500

C8—H8	0.9500	C35—C36	1.386 (3)
C9—C10	1.432 (4)	C35—H35	0.9500
C9—Fe1	2.046 (2)	C36—H36	0.9500
C9—H9	0.9500	C41—C42	1.390 (3)
C10—Fe1	2.048 (2)	C41—C46	1.400 (3)
C10—H10	0.9500	C41—S4	1.7784 (19)
C11—C12	1.388 (3)	C42—C43	1.391 (3)
C11—C16	1.392 (3)	C42—H42	0.9500
C11—S1	1.7731 (19)	C43—C44	1.389 (3)
C12—C13	1.390 (3)	C43—H43	0.9500
C12—H12	0.9500	C44—C45	1.385 (3)
C13—C14	1.384 (3)	C44—H44	0.9500
C13—H13	0.9500	C45—C46	1.386 (3)
C14—C15	1.385 (3)	C45—H45	0.9500
C14—H14	0.9500	C46—H46	0.9500

C5—C1—C2	108.20 (15)	C24—C25—H25	119.9
C5—C1—S1	125.79 (14)	C26—C25—H25	119.9
C2—C1—S1	125.84 (14)	C25—C26—C21	119.73 (19)
C5—C1—Fe1	69.48 (10)	C25—C26—H26	120.1
C2—C1—Fe1	69.16 (10)	C21—C26—H26	120.1
S1—C1—Fe1	123.36 (9)	C32—C31—C36	119.81 (17)
C1—C2—C3	107.66 (15)	C32—C31—S3	124.87 (14)
C1—C2—S2	126.00 (14)	C36—C31—S3	115.05 (14)
C3—C2—S2	126.17 (14)	C33—C32—C31	119.87 (18)
C1—C2—Fe1	69.26 (10)	C33—C32—H32	120.1
C3—C2—Fe1	69.07 (10)	C31—C32—H32	120.1
S2—C2—Fe1	123.49 (9)	C34—C33—C32	120.53 (18)
C4—C3—C2	107.28 (15)	C34—C33—H33	119.7
C4—C3—S3	126.85 (14)	C32—C33—H33	119.7
C2—C3—S3	124.82 (14)	C33—C34—C35	119.52 (18)
C4—C3—Fe1	69.29 (10)	C33—C34—H34	120.2
C2—C3—Fe1	69.09 (10)	C35—C34—H34	120.2
S3—C3—Fe1	117.71 (9)	C36—C35—C34	120.45 (18)
C5—C4—C3	108.55 (15)	C36—C35—H35	119.8
C5—C4—S4	124.71 (14)	C34—C35—H35	119.8
C3—C4—S4	126.71 (14)	C35—C36—C31	119.83 (18)
C5—C4—Fe1	69.54 (10)	C35—C36—H36	120.1
C3—C4—Fe1	69.09 (10)	C31—C36—H36	120.1
S4—C4—Fe1	125.78 (10)	C42—C41—C46	119.61 (17)
C4—C5—C1	108.31 (16)	C42—C41—S4	125.44 (14)
C4—C5—Fe1	69.43 (10)	C46—C41—S4	114.95 (14)
C1—C5—Fe1	69.29 (10)	C41—C42—C43	120.20 (18)
C4—C5—H5	125.8	C41—C42—H42	119.9
C1—C5—H5	125.8	C43—C42—H42	119.9
Fe1—C5—H5	127.0	C44—C43—C42	120.23 (19)
C7—C6—C10	107.8 (2)	C44—C43—H43	119.9
C7—C6—Fe1	70.11 (11)	C42—C43—H43	119.9

C10—C6—Fe1	69.35 (12)	C45—C44—C43	119.42 (18)
C7—C6—H6	126.1	C45—C44—H44	120.3
C10—C6—H6	126.1	C43—C44—H44	120.3
Fe1—C6—H6	126.0	C44—C45—C46	121.02 (18)
C8—C7—C6	109.1 (2)	C44—C45—H45	119.5
C8—C7—Fe1	69.91 (12)	C46—C45—H45	119.5
C6—C7—Fe1	70.21 (11)	C45—C46—C41	119.52 (18)
C8—C7—H7	125.5	C45—C46—H46	120.2
C6—C7—H7	125.5	C41—C46—H46	120.2
Fe1—C7—H7	126.0	C3—Fe1—C2	41.84 (7)
C7—C8—C9	108.4 (2)	C3—Fe1—C1	70.16 (7)
C7—C8—Fe1	70.43 (11)	C2—Fe1—C1	41.58 (7)
C9—C8—Fe1	69.68 (12)	C3—Fe1—C4	41.62 (7)
C7—C8—H8	125.8	C2—Fe1—C4	69.98 (7)
C9—C8—H8	125.8	C1—Fe1—C4	69.47 (7)
Fe1—C8—H8	125.7	C3—Fe1—C5	69.92 (7)
C8—C9—C10	107.4 (2)	C2—Fe1—C5	69.87 (7)
C8—C9—Fe1	70.21 (12)	C1—Fe1—C5	41.23 (7)
C10—C9—Fe1	69.61 (12)	C4—Fe1—C5	41.03 (7)
C8—C9—H9	126.3	C3—Fe1—C9	147.49 (9)
C10—C9—H9	126.3	C2—Fe1—C9	170.02 (10)
Fe1—C9—H9	125.5	C1—Fe1—C9	130.62 (9)
C6—C10—C9	107.3 (2)	C4—Fe1—C9	115.23 (9)
C6—C10—Fe1	70.31 (12)	C5—Fe1—C9	107.99 (8)
C9—C10—Fe1	69.43 (12)	C3—Fe1—C10	169.61 (10)
C6—C10—H10	126.3	C2—Fe1—C10	130.47 (9)
C9—C10—H10	126.3	C1—Fe1—C10	108.38 (8)
Fe1—C10—H10	125.5	C4—Fe1—C10	148.30 (10)
C12—C11—C16	119.25 (18)	C5—Fe1—C10	116.18 (9)
C12—C11—S1	124.52 (14)	C9—Fe1—C10	40.96 (11)
C16—C11—S1	116.23 (15)	C3—Fe1—C8	115.47 (8)
C11—C12—C13	120.04 (18)	C2—Fe1—C8	148.38 (9)
C11—C12—H12	120.0	C1—Fe1—C8	169.37 (9)
C13—C12—H12	120.0	C4—Fe1—C8	108.21 (8)
C14—C13—C12	120.60 (19)	C5—Fe1—C8	130.44 (8)
C14—C13—H13	119.7	C9—Fe1—C8	40.11 (10)
C12—C13—H13	119.7	C10—Fe1—C8	67.80 (9)
C13—C14—C15	119.21 (19)	C3—Fe1—C7	108.45 (8)
C13—C14—H14	120.4	C2—Fe1—C7	116.63 (8)
C15—C14—H14	120.4	C1—Fe1—C7	149.33 (8)
C16—C15—C14	120.60 (19)	C4—Fe1—C7	130.79 (8)
C16—C15—H15	119.7	C5—Fe1—C7	169.01 (8)
C14—C15—H15	119.7	C9—Fe1—C7	67.19 (9)
C15—C16—C11	120.24 (19)	C10—Fe1—C7	67.25 (9)
C15—C16—H16	119.9	C8—Fe1—C7	39.66 (9)
C11—C16—H16	119.9	C3—Fe1—C6	130.44 (8)
C26—C21—C22	120.10 (18)	C2—Fe1—C6	108.56 (8)
C26—C21—S2	121.49 (14)	C1—Fe1—C6	116.90 (8)

C22—C21—S2	118.33 (15)	C4—Fe1—C6	169.34 (8)
C21—C22—C23	119.7 (2)	C5—Fe1—C6	149.22 (8)
C21—C22—H22	120.1	C9—Fe1—C6	67.97 (9)
C23—C22—H22	120.1	C10—Fe1—C6	40.34 (10)
C24—C23—C22	120.0 (2)	C8—Fe1—C6	67.16 (8)
C24—C23—H23	120.0	C7—Fe1—C6	39.68 (8)
C22—C23—H23	120.0	C1—S1—C11	102.60 (9)
C23—C24—C25	120.20 (19)	C2—S2—C21	101.17 (8)
C23—C24—H24	119.9	C3—S3—C31	105.77 (8)
C25—C24—H24	119.9	C4—S4—C41	102.46 (8)
C24—C25—C26	120.2 (2)		

C5—C1—C2—C3	−0.09 (19)	C11—C12—C13—C14	1.9 (3)
S1—C1—C2—C3	175.37 (13)	C12—C13—C14—C15	−0.2 (3)
Fe1—C1—C2—C3	58.57 (12)	C13—C14—C15—C16	−1.8 (3)
C5—C1—C2—S2	−175.67 (13)	C14—C15—C16—C11	2.0 (3)
S1—C1—C2—S2	−0.2 (2)	C12—C11—C16—C15	−0.2 (3)
Fe1—C1—C2—S2	−117.01 (14)	S1—C11—C16—C15	−179.64 (16)
C5—C1—C2—Fe1	−58.66 (12)	C26—C21—C22—C23	0.7 (3)
S1—C1—C2—Fe1	116.80 (14)	S2—C21—C22—C23	177.48 (15)
C1—C2—C3—C4	0.29 (19)	C21—C22—C23—C24	0.6 (3)
S2—C2—C3—C4	175.86 (13)	C22—C23—C24—C25	−1.1 (3)
Fe1—C2—C3—C4	58.98 (12)	C23—C24—C25—C26	0.4 (3)
C1—C2—C3—S3	−168.60 (13)	C24—C25—C26—C21	0.8 (3)
S2—C2—C3—S3	7.0 (2)	C22—C21—C26—C25	−1.4 (3)
Fe1—C2—C3—S3	−109.91 (13)	S2—C21—C26—C25	−178.05 (15)
C1—C2—C3—Fe1	−58.69 (12)	C36—C31—C32—C33	0.7 (3)
S2—C2—C3—Fe1	116.88 (14)	S3—C31—C32—C33	−172.94 (15)
C2—C3—C4—C5	−0.38 (19)	C31—C32—C33—C34	−0.8 (3)
S3—C3—C4—C5	168.22 (13)	C32—C33—C34—C35	0.3 (3)
Fe1—C3—C4—C5	58.48 (12)	C33—C34—C35—C36	0.2 (3)
C2—C3—C4—S4	−178.59 (13)	C34—C35—C36—C31	−0.3 (3)
S3—C3—C4—S4	−10.0 (2)	C32—C31—C36—C35	−0.2 (3)
Fe1—C3—C4—S4	−119.73 (14)	S3—C31—C36—C35	174.06 (15)
C2—C3—C4—Fe1	−58.86 (12)	C46—C41—C42—C43	−0.8 (3)
S3—C3—C4—Fe1	109.74 (14)	S4—C41—C42—C43	179.69 (15)
C3—C4—C5—C1	0.3 (2)	C41—C42—C43—C44	0.3 (3)
S4—C4—C5—C1	178.58 (13)	C42—C43—C44—C45	0.0 (3)
Fe1—C4—C5—C1	58.53 (12)	C43—C44—C45—C46	0.2 (3)
C3—C4—C5—Fe1	−58.20 (12)	C44—C45—C46—C41	−0.8 (3)
S4—C4—C5—Fe1	120.05 (14)	C42—C41—C46—C45	1.1 (3)
C2—C1—C5—C4	−0.1 (2)	S4—C41—C46—C45	−179.43 (15)
S1—C1—C5—C4	−175.62 (13)	C5—C1—S1—C11	−66.45 (17)
Fe1—C1—C5—C4	−58.61 (12)	C2—C1—S1—C11	118.87 (16)
C2—C1—C5—Fe1	58.47 (12)	Fe1—C1—S1—C11	−153.99 (11)
S1—C1—C5—Fe1	−117.00 (14)	C12—C11—S1—C1	−13.77 (19)
C10—C6—C7—C8	0.0 (2)	C16—C11—S1—C1	165.64 (15)
Fe1—C6—C7—C8	−59.29 (14)	C1—C2—S2—C21	−73.60 (17)

C10—C6—C7—Fe1	59.34 (14)	C3—C2—S2—C21	111.62 (16)
C6—C7—C8—C9	−0.1 (2)	Fe1—C2—S2—C21	−161.07 (11)
Fe1—C7—C8—C9	−59.55 (14)	C26—C21—S2—C2	−57.21 (18)
C6—C7—C8—Fe1	59.48 (14)	C22—C21—S2—C2	126.06 (16)
C7—C8—C9—C10	0.1 (2)	C4—C3—S3—C31	84.12 (17)
Fe1—C8—C9—C10	−59.95 (14)	C2—C3—S3—C31	−109.17 (15)
C7—C8—C9—Fe1	60.02 (14)	Fe1—C3—S3—C31	168.05 (9)
C7—C6—C10—C9	0.0 (2)	C32—C31—S3—C3	−15.85 (19)
Fe1—C6—C10—C9	59.81 (14)	C36—C31—S3—C3	170.24 (14)
C7—C6—C10—Fe1	−59.82 (14)	C5—C4—S4—C41	70.06 (17)
C8—C9—C10—C6	0.0 (2)	C3—C4—S4—C41	−112.02 (16)
Fe1—C9—C10—C6	−60.37 (14)	Fe1—C4—S4—C41	158.63 (11)
C8—C9—C10—Fe1	60.33 (14)	C42—C41—S4—C4	8.07 (19)
C16—C11—C12—C13	−1.7 (3)	C46—C41—S4—C4	−171.41 (15)
S1—C11—C12—C13	177.67 (15)		