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# 2-Ferrocenyl-2-[(2-ferrocenylethenyl)(morpholin-4-yl)methyl]-1,3-dithiolane

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The molecular structure of 2-ferrocenyl-2-[(2-ferrocenylethenyl)(morpholin-4yl)methyl]-1,3-dithiolane,  $[Fe_2(C_5H_5)_2(C_{19}H_{21}NOS_2)]$  or  $C_{29}H_{31}Fe_2NOS_2$ , has the ferrocenyl fragments in a *trans* disposition with respect to the vinyl group. One of the methylene groups is disordered over two sites with occupancies of 0.782 (13):0.218 (13). In the crystal, cyclopentadienyl-C-H···O(morpholinyl) interactions feature within helical chains parallel to the *c*-axis direction. The chains are connected by methylene- and cyclopentadienyl-C-H···O(cyclopentadienyl) interactions.



#### Structure description

1,3-Dithiolanes, also known as *S*,*S*-thioacetals, are stable under acidic and basic conditions (Kocieneski *et al.*, 1994). They are of importance in their applications in synthetic, organic and medicinal chemistry (Wuts Peter, 2014) and are used in synthesis as a carbonyl protecting group and for the formation of carbon–carbon bonds through metalation (Gröbel & Seebach, 1977).

The dithiolane fragment is found in antibiotics and antifungals such as luliconazole, which has activity against *Candida albicans*, *Malassezia spp.* and *Aspergillus fumigatus* (Khanna & Bharti, 2014).

The lipophilic character of ferrocene makes it capable of penetrating cell membranes (Ludwig *et al.*, 2019). Therefore, its incorporation into biological molecules represents a matter of great interest in drug development. It has been pointed out that the addition of ferrocene residues in biologically active molecules offers the possibility of improving the efficacy of therapeutic drugs (Patra *et al.*, 2017). In this connection, diferrocenyl-1,3-dithiolane derivatives have pharmacological activity and may be considered as lead candidates for the development of new drugs or as building blocks for new molecules (Mlostoń *et al.*, 2018).

#### Table 1

Hydrogen-bond geometry (Å,  $^\circ).$ 

Cg1-Cg3 are the centroids of the (C10-C14), (C25-C29) and (C15-C19) rings, respectively.

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	$D - H \cdots A$
$C27-H27\cdots O1^{i}$	0.95	2.59	3.492 (7)	158
$C4-H4B\cdots Cg1^{ii}$	0.95	2.89	3.796 (9)	153
$C7 - H7A \cdots Cg2^{iii}$	0.95	2.92	3.733 (6)	140
$C17 - H17 \cdots Cg3^{iv}$	0.95	2.74	3.623 (7)	155

Symmetry codes: (i)  $-x + \frac{3}{2}, -y + 1, z + \frac{1}{2}$ ; (ii) x - 1, y, z; (iii)  $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$ ; (iv)  $x + \frac{1}{2}, -y + \frac{1}{2}, -z$ .

The asymmetric unit of the title compound, Fig. 1, is formed by ferrocenyl vinyl, morpholinyl, ferrocenyl and dithiolate groups. About the C1=C2 vinyl group, the morpholine fragment is cis to the vinyl-bound ferrocenyl residue and trans to the vinyl-H atom. The five-membered dithiolate ring has a twisted conformation at the S1-C3 bond with puckering parameters:  $q_2 = 0.590 (18) \text{ Å}$  and  $\varphi_2 = 14.0 (15)^\circ$ , and asymmetry parameters (Duax et al., 1976):  $\Delta = 343.7 (24), \tau =$ 49.7 (8),  $\Delta Cs(S1) = 61.8$  (5),  $\Delta Cs(C3) = 49.5$  (5) and  $\Delta C2$  $(S1-C3) = 76.6 (6)^{\circ}$ , with bond lengths of 1.858 (5) Å for S1-C3 and C4-C5 of 1.521 (11) Å. On the other hand, the six-membered morpholinyl ring, formed by the O1-C7-C6-N1-C9-C8 atoms, has a chair conformation with puckering parameters (Cremer & Pople, 1975): Q = 0.559 (6) Å,  $\theta =$ 1.6 (5)° and  $\varphi = 24$  (30)° for the calculation starting from the O1 atom through to the C8 atom, and asymmetry parameters:  $\Delta C_2$  (O1–C7) = 1.4 (6),  $\Delta C_2$  (C6–C7) = 3.3 (6),  $\Delta C_2$  (C6–N1) = 2.3 (6),  $\Delta C_2$  (O1–C8) = 2.3 (6),  $\Delta C_s$ (O1) = 0.5 (5),  $\Delta Cs$ (C7) = 2.3 (5),  $\Delta Cs(C6) = 2.6$  (5) and  $\Delta Cs(N1) = 0.5$  (5)° with an average endocyclic torsion angle of 56.7  $(2)^{\circ}$ . The orientations of the five-membered rings about the Fe1 and Fe2 atoms are very close to staggered and eclipsed, respectively.

In the crystal, Fig. 2, cyclopentadienyl-C-H···O(morpholinyl) interactions (Table 1)feature within helical chains parallel to the *c*-axis direction. The chains are connected





Molecular structure of the title compound showing the atom-numbering scheme and displacement ellipsoids for non-H atoms at the 50% probability level.



The crystal array of the title compound showing intermolecular contacts of the type  $C-H\cdots O$  and  $C-H\cdots \pi$  interactions.

within a three-dimensional architecture *via* methylene- and cyclopentadienyl- $C-H \cdots O(cyclopentadienyl)$  interactions.

#### Synthesis and crystallization

1,2-Ethanodithiol (15 mmol) was added to a solution of 1-morpholino-2,3-diferrocenylcyclopropenonylium tetrafluoridoborate (10 mmol) in acetonitrile (30 ml), and the mixture was stirred in a dry inert atmosphere under reflux for 8 h. The solvents were removed *in vacuo*, and the residues underwent chromatography on alumina (hexane–dichloromethane, 4:1 *v:v*). Suitable orange crystals of 2-ferrocenyl-2-[(2-ferrocenylethenyl)(morpholin-4-yl)methyl]-1,3-dithiolane were obtained by the slow evaporation of its saturated dichloromethane/hexane (ratio 1:2 *v/v*) solution. Yield (25%), m.p. 460–461 K. The reaction scheme is shown in Fig. 3.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 274–2.76 (4*H*, *t*, 2NCH<sub>2</sub>, 4 Hz), 3.29–3.35 (2*H*, *m*, SCH<sub>2</sub>), 3.48–3.52 (2*H*, *m*, SCH<sub>2</sub>), 3.55–3.26 (4*H*, *t*, 2OCH<sub>2</sub>, 4 Hz), 4.10 (5*H*, *s*, C<sub>5</sub>H<sub>5</sub>), 4.29 (5*H*, *s*, C<sub>5</sub>H<sub>5</sub>), 4.13 (2*H*, *m*, C<sub>5</sub>H<sub>4</sub>), 4.20 (2*H*, *m*, C<sub>5</sub>H<sub>4</sub>), 4.34 (2*H*, *m*, C<sub>5</sub>H<sub>4</sub>), 4.35 (2*H*, *m*, C<sub>5</sub>H<sub>4</sub>), 6.96 (1*H*, *s*, =CH) p.p.m., <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$ : 39.48 (SCH<sub>2</sub>), 51.16 (NCH<sub>2</sub>), 67.15 (OCH<sub>2</sub>), 69.24 (SCS), 69.13, 69.74 (C<sub>5</sub>H<sub>5</sub>), 67.61, 68.71, 69.93, 70.29 (2 C<sub>5</sub>H<sub>4</sub>), 81.24, 95.89 (C<sub>*ipso*</sub> Fc), 119.84 (2 C), 149.13 (–C=) p.p.m., MS: *m*/*z* 585 [*M*]<sup>+</sup>. Analysis calculated for C<sub>29</sub>H<sub>31</sub>Fe<sub>2</sub>NOS<sub>2</sub>: C, 59.51, H, 5.34, N, 2.39%. Found C, 60.05, H, 5.41, N, 2.45%.



Figure 3 Reaction scheme.

#### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The atoms of the methylene-C4 group are disordered over two sets of sites and were refined with equivalent anisotropic displacement parameters to yield occupancies of 0.782 (13):0.218 (13).

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## Table 2

Experimental details.

Crystal data	
Chemical formula	$[Fe_2(C_5H_5)_2(C_{19}H_{21}NOS_2)]$
$M_{ m r}$	585.37
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	130
a, b, c (Å)	7.5425 (3), 17.6838 (9),
$V(Å^3)$	$2510 \otimes (2)$
7 (A )	2515.8 (2)
Z Padiation type	4 Mo Ka
Kadiation type $(mm^{-1})$	1 24
$\mu$ (IIIII ) Crustel size (mm)	1.54
Crystal size (mm)	0.54 × 0.44 × 0.12
Data collection	
Diffractometer	Xcalibur, Atlas, Gemini
Absorption correction	Analytical (CrysAlis RED;
	Agilent, 2013)
$T_{\min}, T_{\max}$	0.022, 0.250
No. of measured, independent and	9130, 5847, 5231
observed $[I > 2\sigma(I)]$ reflections	
R <sub>int</sub>	0.045
$(\sin \theta / \lambda)_{\rm max} ({\rm \AA}^{-1})$	0.705
Refinement $P(F^2) = P(F^2)$	0.056 0.120 1.06
$R[F > 2\sigma(F)], wR(F), S$	0.056, 0.139, 1.06
No. of reflections	5847
No. of parameters	320
H-atom treatment $(1 - 3)$	H-atom parameters constrained
$\Delta \rho_{\rm max},  \Delta \rho_{\rm min}  ({\rm e \ A}^{-5})$	1.23, -1.23
Absolute structure	Flack x determined using 17/8
	quotients $[(I^{-})-(I^{-})]/[(I^{-})+(I^{-})]$
	(Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.027 (18)

Computer programs: CrysAlis PRO and CrysAlis RED (Agilent, 2013), SHELXT2018 (Sheldrick, 2015a), SHELXL2018 (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012) and Mercury (Macrae et al., 2020).

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# full crystallographic data

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2-Ferrocenyl-2-[(2-ferrocenylethenyl)(morpholin-4-yl)methyl]-1,3-dithiolane

Crystal data

 $[Fe_{2}(C_{5}H_{5})_{2}(C_{19}H_{21}NOS_{2})]$   $M_{r} = 585.37$ Orthorhombic,  $P2_{1}2_{1}2_{1}$  a = 7.5425 (3) Å b = 17.6838 (9) Å c = 18.8920 (11) Å V = 2519.8 (2) Å<sup>3</sup> Z = 4F(000) = 1216

Data collection

Xcalibur, Atlas, Gemini
diffractometer
Graphite monochromator
Detector resolution: 10.4685 pixels mm <sup>-1</sup>
$\omega$ scans
Absorption correction: analytical
(CrysAlis RED; Agilent, 2013)
$T_{\min} = 0.022, \ T_{\max} = 0.250$

#### Refinement

Refinement on  $F^2$ Least-squares matrix: full  $R[F^2 > 2\sigma(F^2)] = 0.056$  $wR(F^2) = 0.139$ S = 1.065847 reflections 320 parameters 0 restraints Primary atom site location: structure-invariant direct methods Secondary atom site location: difference Fourier map  $D_x = 1.543 \text{ Mg m}^{-3}$ Mo K $\alpha$  radiation,  $\lambda = 0.71073 \text{ Å}$ Cell parameters from 3368 reflections  $\theta = 5.2-29.4^{\circ}$  $\mu = 1.34 \text{ mm}^{-1}$ T = 130 KPrism, brown  $0.54 \times 0.44 \times 0.12 \text{ mm}$ 

9130 measured reflections 5847 independent reflections 5231 reflections with  $I > 2\sigma(I)$  $R_{int} = 0.045$  $\theta_{max} = 30.1^{\circ}, \ \theta_{min} = 3.5^{\circ}$  $h = -6 \rightarrow 10$  $k = -15 \rightarrow 24$  $l = -17 \rightarrow 26$ 

Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained  $w = 1/[\sigma^2(F_o^2) + (0.0712P)^2 + 0.1471P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{max} < 0.001$  $\Delta\rho_{max} = 1.23$  e Å<sup>-3</sup>  $\Delta\rho_{min} = -1.23$  e Å<sup>-3</sup> Absolute structure: Flack *x* determined using 1778 quotients  $[(I^+)-(I^-)]/[(I^+)+(I^-)]$  (Parsons *et al.*, 2013) Absolute structure parameter: 0.027 (18)

#### 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.

	x	У	Z	$U_{ m iso}$ */ $U_{ m eq}$	Occ. (<1)
C1	0.6462 (7)	0.3262 (3)	0.2856 (3)	0.0184 (11)	
H1	0.606180	0.278710	0.302928	0.022*	
C2	0.5778 (7)	0.3857 (3)	0.3200 (3)	0.0164 (11)	
C3	0.4556 (7)	0.3753 (3)	0.3847 (3)	0.0176 (10)	
C4	0.1034 (10)	0.3431 (5)	0.3520 (5)	0.034 (2)	0.782 (13)
H4A	0.026843	0.334821	0.393800	0.041*	0.782 (13)
H4B	0.026165	0.351702	0.310356	0.041*	0.782 (13)
C4P	0.177 (4)	0.3480 (18)	0.3075 (19)	0.034 (2)	0.218 (13)
H4PA	0.047803	0.351224	0.298393	0.041*	0.218 (13)
H4PB	0.239322	0.353020	0.261684	0.041*	0.218 (13)
C5	0.2191 (8)	0.2740 (4)	0.3395 (4)	0.0338 (15)	
H5A	0.268795	0.274712	0.291039	0.041*	
H5B	0.148982	0.227075	0.345535	0.041*	
C6	0.5293 (8)	0.4979 (3)	0.2434 (3)	0.0244 (12)	
H6A	0.404142	0.481627	0.239108	0.029*	
H6B	0.593904	0.481116	0.200573	0.029*	
C7	0.5391 (8)	0.5828 (3)	0.2501 (3)	0.0268 (12)	
H7A	0.490242	0.606267	0.206710	0.032*	
H7B	0.465229	0.599228	0.290606	0.032*	
C8	0.7914 (8)	0.5758 (3)	0.3227 (3)	0.0264 (12)	
H8A	0.722502	0.592520	0.364499	0.032*	
H8B	0.914846	0.593825	0.328617	0.032*	
C9	0.7905 (7)	0.4905 (3)	0.3192 (3)	0.0208 (11)	
H9A	0.868833	0.473088	0.280452	0.025*	
H9B	0.835530	0.469225	0.364270	0.025*	
C10	0.7709 (7)	0.3204 (3)	0.2263 (3)	0.0193 (11)	
C11	0.8416 (7)	0.2473 (3)	0.2068 (3)	0.0223 (12)	
H11	0.817860	0.200934	0.230297	0.027*	
C12	0.9524 (7)	0.2565 (3)	0.1467 (3)	0.0235 (12)	
H12	1.015044	0.217531	0.122817	0.028*	
C13	0.9528 (7)	0.3343 (3)	0.1286 (3)	0.0220 (11)	
H13	1.017439	0.356530	0.090791	0.026*	
C14	0.8403 (7)	0.3734 (3)	0.1765 (3)	0.0188 (11)	
H14	0.815352	0.426084	0.175621	0.023*	
C15	0.4455 (8)	0.3252 (4)	0.1031 (4)	0.0330 (15)	
H15	0.382220	0.364764	0.125998	0.040*	
C16	0.5535 (9)	0.3328 (4)	0.0423 (4)	0.0393 (18)	
H16	0.575569	0.378270	0.017001	0.047*	
C17	0.6235 (8)	0.2596 (5)	0.0257 (3)	0.0396 (18)	
H17	0.701159	0.247630	-0.012305	0.048*	
C18	0.5559 (8)	0.2092 (4)	0.0760 (4)	0.0352 (15)	
H18	0.579266	0.156479	0.077488	0.042*	
C19	0.4484 (8)	0.2488 (4)	0.1238 (4)	0.0312 (14)	
H19	0.387975	0.227760	0.163245	0.037*	
C20	0.5469 (6)	0.4080 (3)	0.4483 (3)	0.0186 (11)	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(\hat{A}^2)$ 

C21	0.5531 (8)	0.4860 (3)	0.4679 (3)	0.0233 (12)
H21	0.488755	0.525816	0.445987	0.028*
C22	0.6713 (8)	0.4938 (4)	0.5256 (3)	0.0330 (15)
H22	0.700553	0.539908	0.548606	0.040*
C23	0.7387 (7)	0.4214 (4)	0.5433 (3)	0.0291 (13)
H23	0.819272	0.410200	0.580494	0.035*
C24	0.6634 (7)	0.3687 (4)	0.4949 (3)	0.0228 (12)
H24	0.686980	0.315958	0.493921	0.027*
C25	0.2141 (7)	0.3841 (3)	0.5604 (3)	0.0240 (12)
H25	0.145269	0.362048	0.523752	0.029*
C26	0.3266 (8)	0.3445 (4)	0.6076 (3)	0.0275 (13)
H26	0.345859	0.291407	0.608294	0.033*
C27	0.4053 (8)	0.3984 (4)	0.6536 (3)	0.0285 (13)
H27	0.487580	0.387627	0.690309	0.034*
C28	0.3397 (8)	0.4713 (4)	0.6352 (3)	0.0276 (13)
H28	0.369460	0.517597	0.657731	0.033*
C29	0.2213 (8)	0.4622 (4)	0.5770 (3)	0.0291 (13)
H29	0.158548	0.501472	0.553572	0.035*
Fe1	0.69918 (10)	0.29194 (4)	0.12507 (4)	0.01799 (19)
Fe2	0.46821 (10)	0.42310 (5)	0.55104 (4)	0.01902 (19)
N1	0.6094 (6)	0.4643 (3)	0.3067 (2)	0.0194 (9)
O1	0.7173 (6)	0.6085 (2)	0.2605 (2)	0.0296 (10)
S1	0.24352 (16)	0.42501 (9)	0.36629 (8)	0.0240 (3)
S2	0.39473 (18)	0.27808 (8)	0.40423 (8)	0.0226 (3)

Atomic displacement parameters  $(Å^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.021 (2)	0.020 (3)	0.014 (2)	-0.002 (2)	-0.004 (2)	0.0020 (19)
C2	0.016 (2)	0.020 (3)	0.013 (2)	-0.002 (2)	-0.004(2)	0.0024 (19)
C3	0.016 (2)	0.011 (2)	0.025 (3)	0.001 (2)	-0.001 (2)	0.0024 (19)
C4	0.017 (3)	0.036 (4)	0.050 (6)	-0.005 (3)	-0.006 (3)	-0.012 (4)
C4P	0.017 (3)	0.036 (4)	0.050 (6)	-0.005 (3)	-0.006 (3)	-0.012 (4)
C5	0.028 (3)	0.034 (4)	0.039 (4)	-0.002 (3)	-0.008 (3)	-0.011 (3)
C6	0.024 (3)	0.028 (3)	0.021 (3)	0.001 (3)	-0.003 (2)	0.000 (2)
C7	0.031 (3)	0.026 (3)	0.024 (3)	0.004 (3)	0.002 (3)	0.003 (2)
C8	0.027 (3)	0.027 (3)	0.025 (3)	-0.005 (3)	0.000 (3)	0.000 (2)
C9	0.021 (2)	0.023 (3)	0.019 (3)	-0.005 (2)	-0.001 (2)	0.000 (2)
C10	0.019 (2)	0.021 (3)	0.018 (3)	0.001 (2)	-0.003 (2)	-0.003 (2)
C11	0.021 (3)	0.024 (3)	0.022 (3)	0.003 (2)	0.001 (2)	0.002 (2)
C12	0.020 (2)	0.027 (3)	0.023 (3)	0.006 (2)	-0.001 (2)	-0.006 (2)
C13	0.019 (2)	0.027 (3)	0.019 (3)	-0.001 (2)	0.001 (2)	-0.002 (2)
C14	0.020 (3)	0.020 (3)	0.016 (2)	-0.004 (2)	-0.003 (2)	-0.0015 (19)
C15	0.021 (3)	0.040 (4)	0.038 (4)	0.004 (3)	-0.012 (3)	-0.011 (3)
C16	0.039 (4)	0.041 (4)	0.037 (4)	-0.020 (3)	-0.022 (3)	0.020 (3)
C17	0.023 (3)	0.080 (6)	0.016 (3)	-0.009 (3)	0.000 (3)	-0.014 (3)
C18	0.030 (3)	0.031 (4)	0.044 (4)	-0.003 (3)	-0.009 (3)	-0.011 (3)
C19	0.020 (2)	0.046 (4)	0.027 (3)	-0.011 (3)	-0.005 (3)	0.002 (3)

C20	0.014 (2)	0.023 (3)	0.018 (2)	-0.004 (2)	0.005 (2)	0.001 (2)
C21	0.027 (3)	0.026 (3)	0.017 (3)	-0.008(2)	0.011 (2)	0.000(2)
C22	0.028 (3)	0.046 (4)	0.025 (3)	-0.015 (3)	0.009 (3)	-0.008 (3)
C23	0.018 (2)	0.051 (4)	0.019 (3)	-0.005 (3)	-0.001 (2)	-0.006 (3)
C24	0.015 (2)	0.033 (3)	0.020(3)	0.001 (2)	-0.001 (2)	-0.004 (2)
C25	0.014 (2)	0.036 (3)	0.022 (3)	-0.006 (2)	0.005 (2)	-0.004 (2)
C26	0.027 (3)	0.029 (3)	0.026 (3)	-0.006 (3)	0.006 (3)	0.003 (2)
C27	0.027 (3)	0.040 (4)	0.019 (3)	-0.001 (3)	0.008 (2)	0.000 (2)
C28	0.028 (3)	0.029 (3)	0.026 (3)	-0.007 (2)	0.012 (3)	-0.007(2)
C29	0.023 (3)	0.032 (3)	0.032 (3)	0.004 (3)	0.009 (3)	0.004 (2)
Fe1	0.0182 (3)	0.0201 (4)	0.0156 (4)	-0.0006 (3)	-0.0010 (3)	-0.0012 (3)
Fe2	0.0164 (3)	0.0252 (4)	0.0155 (4)	-0.0026 (3)	0.0021 (3)	-0.0013 (3)
N1	0.017 (2)	0.022 (2)	0.019 (2)	-0.0008 (19)	-0.0028 (19)	0.0033 (18)
01	0.036 (2)	0.021 (2)	0.032 (2)	-0.0023 (19)	0.003 (2)	0.0049 (17)
S1	0.0162 (5)	0.0282 (8)	0.0276 (7)	0.0028 (5)	-0.0020 (5)	-0.0003 (6)
S2	0.0217 (6)	0.0198 (7)	0.0261 (7)	-0.0040 (6)	0.0027 (6)	-0.0003 (5)

Geometric parameters (Å, °)

C1—C2	1.340 (8)	C14—H14	0.9500
C1-C10	1.467 (8)	C15—C19	1.406 (10)
C1—H1	0.9500	C15—C16	1.415 (10)
C2—N1	1.433 (7)	C15—Fe1	2.045 (6)
C2—C3	1.541 (7)	C15—H15	0.9500
C3—C20	1.502 (7)	C16—C17	1.432 (11)
C3—S2	1.817 (5)	C16—Fe1	2.043 (6)
C3—S1	1.858 (5)	C16—H16	0.9500
C4—C5	1.521 (11)	C17—C18	1.399 (10)
C4—S1	1.813 (8)	C17—Fe1	2.044 (6)
C4—H4A	0.9900	C17—H17	0.9500
C4—H4B	0.9900	C18—C19	1.402 (9)
C4P—C5	1.48 (3)	C18—Fe1	2.041 (6)
C4P—S1	1.83 (3)	C18—H18	0.9500
C4P—H4PA	0.9900	C19—Fe1	2.040 (6)
C4P—H4PB	0.9900	C19—H19	0.9500
C5—S2	1.804 (6)	C20—C24	1.424 (8)
C5—H5A	0.9900	C20—C21	1.430 (8)
С5—Н5В	0.9900	C20—Fe2	2.046 (5)
C6—N1	1.466 (7)	C21—C22	1.414 (9)
С6—С7	1.509 (9)	C21—Fe2	2.028 (5)
С6—Н6А	0.9900	C21—H21	0.9500
С6—Н6В	0.9900	C22—C23	1.418 (10)
C7—O1	1.433 (8)	C22—Fe2	2.035 (6)
C7—H7A	0.9900	C22—H22	0.9500
С7—Н7В	0.9900	C23—C24	1.423 (8)
C8—O1	1.425 (7)	C23—Fe2	2.046 (5)
С8—С9	1.511 (8)	С23—Н23	0.9500
C8—H8A	0.9900	C24—Fe2	2.053 (6)

C8—H8B	0.9900	C24—H24	0.9500
C9—N1	1.461 (7)	C25—C26	1.416 (9)
С9—Н9А	0.9900	C25—C29	1.417 (8)
С9—Н9В	0.9900	C25—Fe2	2.044 (5)
C10—C14	1.427 (7)	С25—Н25	0.9500
C10—C11	1.445 (8)	C26—C27	1.420 (9)
C10—Fe1	2.051 (5)	C26—Fe2	2.053 (6)
C11—C12	1.420 (8)	C26—H26	0.9500
C11—Fe1	2.040 (6)	C27—C28	1.423 (9)
С11—Н11	0.9500	C27—Fe2	2.042.(6)
C12-C13	1 417 (8)	C27—H27	0.9500
C12—Fe1	2 051 (6)	$C_{28}$ $C_{29}$	1 426 (9)
C12—H12	0.9500	C28—Fe2	2 048 (6)
C12 - C12	1 421 (8)	C28—H28	0.9500
C13—Fe1	2 055 (5)	C29_Fe2	2.046 (6)
C13—H13	0.9500	$C_{29}$ H29	0.9500
C14—Fe1	2 038 (5)		0.9500
	2.038 (3)		
C2—C1—C10	132.2 (5)	С22—С23—Н23	126.4
C2-C1-H1	113.9	C24—C23—H23	126.4
C10-C1-H1	113.9	Fe2—C23—H23	126.0
C1-C2-N1	127.8 (5)	$C_{23}$ $C_{24}$ $C_{20}$	108.9(5)
C1 - C2 - C3	1213(5)	$C_{23}$ $C_{24}$ $F_{e2}$	694(3)
N1-C2-C3	110.8(4)	$C_{20}$ $C_{24}$ Fe <sup>2</sup>	69.4(3)
$C_{20} = C_{3} = C_{2}^{2}$	1083(4)	$C_{23}$ $C_{24}$ $H_{24}$	125.6
$C_{20} = C_{3} = S_{2}$	108.5(4)	$C_{20}$ $C_{24}$ $H_{24}$	125.6
$C_2 = C_3 = S_2^2$	115.2(4)	$F_{e2}$ $C_{24}$ $H_{24}$	127.2
$C_2 = C_3 = S_2$	113.2(4) 111.2(4)	$C_{26} = C_{25} = C_{29}$	127.2 108 7 (5)
$C_2 = C_3 = S_1$	1081(3)	$C_{26} = C_{25} = C_{25}$	70.1(3)
$S_2 = C_3 = S_1$	105.6(3)	$C_{20} = C_{23} = 1 c_2$	69.8(3)
52 - 63 - 51	109.0(5) 109.3(5)	$C_{25} = C_{25} = 1.02$	125.7
$C_{5} = C_{4} = B_{1}$	109.5 (5)	$C_{20} = C_{23} = H_{23}$	125.7
$C_{3}$	109.8	$E_{23} = E_{23} = E$	125.7
51 - C4 - H4R	109.8	$C_{25} = C_{25} = C_{125}$	120.0
$C_{3}$ $C_{4}$ $H_{4}$ $R_{5}$	109.8	$C_{25} = C_{20} = C_{27}$	107.7(0)
	109.8	$C_{23} = C_{20} = F_{23}$	69.3(3)
$\begin{array}{cccc} \Pi 4A - C 4 - \Pi 4D \\ C 5 - C 4D - S 1 \end{array}$	100.5	$C_{27} = C_{20} = F_{22}$	126.2
$C_5 = C_4 P = U_4 P_4$	100.5	$C_{23}$ $C_{20}$ $C$	126.2
$C_{3}$ $C_{4P}$ $H_{4PA}$	109.5	$C_2/-C_{20}$ -H20	120.2
SI - C4P - H4PA	109.5	re2 - C20 - ri20	120.0
$C_{2}$ $C_{4}$ $C_{4$	109.5	$C_{26} = C_{27} = C_{28}$	108.2 (5)
SI-C4P-H4PB	109.5	$C_{26} = C_{27} = F_{e2}$	/0.1 (3)
H4PA - C4P - H4PB	108.1	C28—C27—Fe2	69.9 (3)
C4r - C5 - S2	113.6 (12)	$C_{20} = C_{27} = H_{27}$	125.9
C4 - C5 - S2	100.5 (5)	$L_{2\delta}$ $L_{2}$ $H_{2}$	125.9
U4—U5—H5A	110.4	$He_2 - U_2 / - H_2 / U_2$	125.7
52—C5—H5A	110.4	$C_2 / - C_2 = C_2 $	10/./(5)
С4—С5—Н5В	110.4	C27—C28—Fe2	69.4 (3)
S2—C5—H5B	110.4	C29—C28—Fe2	69.6 (3)

H5A—C5—H5B	108.6	C27—C28—H28	126.2
N1—C6—C7	108.3 (5)	C29—C28—H28	126.2
N1—C6—H6A	110.0	Fe2—C28—H28	126.5
С7—С6—Н6А	110.0	C25—C29—C28	107.7 (5)
N1—C6—H6B	110.0	C25—C29—Fe2	69.7 (3)
С7—С6—Н6В	110.0	C28—C29—Fe2	69.7 (3)
H6A—C6—H6B	108.4	С25—С29—Н29	126.2
O1—C7—C6	111.9 (5)	С28—С29—Н29	126.2
O1—C7—H7A	109.2	Fe2—C29—H29	126.1
С6—С7—Н7А	109.2	C14—Fe1—C19	138.9 (3)
O1—C7—H7B	109.2	C14—Fe1—C11	68.7 (2)
С6—С7—Н7В	109.2	C19—Fe1—C11	110.7 (2)
H7A—C7—H7B	107.9	C14—Fe1—C18	178.5 (3)
01—C8—C9	111.6 (5)	C19—Fe1—C18	40.2 (3)
O1—C8—H8A	109.3	C11—Fe1—C18	110.2 (3)
C9—C8—H8A	109.3	C14—Fe1—C16	113.3 (3)
01—C8—H8B	109.3	C19—Fe1—C16	67.9 (3)
C9—C8—H8B	109.3	C11—Fe1—C16	177.9(3)
H8A—C8—H8B	108.0	C18—Fe1—C16	677(3)
N1-C9-C8	109 1 (5)	C14—Fe1—C17	1414(3)
N1-C9-H9A	109.9	C19—Fe1—C17	680(3)
C8—C9—H9A	109.9	C11—Fe1—C17	1373(3)
N1—C9—H9B	109.9	C18—Fe1—C17	40 1 (3)
C8—C9—H9B	109.9	C16—Fe1—C17	410(3)
H9A - C9 - H9B	108.3	C14—Fe1—C15	1124(3)
C14-C10-C11	106.5 (5)	C19—Fe1—C15	40.3 (3)
$C_{14}$ $C_{10}$ $C_{1}$	133.8 (5)	C11—Fe1—C15	139.2(3)
$C_{11} - C_{10} - C_{1}$	119.6 (5)	C18—Fe1—C15	67.6(3)
C14— $C10$ — $Fe1$	69.1 (3)	C16—Fe1—C15	40.5 (3)
C11 - C10 - Fe1	68.9(3)	C17—Fe1—C15	68 5 (3)
C1 - C10 - Fe1	124 1 (4)	C14—Fe1—C10	40.9(2)
$C_{12}$ $C_{11}$ $C_{10}$	108.6(5)	C19—Fe1—C10	10.9(2)
C12 $C11$ $E10$	70.1.(3)	C11—Fe1—C10	414(2)
C10-C11-Fe1	69 7 (3)	C18—Fe1—C10	1377(3)
C12-C11-H11	125.7	$C_{16}$ Fe1 $-C_{10}$	137.7(3) 140 3 (3)
C10-C11-H11	125.7	C17—Fe1—C10	1777(3)
Fe1H11	125.7	C15—Fe1—C10	1114(2)
$C_{13}$ $C_{12}$ $C_{11}$	107.8 (5)	C14—Fe1—C12	68.6(2)
C13 - C12 - Fe1	700(3)	C19 - Fe1 - C12	1388(3)
$C_{11}$ $C_{12}$ $F_{e1}$	69 3 (3)	$C11\_Fe1\_C12$	40.6(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	126.1	C18 Fe1 $C12$	111 4 (3)
$C_{11} = C_{12} = H_{12}$	120.1	$C_{16} = 101 - C_{12}$	111.4(3)
$E_{1} = C_{12} = H_{12}$	120.1	C17 - Fe1 - C12	1100(3)
$C_{12}$ $C_{13}$ $C_{14}$	120.2	C15 = Fe1 = C12	170.9(3)
$C_{12} = C_{13} = C_{14}$	60 6 (3)	C10  Fe1  C12	172.0(3)
$C_{12} = C_{13} = F_{c_1}$	69.0 (3)	C10 Fe1 $C12$	40.6(2)
$C_{12} = C_{13} = C_{12}$	125.7	C10  Fe1  C12	1787(2)
$C_{12}$ $C_{13}$ $C_{13}$ $C_{13}$ $C_{14}$ $C_{12}$ $C_{12}$ $C_{13}$ $C$	125.7	$C_{13} = Fe_1 = C_{13}$	1/0.7(3)
UI4-UI3-III3	123.1	011-FCI-013	00.1 (2)

Fe1—C13—H13	127.2	C18—Fe1—C13	140.2 (2)
C13—C14—C10	108.6 (5)	C16—Fe1—C13	113.4 (2)
C13—C14—Fe1	70.3 (3)	C17—Fe1—C13	113.0 (2)
C10-C14-Fe1	70.0 (3)	C15—Fe1—C13	140.6 (3)
C13—C14—H14	125.7	C10—Fe1—C13	68.6 (2)
C10—C14—H14	125.7	C12—Fe1—C13	40.4 (2)
Fe1—C14—H14	125.5	C21—Fe2—C22	40.7 (2)
C19—C15—C16	107.9 (6)	C21—Fe2—C27	157.7 (2)
C19—C15—Fe1	69.7 (4)	C22—Fe2—C27	122.1 (3)
C16—C15—Fe1	69.7 (4)	C21—Fe2—C25	123.2 (2)
С19—С15—Н15	126.1	C22—Fe2—C25	158.9 (3)
C16—C15—H15	126.1	C27—Fe2—C25	68.1 (2)
Fe1—C15—H15	126.1	C21—Fe2—C23	68.8 (3)
C15—C16—C17	107.8 (6)	C22—Fe2—C23	40.7 (3)
C15—C16—Fe1	69.8 (4)	C27—Fe2—C23	107.3 (3)
C17—C16—Fe1	69.5 (4)	$C_{25}$ —Fe2—C23	159.4 (3)
C15—C16—H16	126.1	$C_{21}$ —Fe2—C29	106.7 (3)
C17—C16—H16	126.1	$C^{22}$ —Fe <sup>2</sup> —C <sup>29</sup>	122.3(3)
Fe1—C16—H16	126.2	$C_{27}$ $F_{e2}$ $C_{29}$	685(3)
C18 - C17 - C16	107.0 (6)	$C_{25}$ $F_{e2}$ $C_{29}$	40.5(2)
C18 - C17 - Fe1	69 9 (4)	$C_{23}$ $F_{e2}$ $C_{29}$	1584(3)
$C_{16}$ $C_{17}$ $F_{e1}$	69 5 (4)	$C_{21}$ $F_{e2}$ $C_{20}$	41 1 (2)
C18 - C17 - H17	126.5	$C_{22}$ —Fe2—C20	68.8(2)
$C_{16} - C_{17} - H_{17}$	126.5	$C_{27}$ $F_{e2}$ $C_{20}$	1599(2)
Fe1—C17—H17	125.7	$C_{25}$ $F_{e2}$ $C_{20}$	109.9(2) 108.1(2)
C17 - C18 - C19	109 3 (6)	$C_{23}$ $F_{e2}$ $C_{20}$	690(2)
C17 - C18 - Fe1	70 1 (4)	$C_{29}$ Fe <sup>2</sup> $C_{20}$	1224(2)
C19-C18-Fe1	69 9 (4)	$C_{21}$ $F_{e2}$ $C_{28}$	122.1(2) 121.5(3)
C17 - C18 - H18	125.4	$C^{22}$ Fe <sup>2</sup> $C^{28}$	1065(3)
C19—C18—H18	125.4	$C_{27}$ $F_{e2}$ $C_{28}$	40 7 (2)
Fe1—C18—H18	126.3	$C_{25}$ $F_{e2}$ $C_{28}$	68.2(2)
C18 - C19 - C15	108.1 (6)	$C_{23}$ $F_{e2}$ $C_{28}$	122.2(2)
C18— $C19$ — $Fe1$	70 0 (4)	$C29 - Fe^2 - C28$	40.8 (3)
C15— $C19$ —Fel	70.1 (3)	$C_{20}$ $F_{e2}$ $C_{28}$	1581(2)
C18—C19—H19	126.0	$C_{21}$ —Fe2—C26	159.8 (2)
C15 - C19 - H19	126.0	$C^{22}$ —Fe <sup>2</sup> —C <sup>26</sup>	158.6(3)
Fe1—C19—H19	125.6	$C_{27}$ $F_{e2}$ $C_{26}$	40.6 (2)
$C_{24}$ $C_{20}$ $C_{21}$	106.9 (5)	$C_{25}$ $F_{e^{2}}$ $C_{26}$	40.4(2)
$C_{24}$ $C_{20}$ $C_{21}$ $C_{20}$ $C_{3}$	1262(5)	$C_{23}$ $F_{e2}$ $C_{26}$	1231(3)
$C_{21} - C_{20} - C_{3}$	126.2(5)	$C_{29}$ Fe <sup>2</sup> $C_{26}$	68 3 (3)
$C_{24}$ $C_{20}$ $F_{e^{2}}$	69.9 (3)	$C_{20}$ $F_{e2}$ $C_{26}$	123.8(2)
$C_{21} = C_{20} = F_{e_{2}}$	68 8 (3)	$C_{28}$ —Fe2—C26	684(3)
$C_{3}$ $C_{20}$ $F_{e}^{2}$	132 6 (3)	$C_{21}$ Fe <sup>2</sup> $C_{24}$	68.3(2)
$C_{22} - C_{21} - C_{20}$	108.3 (6)	C22 - Fe2 - C24	68.0 (3)
$C_{22}$ $C_{21}$ $F_{e2}$	69.9 (3)	$C_{27}$ —Fe2—C24	123.8 (3)
$C_{20}$ $C_{21}$ $F_{e2}$	70.2 (3)	C25 - Fe2 - C24	124.0 (2)
C22—C21—H21	125.9	C23—Fe2—C24	40.6 (2)
$C_{20}$ $C_{21}$ $H_{21}$	125.9	$C_{29}$ —Fe2—C24	159.2 (2)
			(2)

Fe2—C21—H21	125.7	C20—Fe2—C24	40.7 (2)
C21—C22—C23	108.7 (6)	C28—Fe2—C24	159.2 (2)
C21—C22—Fe2	69.4 (3)	C26—Fe2—C24	108.9 (3)
C23—C22—Fe2	70.1 (4)	C2—N1—C9	115.7 (4)
C21—C22—H22	125.7	C2—N1—C6	117.8 (4)
C23—C22—H22	125.7	C9—N1—C6	112.9 (4)
Fe2—C22—H22	126.4	C8-01-C7	110.6 (4)
$C^{22}$ $C^{23}$ $C^{24}$	107 3 (5)	C4 - S1 - C3	987(3)
$C_{22} = C_{23} = C_{21}$	69 3 (3)	C4P = S1 = C3	899(9)
$C_{24} = C_{23} = F_{e2}$	70.0(3)	$C_{5}$	94.9(3)
024 025 102	70.0 (5)	05-52-05	)4.) (3)
C10 C1 C2 N1	0.6(0)	$C_{24}$ $C_{20}$ $C_{21}$ $C_{22}$	-0.1(6)
$C_{10} = C_{1} = C_{2} = C_{1}^{2}$	0.0(9)	$C_{24} = C_{20} = C_{21} = C_{22}$	-0.1(0)
C10-C1-C2-C3	-1/6.2(5)	$C_{3}$ $C_{20}$ $C_{21}$ $C_{22}$	-1/2.3(5)
C1 = C2 = C3 = C20	115.7 (5)	$Fe_2 - C_2 0 - C_2 1 - C_2 2$	59.7 (4)
NI = C2 = C3 = C20	-61.7(5)	C24—C20—C21—Fe2	-59.8 (4)
C1—C2—C3—S2	-6.0 (6)	C3—C20—C21—Fe2	128.0 (5)
N1—C2—C3—S2	176.7 (3)	C20—C21—C22—C23	-0.6(6)
C1—C2—C3—S1	-123.8 (5)	Fe2—C21—C22—C23	59.3 (4)
N1—C2—C3—S1	58.9 (5)	C20—C21—C22—Fe2	-59.9 (4)
S1—C4P—C5—S2	-24 (2)	C21—C22—C23—C24	1.1 (6)
S1—C4—C5—S2	43.6 (7)	Fe2—C22—C23—C24	59.9 (4)
N1—C6—C7—O1	56.4 (6)	C21—C22—C23—Fe2	-58.8 (4)
O1—C8—C9—N1	-55.9 (6)	C22—C23—C24—C20	-1.2 (6)
C2-C1-C10-C14	-12.8 (10)	Fe2-C23-C24-C20	58.3 (4)
C2-C1-C10-C11	170.8 (6)	C22—C23—C24—Fe2	-59.5 (4)
C2-C1-C10-Fe1	-105.8 (6)	C21—C20—C24—C23	0.8 (6)
C14—C10—C11—C12	0.4 (6)	C3—C20—C24—C23	173.0 (5)
C1-C10-C11-C12	177.7 (5)	Fe2—C20—C24—C23	-58.3(4)
Fe1—C10—C11—C12	59 5 (4)	$C_{21}$ $C_{20}$ $C_{24}$ $F_{e^{2}}$	59 1 (4)
C14-C10-C11-Fe1	-591(4)	$C_{3}$ $C_{20}$ $C_{24}$ $F_{e2}$	-1287(5)
C1 - C10 - C11 - Fe1	118 1 (5)	$C_{29}$ $C_{25}$ $C_{26}$ $C_{27}$	-0.4(7)
$C_{10} = C_{10} = C_{11} = C_{12}$	110.1(5)	$E_{2} = E_{2} = E_{2$	50 0 (4)
$E_{10} = C_{11} = C_{12} = C_{13}$	50.6(4)	$C_{20} = C_{20} = C_{20} = C_{20} = C_{20}$	-50.3(4)
FeI = CII = CI2 = CI3	59.0 (4)	$C_{29} = C_{23} = C_{20} = F_{22}$	-39.3(4)
C10-C11-C12-Fei	-59.5(4)	$C_{25} = C_{20} = C_{27} = C_{28}$	0.0(7)
CII = CI2 = CI3 = CI4	-1.0(6)	Fe2	59.7 (4)
Fel—C12—C13—C14	58.2 (4)	C25—C26—C27—Fe2	-59.1 (4)
C11—C12—C13—Fel	-59.2 (4)	C26—C27—C28—C29	-0.6 (7)
C12—C13—C14—C10	1.2 (6)	Fe2—C27—C28—C29	59.2 (4)
Fe1—C13—C14—C10	59.8 (4)	C26—C27—C28—Fe2	-59.9 (4)
C12-C13-C14-Fe1	-58.6 (4)	C26—C25—C29—C28	0.0 (7)
C11—C10—C14—C13	-1.0 (6)	Fe2—C25—C29—C28	-59.6 (4)
C1-C10-C14-C13	-177.7 (6)	C26—C25—C29—Fe2	59.5 (4)
Fe1-C10-C14-C13	-60.0 (4)	C27—C28—C29—C25	0.4 (7)
C11-C10-C14-Fe1	59.0 (4)	Fe2—C28—C29—C25	59.5 (4)
C1-C10-C14-Fe1	-117.7 (6)	C27—C28—C29—Fe2	-59.1 (4)
C19—C15—C16—C17	-0.1 (7)	C1—C2—N1—C9	-65.2 (7)
Fe1—C15—C16—C17	59.4 (4)	C3—C2—N1—C9	111.9 (5)
C19-C15-C16-Fe1	-59.4 (4)	C1—C2—N1—C6	72.9 (7)

0.5 (7) 60.1 (4)	C3—C2—N1—C6 C8—C9—N1—C2	-110.0(5) -164.5(5)
-59.5 (4)	C8—C9—N1—C6	55.4 (6)
-0.8 (7)	C7—C6—N1—C2	165.4 (5)
59.0 (4)	C7—C6—N1—C9	-55.4 (6)
-59.8 (4)	C9—C8—O1—C7	58.4 (6)
0.8 (7)	C6—C7—O1—C8	-59.0 (6)
59.9 (4)	C5—C4—S1—C3	-16.1 (7)
-59.1 (4)	C5—C4P—S1—C3	43.3 (18)
-0.4 (7)	C20—C3—S1—C4	-134.0 (5)
-59.9 (4)	C2—C3—S1—C4	107.3 (5)
59.4 (4)	S2—C3—S1—C4	-16.5 (4)
-89.6 (6)	C20—C3—S1—C4P	-165.0 (12)
36.2 (6)	C2—C3—S1—C4P	76.2 (12)
151.8 (4)	S2—C3—S1—C4P	-47.6 (12)
81.2 (6)	C4P—C5—S2—C3	-9.1 (16)
-153.1 (5)	C4—C5—S2—C3	-50.4 (6)
-37.4 (6)	C20—C3—S2—C5	156.7 (4)
175.0 (4)	C2—C3—S2—C5	-81.7 (4)
-59.2 (6)	S1—C3—S2—C5	37.4 (3)
56.4 (6)		
	$\begin{array}{l} 0.5 \ (7) \\ 60.1 \ (4) \\ -59.5 \ (4) \\ -0.8 \ (7) \\ 59.0 \ (4) \\ -59.8 \ (4) \\ 0.8 \ (7) \\ 59.9 \ (4) \\ -59.1 \ (4) \\ -0.4 \ (7) \\ -59.9 \ (4) \\ 59.4 \ (4) \\ 59.4 \ (4) \\ -89.6 \ (6) \\ 36.2 \ (6) \\ 151.8 \ (4) \\ 81.2 \ (6) \\ -153.1 \ (5) \\ -37.4 \ (6) \\ 175.0 \ (4) \\ -59.2 \ (6) \\ 56.4 \ (6) \end{array}$	$\begin{array}{llllllllllllllllllllllllllllllllllll$

# Hydrogen-bond geometry (Å, °)

Cg1-Cg3 are the centroids of the (C10-C14), (C25-C29) and (C15-C19) rings, respectively.

D—H	H···A	D····A	D—H···A	
0.95	2.59	3.492 (7)	158	
0.95	2.89	3.796 (9)	153	
0.95	2.92	3.733 (6)	140	
0.95	2.74	3.623 (7)	155	
	<i>D</i> —H 0.95 0.95 0.95 0.95 0.95	D—H         H···A           0.95         2.59           0.95         2.89           0.95         2.92           0.95         2.74	D—H         H···A         D···A           0.95         2.59         3.492 (7)           0.95         2.89         3.796 (9)           0.95         2.92         3.733 (6)           0.95         2.74         3.623 (7)	D—H         H···A         D···A         D—H···A           0.95         2.59         3.492 (7)         158           0.95         2.89         3.796 (9)         153           0.95         2.92         3.733 (6)         140           0.95         2.74         3.623 (7)         155

Symmetry codes: (i) -x+3/2, -y+1, z+1/2; (ii) x-1, y, z; (iii) -x+1/2, -y+1, z-1/2; (iv) x+1/2, -y+1/2, -z.