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1-[(*E*)-5-Ferrocenylvinyl-2-methylthien-3-yl]-2-(5-formyl-2-methylthien-3-yl)cyclopentene

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In the title molecule, [Fe(C_5H_5)($C_{23}H_{21}OS_2$)], the C=C double bond has a *trans* configuration, and the dihedral angle between the thiophene rings is 66.9 (1)°.

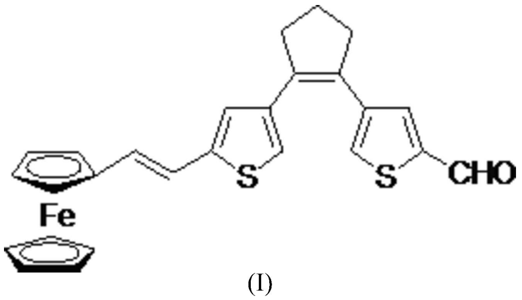
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.040
wR factor = 0.117
Data-to-parameter ratio = 14.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Diarylethenes, notably the bis(thien-3-yl) system, are the most promising photochromic compounds for use in photoelectronic applications such as optical data storage, molecular wires and photo-switching devices because of their fatigue resistance and thermal stability (Irie, 2000). In this paper, we present the crystal structure of (I) which was synthesized by a Wittig reaction of ferrocenylmethylphosphonium bromide (Yuan *et al.*, 2005) with 1,2-bis(5-formyl-2-methylthien-3-yl)-cyclopentene (Lucas *et al.*, 2003).



(I)

The molecular structure of (I) is shown in Fig. 1 and selected bond lengths and angles are given in Table 1. In the ferrocenyl unit, the cyclopentadienyl (Cp) rings are essentially fully eclipsed. The C=C double bond (defined by atoms C17–C19) forms a dihedral angle of 11.2 (3)° with the plane of atoms C19–C23. The two cyclopentadienyl rings are essentially parallel, making a dihedral angle of 0.8 (2)°. The thiophene ring (C12/C13/S2/C16/C15) makes a dihedral angle of 17.1 (2)° with the Cp ring (C19–C23) and the dihedral angle between the two thiophene rings is 66.9 (1)°. The crystal structure is, in part, stabilized by weak C—H···O hydrogen bonds (Table 2).

Experimental

To a slurry of $FcCH_2PPh_3Br$ (1.08 g,2.0 mmol) in THF (50 ml), $NaN(TMS)_2$ [0.6 ml of a 2.5M solution in THF, 1.2 mmol; TMS is bis(trimethylsilyl)amide] was added. The slurry was stirred at room temperature for 30 min, then a solution of 1,2-bis(5-formyl-2-methylthien-3-yl)cyclopentene (0.7 g in 20 ml of THF, 2.21 mmol) was added slowly *via* a syringe and the resulting solution was stirred for 30 min, quenched with 50 ml water, and extracted with Et_2O (3×50 ml). The organic layers were combined and washed with brine, then dried over $MgSO_4$. The solvents were removed *in vacuo*. The crude product was purified by chromatography [silica gel, eluent hexane/CH_2Cl_2 (2:1)], giving the title compound as a red solid (0.30 g, 30%). Crystals appropriate for data collection were obtained by slow diffusion of hexane into a solution of (I) in dichloromethane at 293 K.

Crystal data

$[Fe(C_5H_5)(C_{23}H_{21}OS_2)]$
$M_r = 498.46$
Monoclinic, $P2_1/c$
$a = 25.665$ (3) Å
$b = 7.8952$ (8) Å
$c = 12.1933$ (13) Å
$\beta = 90.996$ (2)°
$V = 2470.4$ (5) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.80$ mm^{-1}
$T = 292$ (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART-CCD diffractometer
Absorption correction: none
11447 measured reflections
4312 independent reflections
3663 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.117$
$S = 1.05$
4312 reflections
301 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.42$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.26$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Fe1—C19	2.046 (3)	C7—C11	1.341 (4)
O1—C1	1.206 (5)	C11—C12	1.471 (4)
S1—C2	1.719 (3)	C16—C17	1.448 (3)
S2—C16	1.729 (3)	C17—C18	1.333 (4)
C1—C2	1.442 (4)	C18—C19	1.458 (4)
C4—C7	1.469 (4)		
O1—C1—C2	125.2 (4)	C18—C17—C16	126.6 (3)
C1—C2—S1	122.4 (3)	C17—C18—C19	124.9 (3)
C6—C5—S1	119.7 (2)	C20—C19—C23	107.2 (3)
C11—C7—C4	129.1 (2)	C20—C19—C18	126.7 (3)
C7—C11—C12	129.2 (3)	C23—C19—C18	126.1 (3)
C14—C13—S2	119.3 (2)	C21—C20—C19	107.6 (3)
C17—C16—S2	122.6 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1$^{\rm i}$	0.93	2.43	3.263 (4)	149
C8—H8D···O1$^{\rm ii}$	0.95	2.50	3.336 (5)	146

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

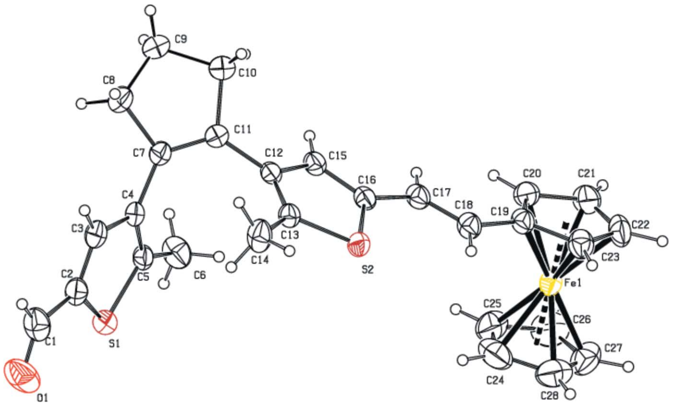


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are represented by circles of arbitrary radius. The minor disorder component is not shown.

Atoms C8, C9 and C10 atoms are disordered over two sites with refined occupancies of 0.60 (3) and 0.40 (3) for the major and minor components, respectively. All H atoms were placed in idealized positions, C—H = 0.96 Å (methyl H), 0.97 Å (methylene H), 0.98 Å (cyclopentadienyl H) or 0.93 Å (all other H), and refined as riding, with $U_{\rm iso}$(H)= 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(C$_{\rm methyl}$).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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