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

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.112
Data-to-parameter ratio = 18.0

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

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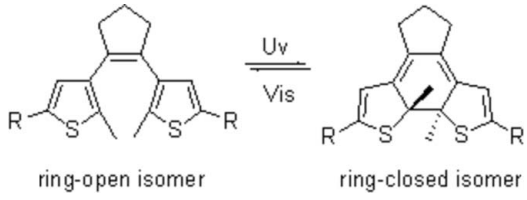
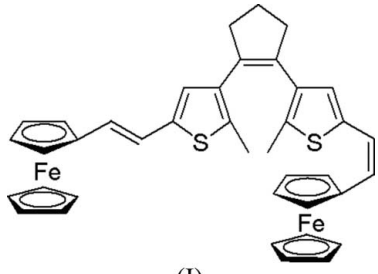
The title molecule, $[Fe_2(C_5H_5)_2(C_{29}H_{26}S_2)]$, contains two ferrocenyl groups bonded through a (*Z*)-CH═CH double bond and an (*E*)-CH═CH double bond.

Comment

Photochromic compounds have attracted increasing attention because of their potential application in optical memory media and switching devices (Irie *et al.*, 2002). Photochromism is defined as a reversible transformation of a chemical species induced in one or both directions by absorption of electromagnetic radiation between two isomers, a ring-open isomer and a ring-closed isomer, having different absorption spectra. The two isomers differ from one another not only in their absorption spectra but also in various physical and chemical properties, such as refractive index, dielectric constant, luminescence, optical rotation, electronic conductivity, oxidation–reduction potential and geometric structure. Among known photochromic systems, diarylethenes bearing two thiophene-derived groups have attracted the most attention, since they are well suited as switching units (Tian & Yang, 2004), and we have focused our attention on this type of material. In this paper, we present the X-ray crystal structure of the title compound, (I), which was synthesized by a Wittig reaction of ferrocenyl methyl phosphonium bromide with 1,2-bis(5-formyl-2-methylthien-3-yl)cyclopentene (Lucas *et al.*, 2003).





(I)

In the molecular structure of (I) (Fig. 1), the two cyclopentadienyl rings C1–C5 and C6–C10 are essentially parallel, with a dihedral angle of 0.8 (2)° between them, as are the C30–

C34 and C35–39 rings, with a dihedral angle of 2.4 (2)° between them. The (*E*)-C11═C12 double bond is slightly twisted from the C6–C10 ring, as indicated by the dihedral angle of 11.7 (3)° formed by the plane of atoms C10–C12 with the C6–C10 ring. On the other hand, the (*Z*)-C28═C29 double bond is essentially coplanar with the C30–C34 ring, as indicated by the dihedral angle of 5.6 (4)° formed by the C28–C30 plane with the C30–C34 ring. The C13–C16/S1 thiophene ring is essentially parallel to the C6–10 ring, as indicated by the dihedral angle of 4.6 (2)°, whereas the dihedral angle formed by the C23–C27/S2 ring with the C30–C34 ring is 51.6 (2)°.

Experimental

The title compound was synthesized according to the literature procedure of Yuan *et al.* (2005). Crystals of (I) appropriate for data collection were obtained by slow diffusion of hexane into a solution of the compound in dichloromethane at 293 K.

Crystal data

$[Fe_2(C_5H_5)_2(C_{29}H_{26}S_2)]$
M_r = 680.50
Monoclinic, $P2_1/c$
a = 16.2228 (11) Å
b = 20.1251 (14) Å
c = 10.2569 (7) Å
β = 105.342 (1)°
V = 3229.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 292 (2) K
0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
26882 measured reflections
7039 independent reflections
5780 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.112
S = 1.08
7039 reflections
390 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

All H atoms were positioned geometrically, with C—H = 0.96 (methyl H), 0.97 (methylene H), 0.98 (cyclopentadienyl H) and 0.93 Å (other H), and were refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{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: *PLATON*.

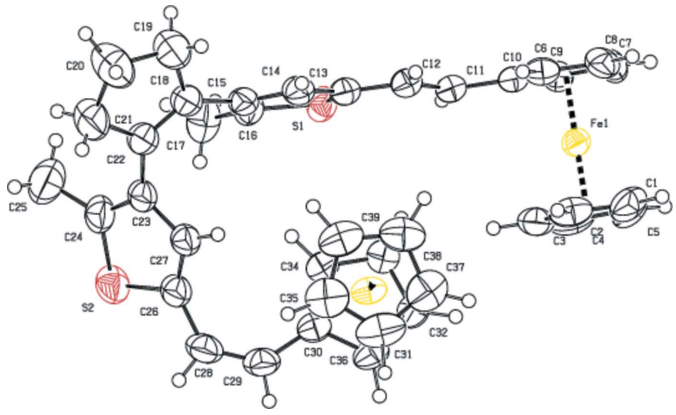


Figure 1
A view of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

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