

1,2-Bis(5-chloro-2-methyl-3-thienyl)cyclopentene

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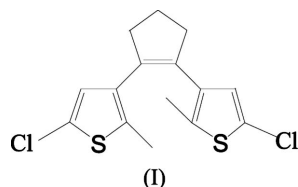
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.056
 wR factor = 0.182
Data-to-parameter ratio = 20.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound, $\text{C}_{15}\text{H}_{14}\text{Cl}_2\text{S}_2$, two substituted thiophene rings are *cis* positioned with respect to the double bond of a cyclopentene ring. The ring skeleton of the molecule is not planar.

Comment

Among many known photochromic systems, diarylethenes bearing two thiophene-derived groups have received the most attention since they are particularly well suited as switching units (Tian & Yang, 2004). Therefore, we have focused on their precursors and analogues. Starting from the title compound, (I), we can easily substitute chlorine by other functional groups and obtain new derivatives. In this paper, we present the crystal structure analysis of (I).



Due to the rigid framework of the cyclopentene ring, atoms C3/C6/C7/C8/C9/C10/C11 should be coplanar. However, due to an overcrowding effect of the two methyl groups, atoms C3 and C11 deviate from the plane of the cyclopentene ring (Fig. 1). Thus, the three five-membered rings are not coplanar. The two heterocyclic rings make a dihedral angle of 59.36 (14) $^\circ$, whereas these two rings make dihedral angles with the cyclopentene ring of 41.43 (17) and 51.09 (17) $^\circ$. Both

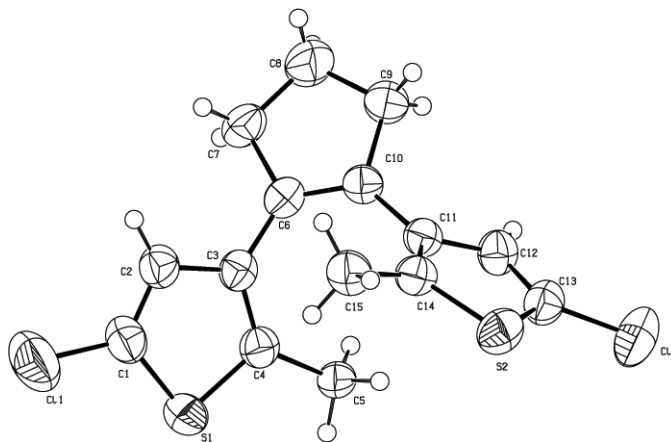


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of an arbitrary size.

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substituents on the thiophene rings (chlorine and methyl groups) are displaced from the planes of the thiophene rings, with a maximum deviation for atom C5 [0.082 (3) Å]. Selected torsion angles describing the molecular conformation are listed in Table 1.

Experimental

The title compound was synthesized according to the literature method of Fürstner *et al.* (1994). Crystals appropriate for data collection were obtained by slow evaporation of an ethanol solution at 277 K.

Crystal data

$C_{15}H_{14}Cl_2S_2$	$D_x = 1.423 \text{ Mg m}^{-3}$
$M_r = 329.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3518 reflections
$a = 8.8423 (8) \text{ \AA}$	$\theta = 2.2\text{--}23.2^\circ$
$b = 12.2784 (11) \text{ \AA}$	$\mu = 0.68 \text{ mm}^{-1}$
$c = 14.4380 (13) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 101.374 (2)^\circ$	Block, colourless
$V = 1536.7 (2) \text{ \AA}^3$	$0.20 \times 0.20 \times 0.10 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2385 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.036$
Absorption correction: none	$\theta_{\text{max}} = 27.5^\circ$
12 983 measured reflections	$h = -11 \rightarrow 11$
3505 independent reflections	$k = -15 \rightarrow 15$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0971P)^2 + 0.2616P]$
$R[F^2 > 2\sigma(F^2)] = 0.056$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.182$	$(\Delta/\sigma)_{\text{max}} = 0.008$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$
3505 reflections	$\Delta\rho_{\text{min}} = -0.44 \text{ e \AA}^{-3}$
174 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

C1—C2	1.354 (5)	C12—C13	1.343 (4)
C1—S1	1.706 (3)	C13—C12	1.710 (3)
C1—Cl1	1.711 (4)	C13—S2	1.720 (3)
C2—C1—C11	126.9 (3)	C12—C13—C12	127.1 (3)
S1—C1—C11	120.2 (2)	C12—C13—S2	121.01 (19)
S1—C1—C2—C3	−1.9 (4)	C11—C12—C13—C12	178.5 (2)
Cl1—C1—C2—C3	178.8 (2)	C11—C12—C13—S2	−1.5 (3)
C2—C3—C4—C5	175.8 (3)	C12—C11—C14—C15	177.6 (3)
C2—C3—C4—S1	−1.8 (3)	C12—C11—C14—S2	−1.2 (3)

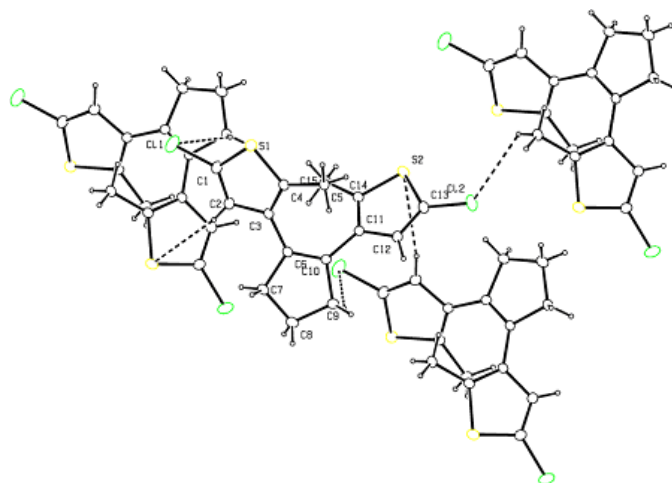


Figure 2

Inter-molecular hydrogen bonding in the crystal structure of (I). Hydrogen-bonding interactions are indicated by dashed lines.

Methyl H atoms were constrained to an ideal geometry, with C—H distances of 0.98 Å and $U_{\text{iso}}(\text{H})$ values of $1.5U_{\text{eq}}(\text{C})$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed at geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–1.00 Å and $U_{\text{iso}}(\text{H})$ values of $1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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