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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.048
 wR factor = 0.129
Data-to-parameter ratio = 12.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

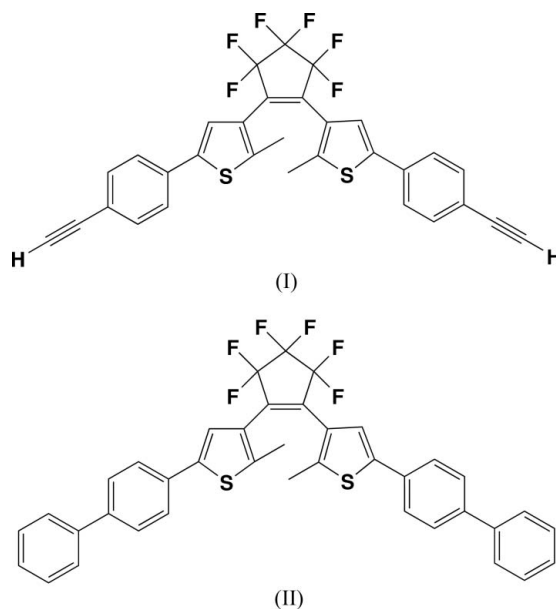
A perfluorocyclopentene dithienylethene based molecular switch: 1,2-bis[5-(4-ethynylphenyl)-2-methylthiophen-3-yl]-3,3,4,4,5,5-hexafluorocyclopentene

The title compound, $\text{C}_{31}\text{H}_{18}\text{F}_6\text{S}_2$, is a molecular switch based on dithienylperfluorocyclopentene. The molecule possesses pseudo- C_2 symmetry and has the open form of the switch. There are a number of intramolecular $\text{C}-\text{H} \cdots \text{F}$ hydrogen bonds, but in the crystal structure there are no interactions between symmetry-related molecules.

Received 21 July 2006
Accepted 15 August 2006

Comment

One of the most promising classes of photochromic materials is that of diarylethenes with attached thiophene rings (dithienylethenes), whose photochromic properties were first described by Irie and Mohri (1988). The most commonly studied dithienylethene has been the one based on dithienylperfluorocyclopentene (Irie, 2000; Fernández-Acebes & Lehn, 1999; Myles & Branda, 2002; Jong *et al.*, 2003; Ern *et al.*, 2002; Krayushkin *et al.*, 2002; Shim *et al.*, 2003). We report here the crystal structure analysis of the precursor, 1,2-bis[5-(4-ethynylphenyl)-2-methylthiophen-3-yl]-3,3,4,4,5,5-hexafluorocyclopentene, (I). Our interest in compound (I) stems from the sheer scope of thiolization of the terminal ethynyl groups and their subsequent immobilization on a gold/silver surface. The investigation of reversible photoswitching in such systems will provide insight into their potential applications in molecular electronics.



The molecular structure of compound (I) is shown in Fig. 1. The bond distances and angles (Table 1) are very close to those observed in similar molecules reported in the

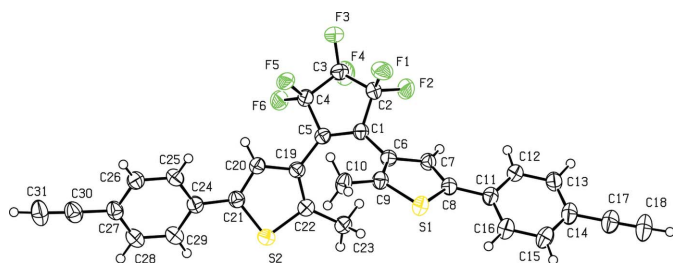


Figure 1

The molecular structure of compound (I), showing the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level.

Cambridge Structural Database (Version 5.27, May 2006 update; Allen, 2002). Compound (I) has pseudo- C_2 symmetry and has the open form of the switch (Fig. 1). The five-membered ring (C1–C5) has an envelope conformation with atom C3 displaced from the least-squares plane through the other four atoms by 0.320 (4) Å. The methyl-attached thiophene groups have an antiparallel conformation and the least-squares planes of the thiophene rings are inclined to one another at 60.38 (12)°. The benzene rings (C11–C16 and C24–C29) are inclined relative to the thiophene rings involving atoms S1 and S2 by 17.45 (11)° and 23.39 (12)°, respectively. The two benzene rings are inclined to one another at 67.25 (12)°. Within the molecule there are some intramolecular C–H...F short contacts (Table 2) that certainly have an influence on the conformation of the central part of the molecule. In the crystal structure of (I), there are no intermolecular hydrogen bonds and no other direction-specific interactions between adjacent molecules.

A diphenyl analogue, (II), was synthesized to serve as a reference molecule to (I) for solution studies. Crystals of compound (II) were of poor quality, diffracting weakly beyond 40° in 2θ and with significant mosaic spread (Iyer *et al.*, 2006). There was positional disorder not only in the central group of fluorine atoms, on atom C3, but also in the biphenyl group on one side of the molecule. However, the overall structure is comparable to that of compound (I).

Experimental

Compound (I) was synthesized according to the procedure published by Osuka *et al.* (2001). Crystals were grown from a solution in dichloromethane.

Crystal data

$C_{31}H_{18}F_6S_2$	$Z = 4$
$M_r = 568.57$	$D_x = 1.467 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 26.7998$ (17) Å	$\mu = 0.27 \text{ mm}^{-1}$
$b = 9.0730$ (5) Å	$T = 173$ (2) K
$c = 10.7628$ (6) Å	Block, pale blue
$\beta = 100.337$ (5)°	$0.40 \times 0.37 \times 0.30 \text{ mm}$
$V = 2574.5$ (3) Å ³	

Data collection

Stoe IPDS-2 diffractometer	4577 independent reflections
ω and φ scans	3722 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.107$
18574 measured reflections	$\theta_{\text{max}} = 25.1^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.129$
 $S = 1.05$
 4577 reflections
 354 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.7289P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} = 0.001$$

$$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$$

Table 1

Selected geometric parameters (Å, °).

S1–C8	1.726 (2)	S2–C21	1.725 (2)
S1–C9	1.714 (3)	S2–C22	1.716 (3)
C8–S1–C9	93.13 (12)	C21–S2–C22	93.41 (12)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C7–H7A...F2	0.95	2.40	2.929 (3)	115
C20–H20A...F5	0.95	2.48	3.073 (3)	120

H atoms were included in calculated positions and treated as riding atoms, with C–H = 0.95–0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times $U_{\text{eq}}(\text{C})$.

Data collection: *X-AREA* (Stoe & Cie, 2004); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2004); 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: *SHELXL97*.

We thank the EU project MWFM (grant No. G5RD-CT-2002–00776) and the Swiss National Science Foundation for financial support.

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