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# 3,3,4,4,5,5-Hexafluoro-1,2-bis(3-methylbenzo[*b*]-2-thienyl)cyclopentene

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The title compound, $C_{23}H_{14}F_6S_2$, was crystallized from a PMMA/chloroform solution (PMMA = polymethylmethacrylate), and its crystal structure was determined. The molecule adopts a photoactive antiparallel conformation. The distance between the two reactive C atoms was determined to be 3.560 (7)Å. The molecule has crystallographic twofold rotation symmetry.

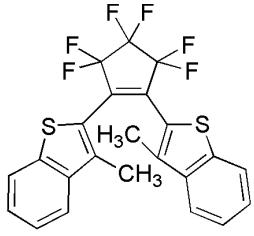
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.061
$wR$ factor = 0.119
Data-to-parameter ratio = 11.6

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

## Comment

As a result of their good thermal stability and high fatigue resistance, photochromic diarylethenes have potential application for opto-electronic devices, such as optical memories and switches (Irie, 2000; Fernandez-Asebes & Lehn, 1999). Diarylethenes usually have one of two conformations in the solid state, parallel or antiparallel (Kobatake *et al.*, 1999; Shibata *et al.*, 2002).




(I)

The title compound (BTPF), (I), is a bis(2-thienyl)perfluorocyclopentene derivative. It has attracted our attention due to its interesting non-linear optical properties (Sun *et al.*, 2002). Unlike most diarylethenes recrystallized from organic solution (Pu *et al.*, 2003), the crystals of BTPF were obtained from a PMMA/chloroform solution. The polymer in chloroform causes deposition of BTPF/PMMA films, which act as a membranous substrate that mediates the growth of BTPF crystals. As a result, well-formed yellow block-shaped single crystals were obtained.

The X-ray crystallographic study showed that BTPF is packed in the antiparallel conformation. The general view of a molecule, together with the atom-numbering scheme, is shown in Fig. 1. The distance between the reactive C atoms (C5 and C5$^{i}$; symmetry code (i) = $-x, y, \frac{1}{2}-z$) is 3.560 (7) Å , which is close enough for a photocyclization reaction (Ramamurthy & Venkatesan, 1987). The molecule has crystallographic twofold rotation symmetry, the axis passing through C3 and the opposite C=C ring of the cyclopentene ring.

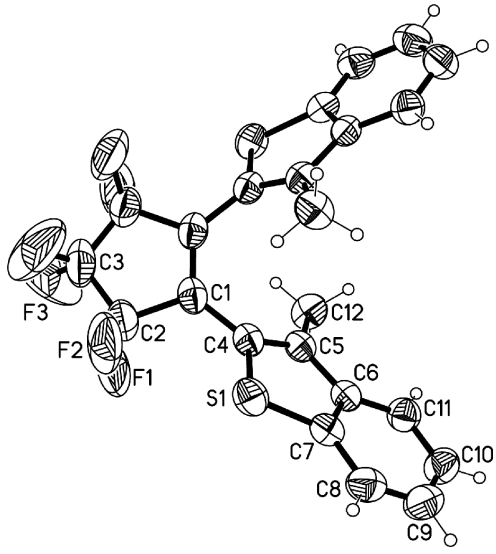



**Figure 1**
View of the molecule of BTPF, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 35% probability level.

## Experimental

The title compound was prepared according to a method described in the literature (Sun *et al.*, 2002). Single crystals were obtained from a PMMA/chloroform solution. The weight ratio of PMMA and BTPF was 5:1.

*Crystal data*

$C_{23}H_{14}F_6S_2$
$M_r$ = 468.46
Monoclinic, $C2/c$
$a$ = 18.8350 (18) Å
$b$ = 9.3507 (9) Å
$c$ = 11.643 (2) Å
$\beta$ = 94.653 (11)°
$V$ = 2043.8 (5) Å$^3$
$Z$ = 4
$D_x$ = 1.522 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 36 reflections
$\theta$ = 3.8–12.6°
$\mu$ = 0.32 mm$^{-1}$
$T$ = 293 (2) K
Block, yellow
0.6 × 0.6 × 0.2 mm

*Data collection*

Bruker $P4$ diffractometer
$\omega$ scans
Absorption correction: none
2244 measured reflections
1644 independent reflections
1198 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 25.0°
$h = -1 \rightarrow 22$
$k = -1 \rightarrow 11$
$l = -13 \rightarrow 13$
3 standard reflections
every 100 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.119
$S$ = 1.00
1644 reflections
142 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.001P)^2 + 7P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$
Extinction correction: *SHELXTL*
Extinction coefficient: 0.00043 (17)

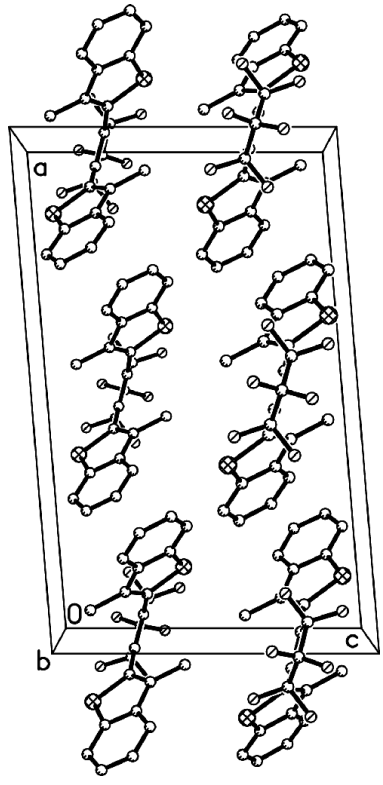



**Figure 2**
A packing view along the $b$ axis.

H atoms were positioned theoretically and refined using a riding model.

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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## References

Bruker (1997). *XSCANS* (Version 2.2) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Fernandez-Asebes, A. & Lehn, J. M. (1999). *Chem. Eur. J.* **5**, 3285–3292.
Irie, M. (2000). *Chem. Rev.* **100**, 1685–1716.
Kobatake, S., Yamada, M., Yamada, T. & Irie, M. (1999). *J. Am. Chem. Soc.* **121**, 8450–8456.
Pu, S., Zhang, F., Sun, F., Wang, R., Zhou, X. & Cheng, X. (2003). *Tetrahedron Lett.* **44**, 1011–1014.
Ramamurthy, V. & Venkatesan, K. (1987). *Chem. Rev.* **87**, 433–481.
Shibata, K., Muto, K., Kobatake, S. & Irie, M. (2002). *J. Phys. Chem. A*, **106**, 209–214.
Sun, F., Zhang, F., Lin, X., Guo, H., Pu, S. & Ma, H. (2002). *SPIE J.* **4930**, 439–442.