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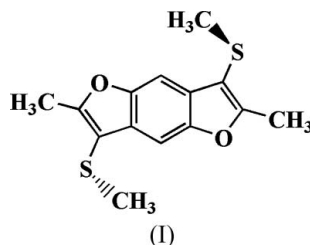
## Key indicators

Single-crystal X-ray study  
T = 298 K  
Mean  $\sigma(C-C)$  = 0.004 Å  
R factor = 0.052  
wR factor = 0.147  
Data-to-parameter ratio = 18.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2,6-Dimethyl-3,7-bis(methylsulfanyl)benzo-  
[1,2-*b*:4,5-*b'*]difuranIn the centrosymmetric molecule of the title compound,  $C_{14}H_{14}O_2S_2$ , the benzo[1,2-*b*:4,5-*b'*]difuran group is almost planar. The structure is stabilized by aromatic  $\pi$ - $\pi$  stacking and  $-CH_2-H \cdots \pi$  interactions.

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## Comment

This work is related to a previously reported communication on the isomeric benzodifuran analogue, 2,5-dimethyl-3,4-bis(methylsulfanyl)benzo[1,2-*b*:4,3-*b'*]difuran (Choi *et al.*, 2006). The title compound, (I), was prepared by the one-pot reaction of hydroquinone with an excess of  $\alpha$ -chloro- $\alpha$ -(methylsulfanyl)acetone in the presence of zinc chloride. In order to determine the overall molecular conformation in the crystal structure, an X-ray crystallographic analysis has been carried out and the results are reported here.The asymmetric unit of (I) consists of one half-molecule (Fig. 1); the molecule is centrosymmetric. The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).Rings *A* (C2–C5/O) and *B* (C1/C1<sup>i</sup>/C2/C2<sup>i</sup>/C3/C3<sup>i</sup>) are each planar, with maximum deviations of 0.0032 (3) (O1) and 0.0015 (2) Å (C2) from the least-squares planes (symmetry code as in Fig. 1). They form a dihedral angle of 0.82 (3)°. Ring *A* has a local pseudo-mirror plane passing through O1 and the mid-point of the C3–C4 bond, as evidenced by the torsion angles (Table 1). The benzo[1,2-*b*:4,5-*b'*]difuran group is nearly planar with a puckering amplitude  $Q_T = 0.0453$  (5) Å (Cremer & Pople, 1975).The crystal structure is stabilized by aromatic  $\pi$ - $\pi$  stacking and  $-CH_2-H \cdots \pi$  interactions (Fig. 2). The separation of the furan groups,  $Cg \cdots Cg^{iii}$ , is 3.582 (1) Å ( $Cg$  is the centroid of the C2–C5/O1 ring; symmetry code as in Fig. 2), which clearly indicates the presence of a  $\pi$ - $\pi$  stacking interaction. The nearest ring centroid separation of  $Cg \cdots Cg^{iii}$  is 3.614 (3) Å (symmetry code as in Fig. 2). The packing of the molecules is additionally stabilized by  $-CH_2-H \cdots \pi$  interactions between adjacent furan rings, with a  $-C6-H6C \cdots Cg^{ii}$  distance of 2.91 Å (symmetry code as in Fig. 2).

## Experimental

The title compound, (I), was prepared according to the method described previously for the benzodifuran analogue, 2,5-dimethyl-3,4-bis(methylsulfanyl)benzo[1,2-*b*:4,3-*b'*]difuran (Choi *et al.*, 2006) [m.p. 452–452 K;  $R_F = 0.60$  (CCl<sub>4</sub>)]. Crystals were obtained by recrystallization from cyclohexane.

### Crystal data

C <sub>14</sub> H <sub>14</sub> O <sub>2</sub> S <sub>2</sub>	$V = 333.91$ (5) Å <sup>3</sup>
$M_r = 278.37$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.384$ Mg m <sup>-3</sup>
$a = 5.2073$ (5) Å	Mo $K\alpha$ radiation
$b = 8.2548$ (6) Å	$\mu = 0.39$ mm <sup>-1</sup>
$c = 8.5234$ (6) Å	$T = 298$ (2) K
$\alpha = 105.616$ (6)°	Prism, colourless
$\beta = 98.690$ (7)°	0.50 × 0.31 × 0.29 mm
$\gamma = 103.564$ (6)°	

### Data collection

Stoe Stadi-4 diffractometer	1339 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$\theta_{\max} = 27.5^\circ$
Absorption correction: none	3 standard reflections
1530 measured reflections	frequency: 60 min
1530 independent reflections	intensity decay: 1.6%

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0799P)^2 + 0.3086P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.147$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.01$	$\Delta\rho_{\max} = 0.44$ e Å <sup>-3</sup>
1530 reflections	$\Delta\rho_{\min} = -0.41$ e Å <sup>-3</sup>
82 parameters	
H-atom parameters constrained	

**Table 1**

Selected torsion angles (°).

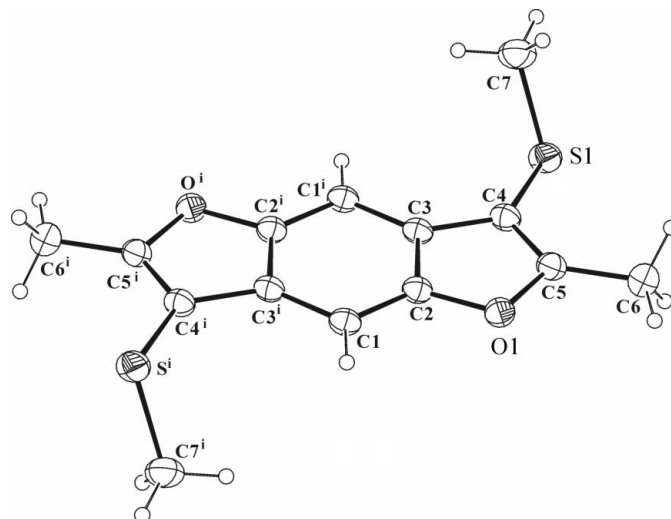
C3–C2–O1–C5	0.6 (2)	C5–C4–C3–C2	0.0 (3)
C2–O1–C5–C4	–0.6 (3)	C4–C3–C2–O1	–0.4 (2)
O1–C5–C4–C3	0.3 (2)		

H atoms were positioned geometrically, with C–H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *STADIA* (Stoe & Cie, 1996); cell refinement: *STADIA*; data reduction: *X-RED32* (Stoe & Cie, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

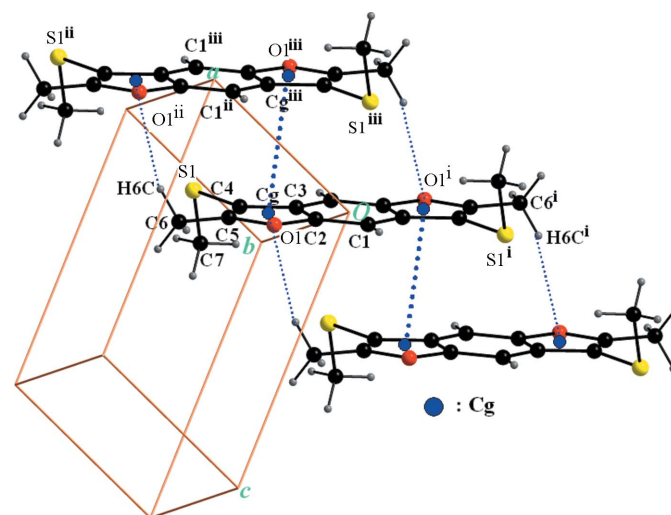
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**Figure 1**

The molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i)  $-x, -y, -z$ .]



**Figure 2**

A partial packing diagram of (I).  $-\text{CH}_2-\text{H} \cdots \pi$  and  $\pi-\pi$  interactions are shown as thin and thick dotted lines, respectively. Cg is the centroid of the (C2–C5/O) ring. [Symmetry codes: (i)  $-x, -y, -z$ ; (ii)  $x - 1, y, z$ ; (iii)  $1 - x, -y, -z$ .]

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