

Hong Dae Choi,^a Byoung Won Kang,^a Pil Ja Seo,^a Byeng Wha Son^b and Uk Lee^{b*}^aDepartment of Chemistry, Dongeui University, San 24 Kaya-dong Busanjin-ku, Busan 614-714, Republic of Korea, and ^bDepartment of Chemistry, Pukyong National University, 599-1 Daeyeon-3dong Nam-ku, Busan 608-737, Republic of Korea

Correspondence e-mail: uklee@pknu.ac.kr

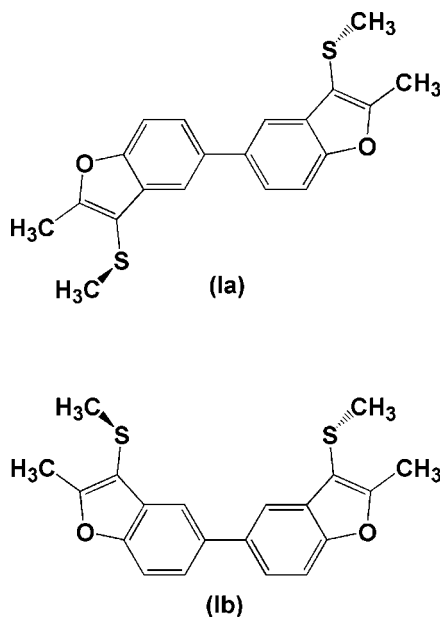
Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.009$ Å
 R factor = 0.103
 wR factor = 0.214
Data-to-parameter ratio = 18.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

2,2'-Dimethyl-3,3'-bis(methylsulfanyl)-5,5'-bis(1-benzofuran)

The title compound, $\text{C}_{20}\text{H}_{18}\text{O}_2\text{S}_2$, was obtained from the reaction of 4,4'-biphenol with α -chloro- α -(methylsulfanyl)-acetone in the presence of zinc chloride. The interplanar dihedral angle between the two 1-benzofuran groups is $39.2(2)^\circ$. The structure is stabilized by π - π stacking and $\text{C}-\text{H}\cdots\pi$ interactions.Received 5 April 2006
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Comment

Bisbenzofuran derivatives have attracted attention because of their chemical properties and application to photonic devices, and some have been studied by X-ray diffraction methods (Rodier *et al.*, 1994; Liao *et al.*, 2003; Yamaguchi & Irie, 2005). A bisbenzofuran structurally related to disodium cromoglycate, which is useful against asthma, has also been prepared (Sunder & Peet, 1980).

We report here the crystal structure of the title bisbenzofuran compound, (1a) (Fig. 1 and Table 1). Both 1-benzofuran groups are planar, with mean deviations from the least-squares planes of 0.009 (C1–C8/O1) and 0.013 Å (C11–C18/O2). The interplanar dihedral angle between the two 1-benzofuran groups is $39.2(2)^\circ$. We predicted two possible isomers for this structure, (1a) and (1b). The actual structure was confirmed as (1a), with the methyl groups of the methylsulfanyl substituents pointing in opposite directions with respect to the overall molecular plane. The S atoms are 0.116 (7) and 0.036 (7) Å out of the C1–C8/O1 and C11–C18/O2 planes, respectively.

Fig. 2 shows the aromatic π - π stacking and $\text{C}-\text{H}\cdots\pi$ interactions that stabilize the packing in the crystal structure.

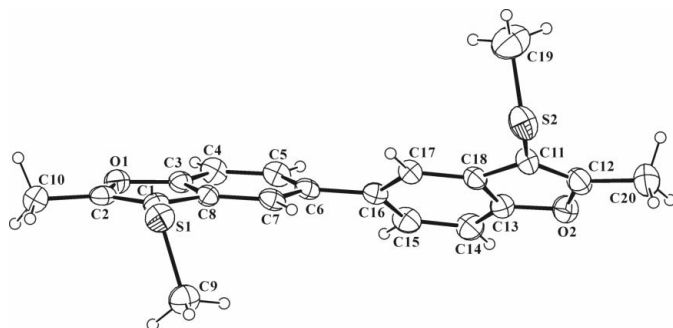


Figure 1
A view of the structure of (Ia), with 30% probability displacement ellipsoids.

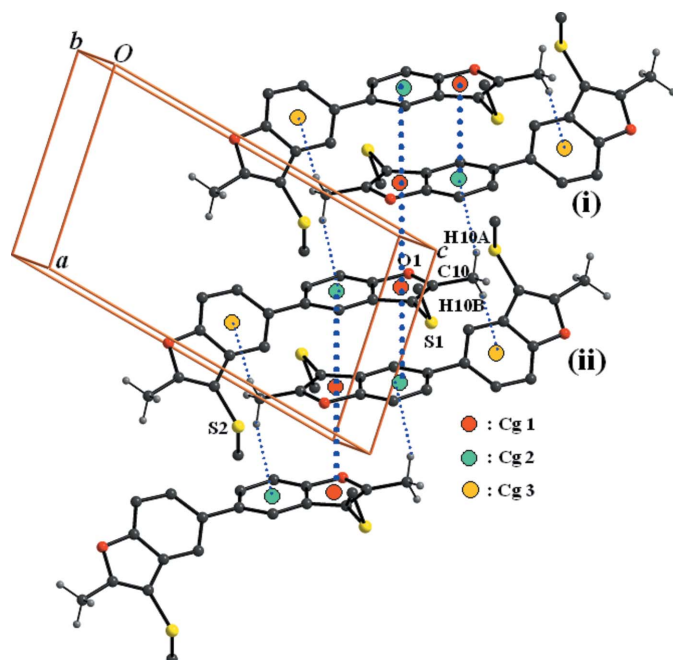


Figure 2
A packing diagram for (Ia), with C–H... π interactions drawn as thin dotted lines and π – π interactions shown as thick dotted lines. Cg1 is the centroid of the C1–C3/C8/O1 ring, Cg2 is the centroid of the C3–C8 ring and Cg3 is the centroid of the C13–C18 ring [Symmetry codes: (i) $-x, 2 - y, 2 - z$; (ii) $1 - x, 2 - y, 2 - z$].

The ring centroid separations $Cg1 \cdots Cg1^i$ and $Cg1 \cdots Cg2^{ii}$ are 3.608 (4) and 3.746 (4) Å, respectively, clearly indicating π – π stacking interactions [Cg1 is the centroid of the C1–C3/C8/O1 ring and Cg2 is the centroid of the C3–C8 ring; symmetry codes: (i) $-x, 2 - y, 2 - z$; (ii) $1 - x, 2 - y, 2 - z$]. In addition, C–H... π interactions further stabilize inversion-related dimers, with H10A...Cg2ⁱ and H10B...Cg3ⁱⁱ distances of 2.88 and 3.11 Å, respectively (Cg3 is the centroid of the C13–C18 ring).

Experimental

The title compound was prepared by a procedure previously used for substituted 1-benzofurans (Choi *et al.*, 1998) and naphtho[*b*]furans (Choi *et al.*, 1999). Zinc chloride (680 mg, 5.0 mmol) was added at room temperature to a stirred solution of α -chloro- α -(methyl-

sulfanyl)acetone (693 mg, 5.0 mmol) and 4,4'-biphenol (466 mg, 2.5 mmol) in dichloromethane (30 ml) and tetrahydrofuran (5 ml), and stirred for 40 min. The mixture was quenched with water and the organic layer was separated, dried over magnesium sulfate, filtered and concentrated in vacuum. The residue was purified by column chromatography (hexane–ethyl acetate 4:1) to afford the title compound in 26% yield. Crystals suitable for X-ray diffraction analysis were grown by slow evaporation of a benzene solution [m.p. 394–395 K; $R_F = 0.82$ (hexane–ethyl acetate, 4:1)].

Crystal data

$C_{20}H_{18}O_2S_2$	$V = 883.5$ (7) Å ³
$M_r = 354.46$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.332$ Mg m ⁻³
$a = 7.830$ (4) Å	Mo $K\alpha$ radiation
$b = 8.695$ (3) Å	$\mu = 0.31$ mm ⁻¹
$c = 14.046$ (6) Å	$T = 298$ (2) K
$\alpha = 78.37$ (3)°	Plate, colourless
$\beta = 73.94$ (4)°	$0.21 \times 0.12 \times 0.03$ mm
$\gamma = 76.38$ (3)°	

Data collection

Stoe STADI-4 diffractometer	1942 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$\theta_{\max} = 27.5^\circ$
Absorption correction: none	3 standard reflections
4038 measured reflections	frequency: 60 min
4038 independent reflections	intensity decay: 3.4%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 2.2293P]$
$R[F^2 > 2\sigma(F^2)] = 0.103$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.214$	$(\Delta\sigma)_{\max} < 0.001$
$S = 1.17$	$\Delta\rho_{\max} = 0.26$ e Å ⁻³
4038 reflections	$\Delta\rho_{\min} = -0.29$ e Å ⁻³
218 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

S1–C1	1.741 (6)	O1–C3	1.378 (7)
S1–C9	1.783 (7)	O1–C2	1.399 (7)
S2–C11	1.746 (7)	O2–C13	1.377 (8)
S2–C19	1.804 (9)	O2–C12	1.398 (8)
C1–S1–C9	100.8 (3)	C11–S2–C19	101.4 (4)

All H atoms were positioned geometrically in ideal positions and refined using a riding model, with C–H = 0.93 Å for aromatic and 0.96 Å for methyl H atoms, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms or $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. The crystal used for data collection was very small and weakly diffracting. This accounts for the relatively high R factor and standard uncertainties reported here.

Data collection: *STADI4* (Stoe & Cie, 1996); cell refinement: *STADI4*; data reduction: *X-RED* (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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