

Hong Dae Choi,^a Hyun Mi Woo,^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 3-dong Nam-ku, Busan 608-737, Republic of Korea

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

Key indicators

Single-crystal X-ray study
T = 120 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.030
wR factor = 0.083
Data-to-parameter ratio = 16.7

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

5-(4-Bromophenyl)-3-methylsulfanyl-2-phenyl-1-benzofuran

The title compound, $\text{C}_{21}\text{H}_{15}\text{BrOS}$, was prepared by the Lewis acid-catalysed reaction of 4'-bromo-1,1'-biphenyl-4-ol with 2-chloro-2-(methylsulfanyl)acetophenone. The structure is stabilized by intermolecular (benzofuran)C—H \cdots O(furan) hydrogen bonds and by aromatic $\pi(\text{benzene ring of benzofuran})\cdots\text{H}-\text{C}(4\text{-bromophenyl})$ interactions.

Received 10 July 2006
Accepted 19 September 2006

Comment

This work is related to the previous communication on the isomeric benzofuran analogue, 5-(4-bromophenyl)-2-methyl-3-(methylsulfanyl)-1-benzofuran (Choi *et al.*, 2006). The title compound, (I), was prepared by the one-pot reaction of 4'-bromo-1,1'-biphenyl-4-ol with 2-chloro-2-(methylsulfanyl)acetophenone in the presence of zinc chloride. In order to determine the overall molecular conformation in the crystal structure, an X-ray crystallographic analysis of this isomer has been carried out and the results are reported here (Fig. 1). The dihedral angles between the mean plane of the 1-benzofuran group and the 4-bromophenyl ring and the phenyl ring are 38.49 (6) and 21.22 (7)°, respectively.

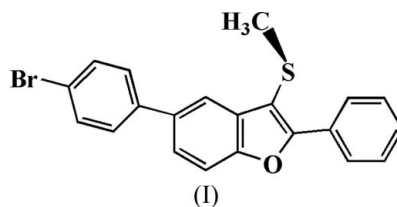


Fig. 2 shows the packing and intermolecular interactions. An effective $\pi-\pi$ stacking interaction was not found because of the large dihedral angles between the mean planes of the benzofuran group and the 4-bromophenyl and phenyl rings. The packing is stabilized by intermolecular C9—H9 \cdots Oⁱ hydrogen bonds (2.61 Å), and by a Cg \cdots H2ⁱⁱ—C2ⁱⁱ π interaction (2.97 Å) (symmetry code as in Fig. 2; Cg is the centroid of the C7—C10/C13—C14 ring).

Experimental

Compound (I) was prepared according to the method described previously for the benzofuran analogue 5-(4-bromophenyl)-2-methyl-3-(methylsulfanyl)-1-benzofuran (Choi *et al.*, 2006), but utilizing 2-chloro-2-(methylsulfanyl)acetophenone in place of α -chloro- α -(methylsulfanyl)acetone. Crystals suitable for an X-ray analysis were grown by slow evaporation of a tetrahydrofuran solution [yield 51%, m.p. 412–413 K; $R_{\text{F}} = 0.72$ (CCl_4)].

Crystal data

$C_{21}H_{15}BrOS$
 $M_r = 395.30$
 Triclinic, $P\bar{1}$
 $a = 7.7452$ (5) Å
 $b = 9.2404$ (6) Å
 $c = 12.6789$ (9) Å
 $\alpha = 101.476$ (1)°
 $\beta = 107.091$ (1)°
 $\gamma = 90.929$ (1)°

$V = 847.3$ (1) Å³
 $Z = 2$
 $D_x = 1.549$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 2.55$ mm⁻¹
 $T = 120$ (2) K
 Block, colorless
 $0.64 \times 0.60 \times 0.40$ mm

Data collection

Bruker SMART CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1999)
 $T_{min} = 0.198$, $T_{max} = 0.357$

7306 measured reflections
 3629 independent reflections
 3270 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.045$
 $\theta_{max} = 27.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.083$
 $S = 0.98$
 3629 reflections
 217 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 0.2432P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.46$ e Å⁻³
 $\Delta\rho_{min} = -0.55$ e Å⁻³

All H atoms were positioned geometrically and refined using a riding model, with C–H = 0.93 Å for aromatic and 0.96 Å for methyl H atoms, and with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms and $1.5U_{eq}(C)$ for methyl H atoms.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); 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.

References

Brandenburg, K. (1998). DIAMOND, Version 2.1. Crystal Impact GbR, Bonn, Germany.
 Bruker (1997). SMART and SAINT. Versions 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.

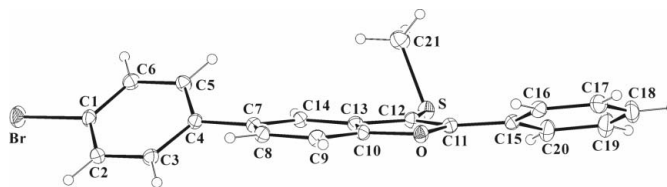


Figure 1
 The molecular of (I), with 30% probability displacement ellipsoids.

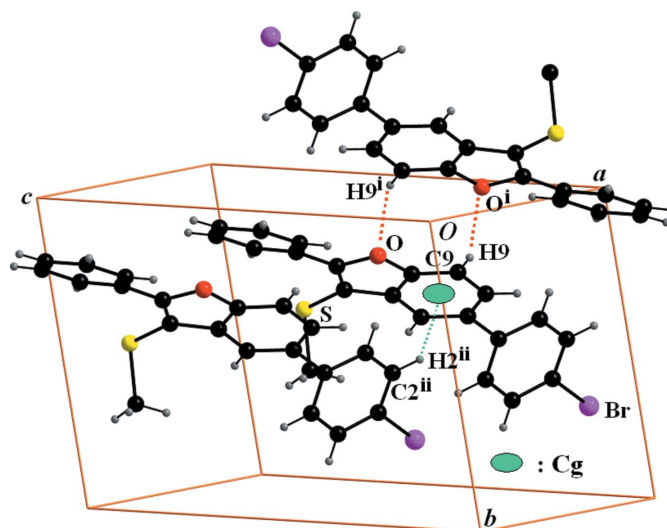


Figure 2
 A partial packing diagram for (I), with the C9–H9···Oⁱ hydrogen bond and the C2ⁱⁱ–H2ⁱⁱ···Cg π interactions drawn as dotted lines. Cg is the centroid of the C7–C10/C13–C14 benzene ring. [Symmetry codes: (i) $-x, -y, -z$; (ii) $x - 1, y, z$.]

Choi, H. D., Woo, H. M., Seo, P. J., Son, B. W. & Lee, U. (2006). *Acta Cryst.* **E62**, o4253–o4254.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Sheldrick, G. M. (1999). SADABS. University of Göttingen, Germany.