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5-Methyl-2,3-diphenyl-1-benzofuran

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.083
wR factor = 0.184
Data-to-parameter ratio = 17.7

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

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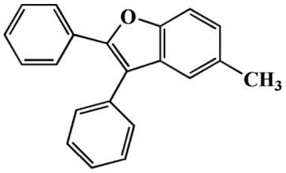
The title compound, $C_{21}H_{16}O$, was synthesized by the Lewis acid-catalysed reaction of *p*-cresol with 2-chloro-2-methylsulfanyl-2-phenylacetophenone. The 1-benzofuran ring system is almost planar. The structure is stabilized by $-CH_2-H\cdots\pi$ interactions.

Comment

1-Benzofuran derivatives occur widely in synthetic substances, as well as in natural products, and numerous examples are known to exhibit interesting pharmacological properties (Ward, 1997; Howlett *et al.*, 1999). The chemistry of 1-benzofuran ring derivatives has been extensively studied and discussed elsewhere (Cagniant & Cagniant, 1975). Although there are several different methods for preparing the 2,3-diphenyl-1-benzofuran analogue (Koenigkramer & Zimmer, 1980; Brady & Giang, 1986; Morrison & Musgrave, 2002), the crystal structures of these compounds have not been investigated.



(I)

With our ongoing interest in the syntheses and structures of 1-benzofuran derivatives (Choi *et al.*, 2001, 2003, 2006; Seo *et al.*, 2004), we report here the crystal structure of the title compound, (I) (Fig. 1 and Table 1), which was directly prepared by the one-pot reaction of *p*-cresol with 2-chloro-2-methylsulfanyl-2-phenylacetophenone in the presence of a Lewis acid.

The 1-benzofuran ring system *A* (O/C1–C4/C17–C20) is planar with a puckering amplitude $Q_T = 0.038$ (1) Å (Cremer & Pople, 1975). The dihedral angles between the planar rings *B* (C5–C10), *C* (C11–C16) and *A* are $A/B = 30.9$ (1)°, $A/C = 57.95$ (9)° and $B/C = 63.43$ (9)°.

The packing of the molecules (Fig. 2) is stabilized by $-CH_2-H\cdots\pi$ interations between adjacent molecules, with a $-C21H_2-H21C\cdots Cg^i$ distance of 2.99 Å [Symmery code: (i) $x + 1, y, z$; *Cg* is the centroid of the C1–C4/O ring]. As a result of the conformational hindrance of the two phenyl rings, no aromatic π–π stacking interactions were found in (I).

Experimental

The title compound was obtained from *p*-cresol with 2-chloro-2-methylsulfanyl-2-phenylacetophenone utilizing successive dehydrocyclization and concurrent elimination of methylsulfanyl group *via* a

Friedel–Crafts reaction intermediater under Lewis acid conditions (Choi *et al.*, 2001). Crystals suitable for X-ray analysis were grown by slow evaporation of a chloroform solution.

Crystal data

$C_{21}H_{16}O$
$M_r = 284.34$
Triclinic, $P\bar{1}$
$a = 6.047$ (1) Å
$b = 7.591$ (2) Å
$c = 17.112$ (3) Å
$\alpha = 94.46$ (3)°
$\beta = 94.22$ (3)°
$\gamma = 98.86$ (3)°
$V = 770.8$ (3) Å^3
$Z = 2$
$D_x = 1.225$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 298$ (2) K
Plate, colorless
0.62 × 0.58 × 0.21 mm

Data collection

Stoe Stadi-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3532 measured reflections
3532 independent reflections
1778 reflections with $I > 2\sigma(I)$
$\theta_{max} = 27.5°$
3 standard reflections
frequency: 60 min
intensity decay: 3.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.083$
$wR(F^2) = 0.184$
$S = 1.19$
3532 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.194P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O—C4	1.380 (4)	C1—C5	1.460 (4)
O—C1	1.398 (3)	C2—C11	1.479 (4)
C4—O—C1	106.0 (2)	O—C1—C5	114.8 (3)
C2—C1—O	110.8 (3)	C1—C2—C11	127.9 (3)
C2—C1—C5	134.3 (3)		

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 $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.2$ for aromatic H and $x = 1.5$ for methyl H atoms.

Data collection: *STADI4* (Stoe & Cie, 1996); cell refinement: *STADI4*; data reduction: *X-RED32* (Stoe & Cie, 1996); 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*.

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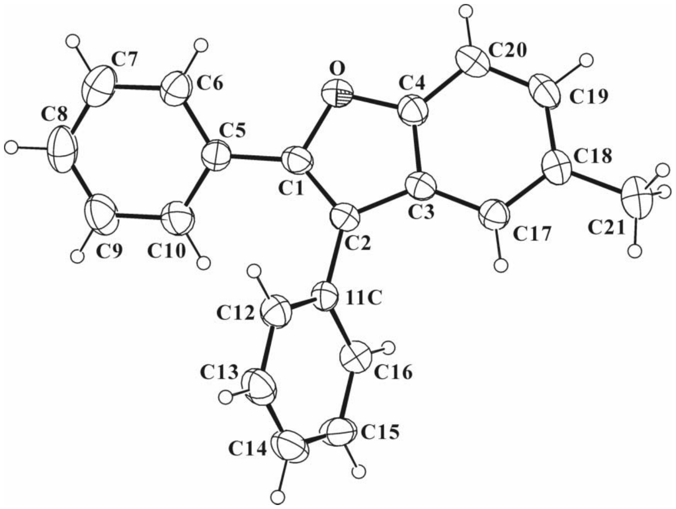

Figure 1
The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

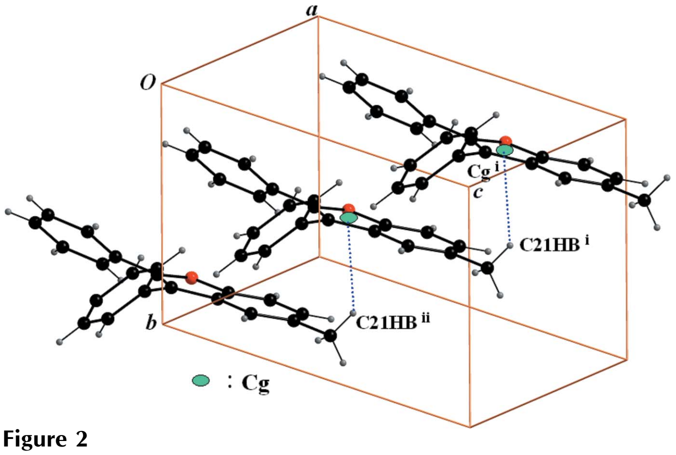

Figure 2
A packing diagram of (I). $-CH_2-H\cdots\pi$ interactions are shown as dashed lines. *Cg* is the centroid of the C1–C4/O ring. [Symmetry codes: (i) $x + 1, y, z$; (ii) $x - 1, y, z$.]

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