Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination.* University of Cambridge, England.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.

Acta Cryst. (1996). C**52**, 94–95

5-Methyl-3-(1-phenylethylidene)-2,3-dihydrobenzo[*b*]furan-2-one

S. Selladurai,[a] K. Subramanian,[b] S. Lakshmi,[b] Yu-Sheng Chen,[c] Elizabeth J. Holt[d] and S. Narasinga Rao[c]

[a]*Division of Applied Sciences, MIT Campus, Anna University, Madras 25, India,* [b]*Department of Physics, Anna University, Madras, India,* [c]*Department of Physics, University of Central Oklahoma, Edmond, Oklahoma, USA, and* [d]*Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma, USA*

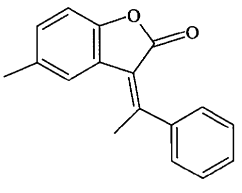
(*Received 12 December 1994; accepted 24 July 1995*)

Abstract

The benzofuran ring in the title compound, $C_{17}H_{14}O_2$, is planar with a methyl group substituted in the 5-position. The 5-methyl and 3-ethylidene groups are in *trans* positions with respect to the benzofuran ring. The structure is stabilized by intermolecular van der Waals interactions.

Comment

The title compound, (I), was prepared as part of a study of diastereoselectivities of free-radical reactions. The crystal structure was determined in order to establish whether a phenylethylidene group would be formed *trans* or *gauche* to the benzofuran ring.



(I)

The benzofuran ring is planar (with a maximum deviation from the plane of 0.75 Å for C8) and shows typical aromaticity and delocalization of π electrons. The phenyl ring is twisted out of the plane of the benzofuran moiety by 130°. The 5-methyl and ethylidene groups are in *trans* positions with respect to the benzofuran ring. Bond lengths and bond angles are as expected.

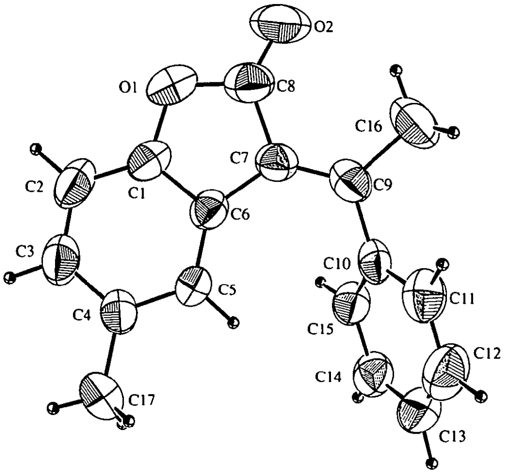


Fig. 1. View of the title molecule with displacement ellipsoids plotted at the 50% probability level.

Experimental

Crystal supplied by S. Selladurai.

Crystal data

$C_{17}H_{14}O_2$
$M_r = 250.3$
Triclinic
$P\bar{1}$
$a = 9.890\,(5)$ Å
$b = 9.258\,(4)$ Å
$c = 8.878\,(5)$ Å
$\alpha = 108.26\,(4)^\circ$
$\beta = 78.48\,(4)^\circ$
$\gamma = 67.38\,(4)^\circ$
$V = 663.3\,(6)$ Å^3
$Z = 2$
$D_x = 1.253$ Mg m^{-3}
$D_m = 1.249$ Mg m^{-3}
D_m measured by flotation

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 11.5$–15°
$\mu = 0.0757$ mm^{-1}
$T = 293$ K
Block
0.35 × 0.29 × 0.12 mm
Red

Data collection

Syntex *P*3 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
1901 measured reflections
1705 independent reflections
913 observed reflections $[I > 3\sigma(I)]$

$\theta_{\max} = 25^\circ$
$h = -11 \rightarrow 11$
$k = 0 \rightarrow 10$
$l = -10 \rightarrow 10$
3 standard reflections monitored every 97 reflections intensity decay: <5%

Refinement

Refinement on *F*
$R = 0.063$
$wR = 0.083$
$S = 1.271$
913 reflections
214 parameters
H-atom parameters not refined

$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{\max} = 0.58$
$\Delta\rho_{\max} = 2.2$ e Å^{-3}
$\Delta\rho_{\min} = 0.6$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from Cromer & Mann (1968)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* ($Å^2$)

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
O1	0.9740 (5)	0.2628 (6)	0.0957 (6)	5.91 (4)
O2	0.8125 (6)	0.5375 (7)	0.1544 (7)	7.86 (5)
C1	1.1089 (7)	0.1762 (8)	0.1242 (7)	4.66 (5)
C2	1.1805 (8)	0.0033 (8)	0.0839 (8)	5.68 (6)
C3	1.3105 (8)	−0.0611 (8)	0.1265 (9)	5.34 (6)
C4	1.3667 (6)	0.0457 (7)	0.2113 (7)	4.30 (5)
C5	1.2910 (7)	0.2192 (7)	0.2476 (7)	4.00 (5)
C6	1.1578 (6)	0.2902 (7)	0.2049 (7)	3.91 (5)
C7	1.0496 (6)	0.4611 (7)	0.2300 (7)	4.33 (5)
C8	0.9304 (8)	0.4357 (7)	0.1615 (9)	5.53 (6)
C9	1.0463 (6)	0.6157 (7)	0.2951 (7)	4.48 (5)
C10	1.1818 (7)	0.6236 (7)	0.3337 (8)	4.07 (4)
C11	1.1625 (8)	0.7307 (8)	0.4962 (8)	5.66 (6)
C12	1.2904 (11)	0.7367 (10)	0.5310 (9)	6.70 (7)
C13	1.4390 (9)	0.6420 (9)	0.4052 (10)	5.98 (6)
C14	1.4581 (7)	0.5413 (8)	0.2434 (8)	5.16 (6)
C15	1.3293 (7)	0.5321 (7)	0.2095 (8)	4.54 (5)
C16	0.9114 (8)	0.7863 (9)	0.3303 (9)	5.68 (6)
C17	1.5059 (7)	−0.0279 (8)	0.2559 (9)	6.10 (6)

Table 2. *Selected geometric parameters* (Å, °)

C1—C2	1.363 (10)	C8—O1	1.369 (10)
C1—O1	1.388 (9)	C8—O2	1.213 (10)
C1—C6	1.385 (11)	C9—C10	1.470 (10)
C2—C3	1.378 (11)	C9—C16	1.509 (9)
C3—C4	1.407 (11)	C10—C11	1.395 (9)
C4—C5	1.378 (8)	C10—C15	1.373 (8)
C4—C17	1.477 (10)	C11—C12	1.378 (15)
C5—C6	1.414 (9)	C12—C13	1.385 (11)
C6—C7	1.442 (8)	C13—C14	1.372 (11)
C7—C8	1.492 (12)	C14—C15	1.393 (11)
C7—C9	1.349 (10)		
O1—C1—C2	124.6 (7)	C7—C8—O1	108.4 (6)
O1—C1—C6	110.8 (6)	C7—C8—O2	131.6 (8)
C2—C1—C6	124.5 (6)	O1—C8—O2	120.0 (8)
C1—C2—C3	117.2 (7)	C8—O1—C1	108.6 (6)
C2—C3—C4	122.1 (6)	C7—C9—C10	119.6 (5)
C3—C4—C5	118.3 (6)	C7—C9—C16	124.3 (6)
C3—C4—C17	120.5 (6)	C10—C9—C16	116.0 (6)
C5—C4—C17	121.2 (6)	C9—C10—C11	120.8 (5)
C4—C5—C6	121.3 (6)	C9—C10—C15	121.1 (6)
C5—C6—C1	116.5 (6)	C11—C10—C15	118.1 (7)
C5—C6—C7	135.6 (6)	C10—C11—C12	120.3 (5)
C1—C6—C7	107.8 (5)	C11—C12—C13	121.0 (7)
C6—C7—C8	104.3 (6)	C12—C13—C14	119.1 (8)
C6—C7—C9	132.2 (6)	C13—C14—C15	119.8 (6)
C8—C7—C9	123.5 (6)	C14—C15—C10	121.7 (6)
C1—C2—C3—C4	0.9 (4)	C10—O1—C11—C12	−2.6 (4)
C2—C3—C4—C5	0.2 (4)	C12—C13—C14—C15	−0.3 (3)
C3—C4—C5—C6	−0.6 (3)	C13—C14—C15—C16	−1.8 (7)
C4—C5—C6—C1	0.4 (4)	C14—C15—C16—C11	1.7 (6)
C5—C6—C1—C2	0.7 (3)	C15—C16—C11—C12	−180 (3)
C6—C1—C2—C3	−1.0 (3)	C16—C11—C12—C13	−2.8 (6)
C9—C10—O11—C11	3.2 (3)	C17—C14—C13—C12	178.6 (2)
C9—C12—C11—O1	−0.7 (5)	C16—C11—C12—C9	−175.3 (4)

Data were collected using a variable scan rate and a scan width of 1.2° below $K\alpha_1$ and 1.2° above $K\alpha_2$. Backgrounds were measured at each side of the scan for a combined time equal to the total scan time. Data were corrected for Lorentz, polarization, centering and background effects (Blessing, 1986). The non-H atoms were located by direct methods using *MULTAN*80 (Main *et al.*, 1980). Refinement (*XRAY*; Stewart, 1980) of the scale factor and positional and anisotropic displacement parameters for these atoms was carried out to convergence. H atoms were located from a difference Fourier synthesis and were included in the final cycles of refinement in fixed positions and with fixed isotropic displacement parameters.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: SZ1043). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Blessing, R. H. (1986). *Crystallogr. Rev.* **1**, 3–58.

Cromer, D. T. & Mann, I. B. (1968). *Acta Cryst.* A**24**, 321–324.

Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Universities of York, England, and Louvain, Belgium.

Stewart, J. M. (1980). Editor. *The XRAY System of Crystallographic Programs.* Version of 1980. Computer Science Center, University of Maryland, College Park, Maryland, USA.

Acta Cryst. (1996). C**52**, 95–97

1-Bromo-2,7-dimethylnaphthalene

LAURIE A. BROWN, RAVI K. LAXMAN, ANDREW W. MAVERICK AND FRANK R. FRONCZEK

Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803-1804, USA

(*Received 20 March 1995; accepted 24 July 1995*)

Abstract

The naphthalene moiety of the title compound, $C_{12}H_{11}Br$, is planar within 0.052 (4) Å. The Br, C11 and C12 atoms deviate by −0.1711 (5), 0.065 (5) and 0.182 (4) Å, respectively, from this plane. The C—Br distance is 1.911 (3) Å.

Comment

The bond lengths and angles (Table 2) within the aromatic nucleus of the title compound, (I), differ in some respects from those described by Cruickshank (1957) for naphthalene. The largest deviations occur where the ring is the most substituted, at atoms C1 and C2. The C1—C2 bond distance in the title compound is 0.029 (6) Å longer than that in naphthalene. The C2—C1—C9 angle is 3.2 (4)° larger, the C2—C3—C4 angle 2.8 (3)° larger, while the C1—C2—C3 angle is smaller by 4.3 (3)° than the corresponding angles in naphthalene. The largest deviation from the naphthalene (C1–C10) least-squares plane is observed at atom C12