Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-[2-(4-Hydroxyphenyl)-4,6-dimethoxy-1-benzofuran-3-yl]ethanone

Xiao-Xiao Li, Yu-Ping Wei, Ye-Fei Nan, Chang-Hua Hua and Liang-Dong Sun*

Department of Chemistry, College of Sciences, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: doristju@gmail.com

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.147
Data-to-parameter ratio = 15.9

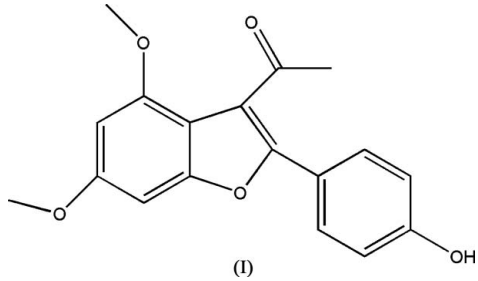
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 April 2006
Accepted 10 May 2006

In the crystal structure of the title compound, $C_{18}H_{16}O_5$, O—H···O hydrogen bonds connect the molecules into centrosymmetric dimers that form stacks down the *a* axis.

Comment

The structure of the title compound, (I), a 2-phenylbenzofuran derivative prepared by oxidation of the corresponding substituted flavylium salt (Jurd, 1964) is presented here (Fig. 1 and Table 1).



(I)

The atoms of the benzofuran ring system are almost coplanar, the mean deviation from the C1–C8/O1 mean plane being 0.0102 (2) Å. The benzofuran system and its hydroxyphenyl substituent are inclined at a dihedral angle of 33.5 (1)°, with a C4—O1—C1—C9 torsion angle of 179.78 (12)°. The angles about C1 are significantly distorted from trigonal geometry (Table 1). In particular, the widening of the C2—C1—C9 angle [136.80 (16)°] may reflect steric interaction beween the hydroxyphenyl and ethanone substituents.

In the crystal structure, O—H···O hydrogen bonds link adjacent molecules into centrosymmetric dimers (Table 2). An intermolecular π-stacking interaction, with a centroid–centroid distance of 3.566 (2) Å, between the furan ring and the fused benzene ring of an adjacent molecule, forms stacks along the *a* axis (Fig. 2).

Experimental

The title compound was prepared according to the procedure of Jurd (1964). Suitable crystals were obtained by evaporation of an ethyl acetate/hexane (1:1 *v*/*v*) solution (m.p. 446 K).

Crystal data

$C_{18}H_{16}O_5$
M_r = 312.32
Monoclinic, $P2_1/a$
a = 7.8442 (12) Å
b = 18.365 (3) Å
c = 10.7516 (18) Å
β = 105.781 (7)°
V = 1490.5 (4) Å^3
Z = 4
D_x = 1.392 Mg m^{-3}
Mo *Kα* radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colorless
0.26 × 0.24 × 0.20 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.974, T_{max} = 0.980
9260 measured reflections
3401 independent reflections
2251 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.147
S = 1.04
3401 reflections
214 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0789P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond and torsion angles (°).

O1—C1—C2	110.54 (14)	C2—C1—C9	136.80 (16)
O1—C1—C9	112.66 (14)		
C4—O1—C1—C9	−179.78 (12)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3^{i}	0.94 (3)	1.85 (3)	2.781 (2)	170 (3)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.96 Å); for the CH and CH_2 groups, U_{iso}(H) values were set equal to $1.2U_{eq}$(C) [$1.5U_{eq}$(C) for the methyl groups].

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure*.

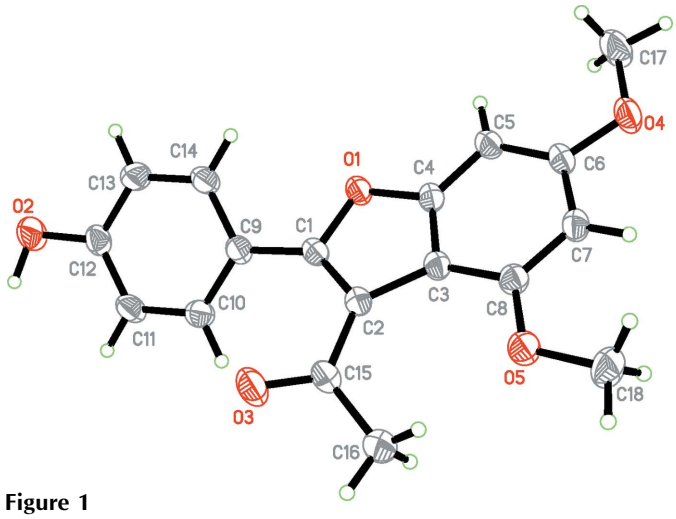


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids at the 35% probability level.

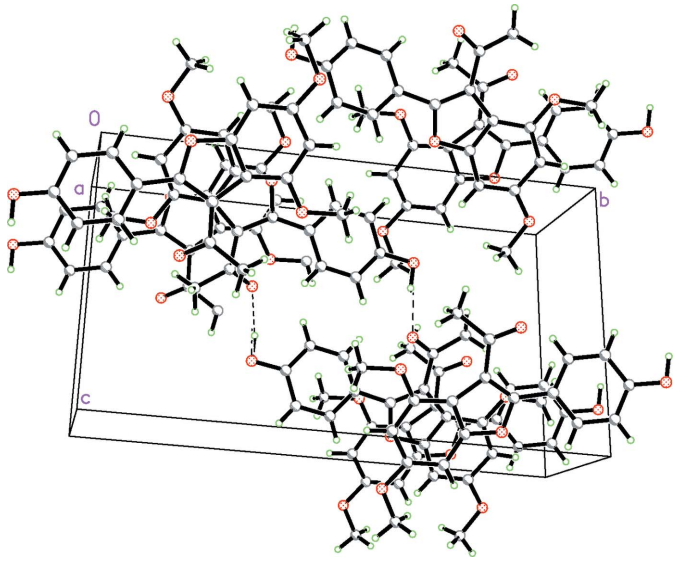


Figure 2
The crystal packing of (I), viewed approximately down the *a* axis. Hydrogen bonds are shown as dashed lines.

References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Jacobson, R. (1998). *REQAB*. Private communication to Rigaku Corporation, Tokyo, Japan.
Jurd, L. (1964). *J. Org. Chem.* **29**, 2602–2605.
Molecular Structure Corporation & Rigaku (1999). *CrystalClear*. Version 1.3.6. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA, and Rigaku, 3-9-12 Akishima, Tokyo, Japan.
Rigaku/MSC (2005). *CrystalStructure*. Version 3.7.0. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA .
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.