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2-Acetylbenzo[*b*]furan

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The benzofuran moiety of the title molecule, $C_{10}H_8O_2$, is planar and forms a dihedral angle of 6.69 (9)° with the attached acetyl group. In the crystal structure, symmetry-related molecules are linked to form chains by C—H···O intermolecular hydrogen bonds involving the furan H atom and the O atom of the acetyl group. Adjacent chains are interlinked through weak C—H···π interactions involving the furan ring.

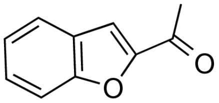
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.092
Data-to-parameter ratio = 13.0

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

Comment

A convenient method of preparing 2-acetylbenzofuran, (I), from 2-hydroxybenzaldehyde and chloroacetone in the presence of KOH has been reported (Elliott, 1951). We have obtained (I) using a phase-transfer catalytic method. The present X-ray diffraction study was undertaken to understand the geometry of the benzofuran ring system and the effect of acetyl group substitution at position 2 of the furan ring.



(I)

In (I), the benzofuran moiety is planar and the acetyl group is slightly twisted about the C2—C21 bond, as seen from the torsion angles O1—C2—C21—O21 = 5.9 (3)° and C3—C2—C21—C22 = 6.7 (3)°. The geometry of the benzofuran ring is comparable to that found in ethyl 3-hydroxybenzo[*b*]furan-2-carboxylate (Gould *et al.*, 1998). In the solid state, the symmetry-related molecules are linked by C3—H3···O21($\frac{3}{2}-x, -y, -\frac{1}{2}+z$) hydrogen bonds to form chains along the *c* axis. Adjacent chains related by the symmetry operation ($-\frac{1}{2}+x, y, \frac{3}{2}-z$) are linked by C—H···$\pi$ hydrogen bonds involving the furan ring (Table 1), to form double-chain structures.

Experimental

The title compound was synthesized employing a phase-transfer catalytic technique. Salicylaldehyde (6.12 ml, 0.05 mol) and chloroacetone (4.0 ml, 0.05 mol) were added to benzene (30 ml) and the reaction mixture was magnetically stirred for 3 h with 20% aqueous potassium carbonate (20 ml) solution in the presence of a catalytic amount of tetrabutylammonium hydrogen sulfate (200 mg) as a phase-transfer catalyst. The resulting solid was filtered off and dried in air. Recrystallization from 1,4-dioxane afforded the crystals. The yield of the isolated product was 86%.

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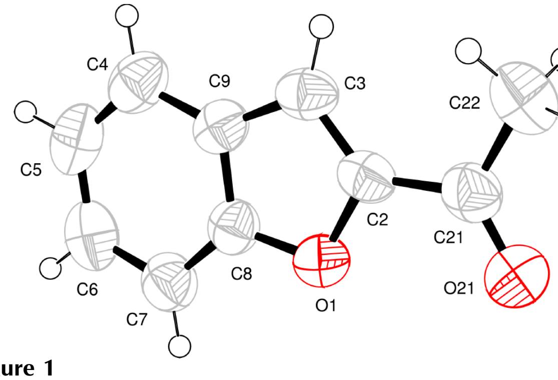

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids (Farrugia, 1997).

Crystal data

$C_{10}H_8O_2$
$M_r = 160.16$
Orthorhombic, *Pbca*
$a = 8.3865$ (13) Å
$b = 18.273$ (4) Å
$c = 10.652$ (2) Å
$V = 1632.4$ (5) Å^3
$Z = 8$
$D_x = 1.303$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10$–15°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Block, light brown
0.3 × 0.3 × 0.3 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
1419 measured reflections
1419 independent reflections
907 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 25.0°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 21$
$l = 0 \rightarrow 12$
2 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.092$
$S = 1.03$
1419 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 0.2715P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.10$ e Å^{-3}
$\Delta\rho_{\min} = -0.12$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O21$^{\rm i}$	0.93	2.42	3.190 (2)	140
C7—H7···$Cg1^{\rm ii}$	0.93	2.89	3.431 (2)	119

Symmetry codes: (i) $\frac{3}{2} - x, -y, z - \frac{1}{2}$; (ii) $x - \frac{1}{2}, y, \frac{3}{2} - z$.

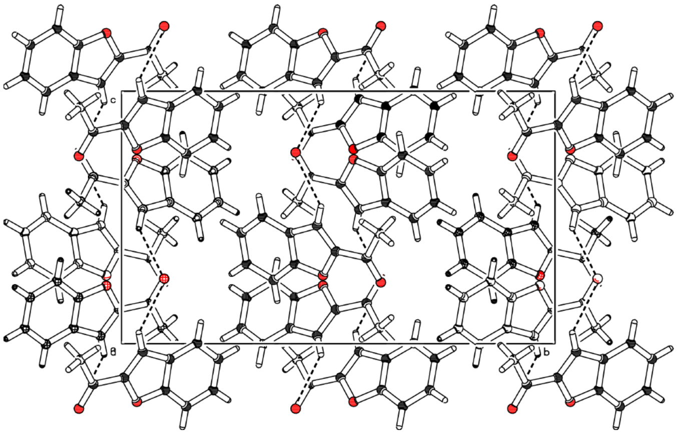

Figure 2
The molecular packing of (I), viewed down the *a* axis (Spek, 1990).

The H atoms were fixed geometrically and were treated as riding on their parent C atoms, with isotropic displacement parameters. The methyl group was found to be disordered over two positions rotated from each other by 60°. It was refined as an idealized disordered methyl group.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1994); cell refinement: *MolEN* (Fair, 1990); data reduction: *MolEN*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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