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2-Acetyl-3-(benzoylamino)-1-benzofuran

Nazan Ocak İskeleli,[a]* Canan Kazak,[a] Cumhur Kırılmış[b] and Murat Koca[b]

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit–Samsun, Turkey, and [b]Fırat University, Faculty of Science and Art, Department of Chemistry, TR-23169 Elazığ, Turkey

Correspondence e-mail: nocak@omu.edu.tr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.073
wR factor = 0.195
Data-to-parameter ratio = 13.7

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

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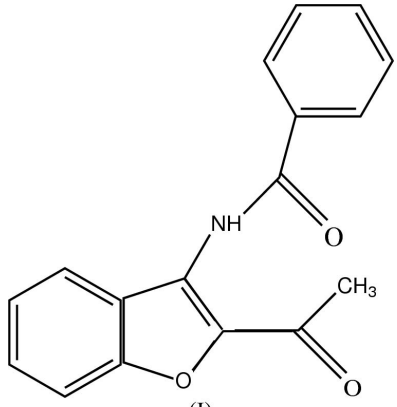
The title compound, $C_{17}H_{13}NO_3$, displays the characteristic features of benzofuran derivatives. The molecule is nearly planar. An intramolecular N—H···O hydrogen bond, together with π—π stacking interactions, helps to stabilize the structure.

Comment

The 2- and 3-substituted benzofuran nucleus is a central component of a diverse class of heterocyclic natural and synthetic products that exhibit a broad range of biological activities (Nicolaou *et al.*, 2000; Gölitzer & Kramer, 2000). The title compound, (I), was synthesized from the reaction of 2-acetyl-3-aminobenzofuran (Ocak Iskeleli *et al.*, 2005) with benzoyl chloride in dry acetone.



(I)

The benzofuran ring system of the title compound, (I), is planar, with a maximum deviation from the plane of 0.050 (6) Å for atom C4 (Fig. 1). The dihedral angle between the benzofuran ring system and the phenyl ring is 2.47 (13)°. The C═O bond lengths [C11—O3 = 1.232 (5) Å and C9—O2 = 1.239 (5) Å] agree with values reported in the literature (Ocak Iskeleli *et al.*, 2005).

The crystal structure is stabilized by an intramolecular N1—H1···O2 hydrogen bond and two π–π stacking interactions. These interactions are between *Cg*1(O1–C8) at (*x*, *y*, *z*) and *Cg*1 at (1 − *x*, −*y*, −*z*) [*Cg*1···*Cg*1^{i} = 3.500 (3) Å], *Cg*3(C12–C17) at (*x*, *y*, *z*) and *Cg*2(C1–C6) at (1 − *x*, 1 − *y*, −*z*) [*Cg*3···*Cg*2^{ii} = 3.691 (3) Å].

Experimental

A mixture of 2-acetyl-3-aminobenzofuran (1.75 g, 10 mmol) and benzoyl chloride (1.54 g, 11 mmol) in absolute acetone (200 ml) was stirred at room temperature for 5 h. The reaction mixture was poured

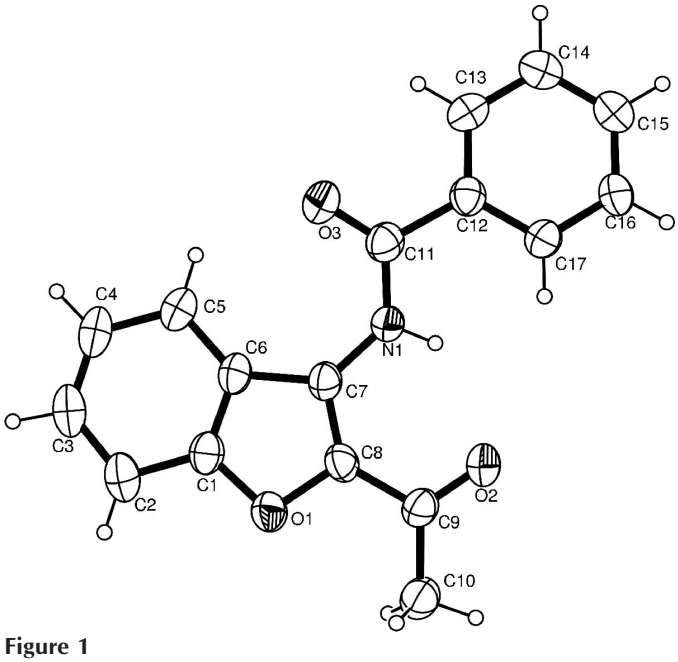


Figure 1
The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of fixed radius.

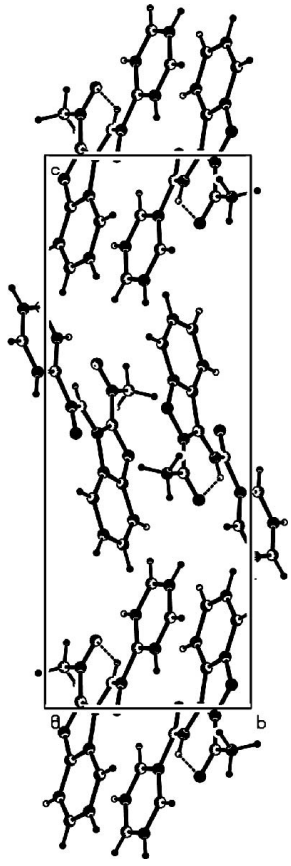


Figure 2
A packing diagram of compound (I) viewed along the *a* axis.

into water (400 ml) and neutralized with ammonia (5%). The title compound was filtered off, washed with water, dried and recrystallized from acetone (86%) to yield colourless crystals.

Crystal data

$C_{17}H_{13}NO_3$	D_x = 1.380 Mg m^{-3}
M_r = 279.28	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 7057 reflections
a = 8.9283 (12) Å	θ = 2.0–26.9°
b = 7.4852 (12) Å	μ = 0.10 mm^{-1}
c = 20.273 (3) Å	T = 293 (2) K
β = 97.032 (11)°	Plate, colourless
V = 1344.7 (3) Å^3	0.80 × 0.34 × 0.08 mm
Z = 4	

Data collection

Stoe IPDS-2 diffractometer	2615 independent reflections
ω scans	964 reflections with $I > 2\sigma(I)$
Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)	R_{int} = 0.141
	θ_{max} = 26.0°
T_{min} = 0.953, T_{max} = 0.994	$h = -11 \rightarrow 10$
7795 measured reflections	$k = -9 \rightarrow 9$
	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0791P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.073	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.195	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
S = 0.84	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
2615 reflections	Extinction correction: *SHELXL97*
191 parameters	Extinction coefficient: 0.015 (3)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

C1—C6	1.361 (6)	C6—C7	1.464 (5)
C1—O1	1.382 (5)	C7—C8	1.347 (6)
C1—C2	1.415 (6)	C7—N1	1.376 (5)
C2—C3	1.383 (7)	C8—O1	1.412 (5)
C3—C4	1.346 (7)	C9—O2	1.239 (5)
C4—C5	1.405 (6)	C11—O3	1.232 (5)
C5—C6	1.399 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	2.13	2.768 (5)	131

H atoms were positioned geometrically and treated using a riding model, with aromatic C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å and an N—H distance of 0.86 Å. U_{iso}(H) values were set at xU_{eq}(carrier atom), where x = *1.5* for methyl H and 1.2 for other H atoms. Owing to the poor quality of the crystal, the R_{int} and R values are somewhat high.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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