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2-Acetyl-3-amino-1-benzofuran

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Key indicators

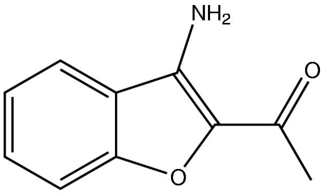
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.103
Data-to-parameter ratio = 13.1

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

The title compound, $C_{10}H_9NO_2$, displays the characteristic features of a benzofuran derivative. The molecular structure is nearly planar with an intramolecular N—H···O hydrogen bond involving the amino group and the acetyl carbonyl O atom. In the crystal structure, there are intermolecular N—H···O and C—H···O interactions, which help to stabilize the structure.

Comment

Benzofuran derivatives possess analgesic, antimicrobial, bacteriostatic, bactericidal, fungistatic and fungicidal activities (Hassaneen *et al.*, 2002). Many natural benzofurans have physiological, pharmacological and toxic properties and, as a result, there is continuing interest in their chemical synthesis (Kappe *et al.*, 1997; Arıcı *et al.*, 2004). The title compound, (I), was synthesized by the condensation of 1-chloroacetone with 2-cyanophenol in the presence of K_2CO_3.



(I)

The molecular structure of (I) is illustrated in Fig. 1 and selected bond distances and angles are given in Table 1. The molecule is nearly planar, with atom C1 displaced by 0.249 (2) Å from the mean plane through the benzofuran moiety and atoms O1, N1 and C2 (maximum deviation 0.059 Å for atom C2). In the benzofuran ring system, all the bond lengths agree with values reported in the literature (Arıcı *et al.*, 2004).

There is one intramolecular hydrogen bond and three intermolecular hydrogen bonds (Table 2 and Fig. 2). Atom O1 is involved as a acceptor in two intermolecular hydrogen bonds and in an intramolecular trifurcated hydrogen bond. The other C—H···O intermolecular interactions, shown in Fig. 2, help to stabilize the structure.

Experimental

2-Cyanophenol (11.91 g, 0.1 mol), potassium carbonate (20.00 g, 0,145 mol) and dry acetone (200 ml) were placed in a 500 ml two-necked flask fitted with a reflux condenser, and the mixture was stirred for 1 h at room temperature. To this solution, 1-chloroacetone (9.34 g, 8.05 ml, 0.101 mol) was added and the mixture refluxed for

4 h. The course of the reaction was monitored by IR spectroscopy. The mixture was allowed to cool to room temperature and was then poured into 500 ml of water and precipitated twice from water. The solid was filtered and recrystallized from ethanol (yield 12.70 g, 72.57%).

Crystal data

$C_{10}H_9NO_2$
$M_r = 175.18$
Monoclinic, $P2_1/c$
$a = 5.1800$ (4) Å
$b = 16.5600$ (14) Å
$c = 10.2271$ (8) Å
$\beta = 104.020$ (6)°
$V = 851.16$ (12) Å^3
$Z = 4$

$D_x = 1.367$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12 005 reflections
$\theta = 2.1$–27.6°
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.65 × 0.42 × 0.35 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: none
13 507 measured reflections
1932 independent reflections
1547 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.071$
$\theta_{\rm max} = 27.4°$
$h = -6 \rightarrow 6$
$k = -21 \rightarrow 21$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.103$
$S = 1.07$
1932 reflections
147 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 0.0487P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.18$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.117 (14)

Table 1
Selected bond distances (Å).

C2—O1	1.2425 (15)	C5—C6	1.4020 (16)
C3—C4	1.3789 (15)	C6—C7	1.3761 (19)
C3—O2	1.3980 (14)	C7—C8	1.399 (2)
C4—N1	1.3363 (16)	C8—C9	1.3794 (18)
C4—C5	1.4411 (16)	C9—C10	1.3807 (18)
C5—C10	1.3931 (16)	C10—O2	1.3601 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1D···O1	0.86	2.28	2.8496 (14)	124
N1—H1E···O1$^{\rm i}$	0.86	2.10	2.9122 (13)	158
C1—H1B···O1$^{\rm ii}$	0.95 (2)	2.60 (2)	3.5473 (19)	174.3 (17)
C9—H9···O2$^{\rm iii}$	1.004 (16)	2.545 (16)	3.5395 (16)	170.8 (12)

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

The amino H atoms were included in calculated positions and refined using a riding model [N—H = 0.86 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(N)]. The remainder of the H atoms were located in difference electron-density maps and refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); 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).

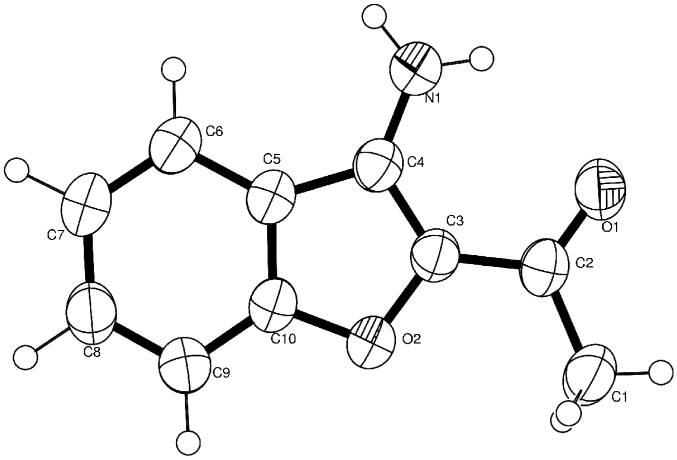


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

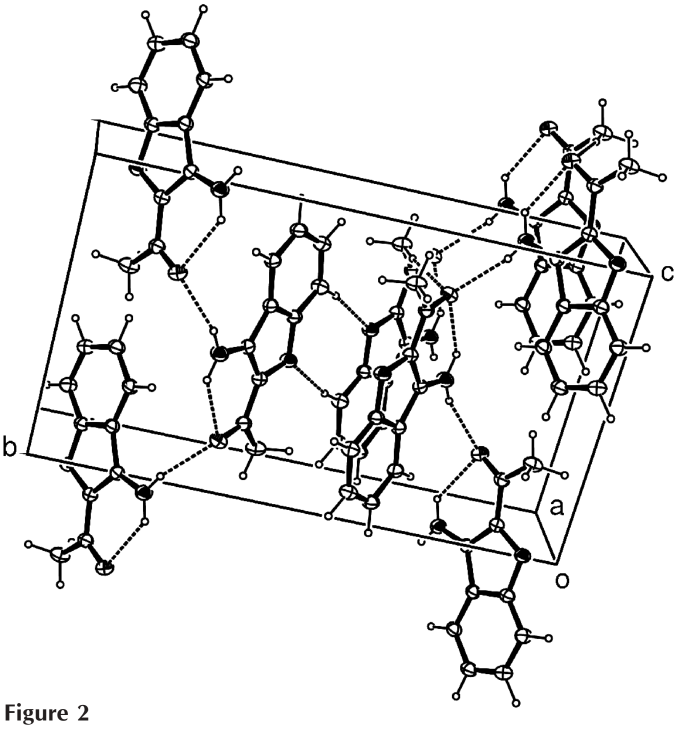


Figure 2
A view of the crystal packing of (I), showing the intra- and intermolecular hydrogen bonds (dashed lines).

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