organic papers

3-(3-Pyridylamino)isobenzofuran-1(3H)-one

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The crystal packing of the title compound, $C_{13}H_{10}O_2N_2$, is stabilized by one N—H$\cdots$N and two C—H$\cdots$O intermolecular hydrogen bonds and also by two C—H$\cdots\pi$ interactions. The N—H$\cdots$N and C—H$\cdots$O hydrogen bonds generate an edge-fused $R_3^3(19)$ ring motif and the phthalide section of the molecule is planar. The dihedral angle between the phthalide group and the pyridyl ring is 87.28 (10)°.

Comment

In separate papers, we have reported the synthesis and crystal structures of 3-(*p*-chloroanilino)phthalide (Büyükgüngör & Odabaşoğlu, 2006), 3-(*o*-methoxyanilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*a*), 3-(*p*-methoxyanilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*b*) and 3-(*p*-hydroxyanilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*c*). Here, we report the structure of 3-(pyridin-3-ylamino)isobenzofuran-1(3*H*)-one, (I) (Fig. 1 and Table 1).


(I)
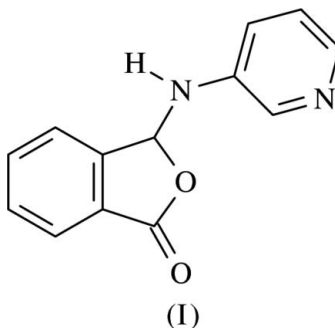
The phthalide group of (I) (atoms C1–C8/O2) is essentially planar, the largest deviation from the mean plane being 0.014 (2) Å for atom C8. The dihedral angle between the mean planes of the phthalide group and the pyridyl ring is 87.28 (10)°.

The crystal packing of (I) is stabilized by N—H$\cdots$N and C—H$\cdots$O intermolecular hydrogen bonds, which generate an edge-fused $R_3^3(19)$ ring motif (Etter, 1990), and by C—H$\cdots\pi$ interactions (Fig. 2 and Table 2).

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006*c*), using phthalaldehydic acid and 3-aminopyridine as starting materials (yield 85%; m.p. 432–433 K). Crystals of (I) suitable for X-ray crystal structure analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.
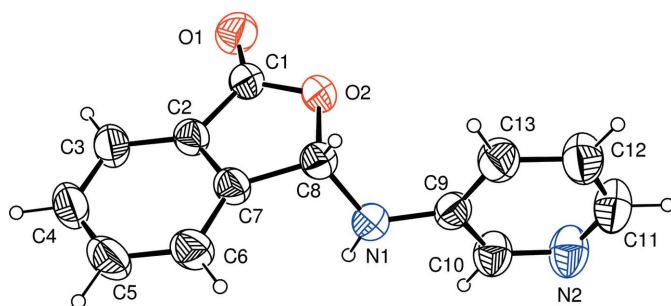
Figure 1
A view of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

Crystal data

$C_{13}H_{10}N_2O_2$
$M_r = 226.23$
Orthorhombic, $P2_12_12_1$
$a = 5.8236$ (5) Å
$b = 7.9820$ (7) Å
$c = 24.5229$ (17) Å
$V = 1139.92$ (16) Å^3

$Z = 4$
$D_x = 1.318$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Plate, colourless
$0.74 \times 0.52 \times 0.09$ mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration
  (*X-RED32*; Stoe & Cie, 2002)
  $T_{min} = 0.939$, $T_{max} = 0.992$

9694 measured reflections
1327 independent reflections
1110 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.091$
$S = 1.07$
1327 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.0337P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.047 (8)

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.206 (3)	C7—C8	1.493 (3)
C1—O2	1.350 (3)	C8—N1	1.408 (2)
C2—C7	1.377 (3)	C9—N1	1.395 (3)
O1—C1—O2	121.04 (19)	N1—C8—O2	111.24 (16)
O1—C1—C2	130.2 (2)		

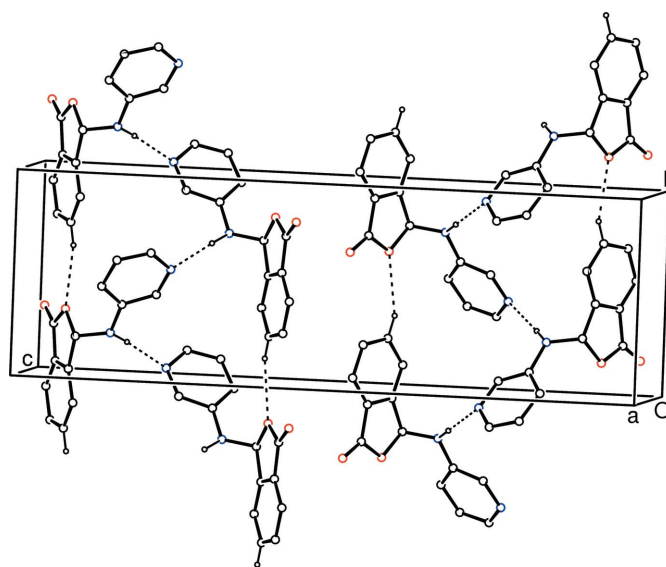**Table 2**
Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C9–C13 and C2–C7 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$N2^i	0.98 (3)	2.04 (3)	2.996 (3)	165 (2)
C5—H5$\cdots$O2^{ii}	0.93	2.52	3.366 (3)	152
C13—H13$\cdots$O1^{iii}	0.93	2.59	3.512 (3)	170
C4—H4$\cdots$Cg1^{iv}	0.93	3.35	4.075 (3)	137
C11—H11$\cdots$Cg2^v	0.93	2.83	3.746 (3)	170

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

Figure 2
A packing diagram for (I), with hydrogen bonds drawn as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

In the absence of significant anomalous dispersion effects, Freidel pairs were merged. All C-bound H atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic H and 0.98 Å for methine H, and with $U_{iso}(H) = 1.2U_{eq}(C)$. The N-bound H atom was located in a difference Fourier map and refined freely with an isotropic displacement parameter.

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, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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