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## Key indicators

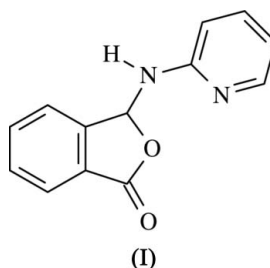
Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.062  
 $wR$  factor = 0.132  
Data-to-parameter ratio = 12.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.3-(2-Pyridylamino)isobenzofuran-1(3*H*)-oneThe crystal structure of the title compound,  $\text{C}_{13}\text{H}_{10}\text{O}_2\text{N}_2$ , is stabilized by  $\text{N}-\text{H}\cdots\text{N}$  intermolecular hydrogen bonds which generate  $C(4)$  chains. The phthalide system is planar and the dihedral angle between this plane and that of the pyridine ring is  $73.55(13)^\circ$ .

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3-Substituted phthalides. Part  
VI

## Comment

In a previous paper, we reported the synthesis and crystal structure of 3-(3-pyridylamino)isobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2006*b*). In the present paper, we report the structure of 3-(2-pyridylamino)isobenzofuran-1(3*H*)-one [or 3-(2-pyridylamino)phthalide], (I) (Fig. 1).The crystal packing is stabilized by  $\text{N}-\text{H}\cdots\text{N}$  intermolecular hydrogen bonds (Table 2), forming  $C(4)$  chains (Etter, 1990) running parallel to the  $a$  axis (Fig. 2). The phthalide system ( $\text{C}1-\text{C}8/\text{O}2$ ) of the molecule is essentially planar, the largest deviation from the mean plane being  $0.020(3)$  Å for atom C8. The dihedral angle between the mean planes of the phthalide unit and the pyridine ring is  $73.55(13)^\circ$ .

## Experimental

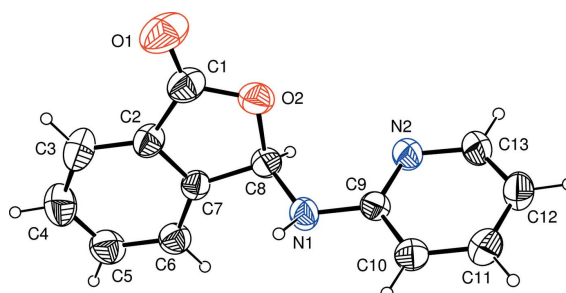
The title compound was prepared as described by Kubota & Tatsuno (1971) and Odabaşoğlu & Büyükgüngör (2006*a*) using phthalaldehyde.

Figure 1

A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

hydric acid and 2-aminopyridine as starting materials (yield 95%; m.p. 479–480 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.

Crystal data

$C_{13}H_{10}N_2O_2$   $Z = 8$   
 $M_r = 226.23$   $D_x = 1.333 \text{ Mg m}^{-3}$   
 Orthorhombic, *Pbca* Mo  $K\alpha$  radiation  
 $a = 8.6366 (5) \text{ \AA}$   $\mu = 0.09 \text{ mm}^{-1}$   
 $b = 18.1462 (12) \text{ \AA}$   $T = 296 \text{ K}$   
 $c = 14.3885 (11) \text{ \AA}$  Plate, colorless  
 $V = 2255.0 (3) \text{ \AA}^3$   $0.78 \times 0.31 \times 0.04 \text{ mm}$

Data collection

Stoe IPDS-2 diffractometer 23991 measured reflections  
 $\omega$  scans 1991 independent reflections  
 Absorption correction: integration 1173 reflections with  $I > 2\sigma(I)$   
 (*X-RED32*; Stoe & Cie, 2002)  $R_{\text{int}} = 0.154$   
 $T_{\text{min}} = 0.961, T_{\text{max}} = 0.996$   $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on  $F^2$   $w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.1489P]$   
 $R[F^2 > 2\sigma(F^2)] = 0.062$  where  $P = (F_o^2 + 2F_c^2)/3$   
 $wR(F^2) = 0.132$   $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $S = 1.04$   $\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$   
 1991 reflections  $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$   
 158 parameters  
 H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected geometric parameters ( $\text{\AA}, ^\circ$ ).

C1–O1	1.211 (4)	C7–C8	1.503 (4)
C1–O2	1.363 (4)	C8–N1	1.419 (4)
C2–C7	1.370 (4)		
O1–C1–O2	120.9 (3)	N1–C8–O2	111.3 (2)
O1–C1–C2	130.3 (4)		

Table 2

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1–H1 $\cdots$ N2 <sup>i</sup>	0.89 (4)	2.12 (4)	2.981 (4)	161 (3)

Symmetry code: (i)  $x - \frac{1}{2}, y, -z + \frac{1}{2}$ .

There did not appear to be any problem with the crystal quality in terms of the physical appearance and diffraction spots. However, the compound crystallized as very thin plate-shaped crystals and so, although the exposure time was set to a high value (5 min), the value of  $R_{\text{int}}$ , 0.154, is due to the weakness of the diffraction. All C-bound H atoms were refined using the riding-model approximation, with C–

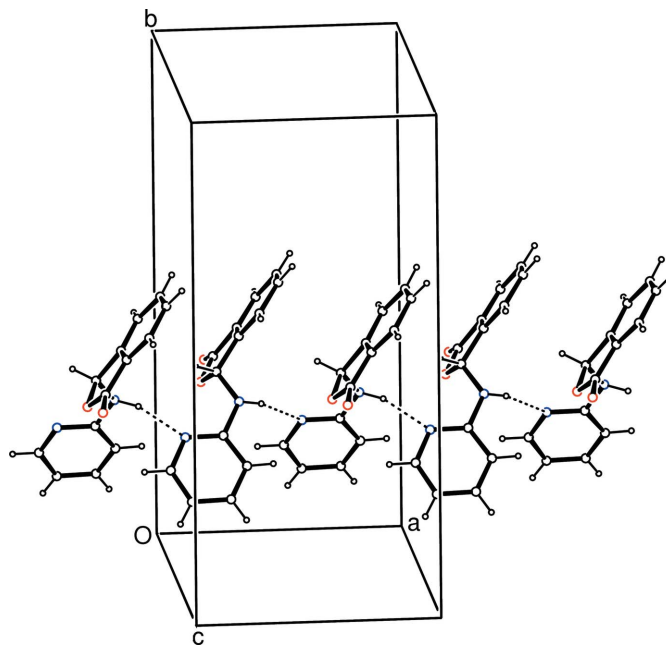


Figure 2

A partial packing diagram of (I), showing the hydrogen bonds as dashed lines.

H = 0.93  $\text{\AA}$  for aromatic and C–H = 0.98  $\text{\AA}$  for methine H atoms [ $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ ]. The N-bound H atom was located in a Fourier difference map and was allowed to refine freely.

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

- Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
 Kubota, Y. & Tatsuno, T. (1971). *Chem. Pharm. Bull.* **19**, 1226–1233.  
 Odabaşoğlu, M. & Büyükgüngör, O. (2006a). *Acta Cryst.* **E62**, o1879–o1881.  
 Odabaşoğlu, M. & Büyükgüngör, O. (2006b). *Acta Cryst.* **E62**, o2088–o2089.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. Univ. of Göttingen, Germany.  
 Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.