

Mustafa Odabaşoğlu^{a*} and
Orhan Büyükgüngör^b

^aDepartment of Chemistry, Faculty of Arts & Science, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, and ^bDepartment of Physics, Faculty of Arts & Science, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey

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

Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(C-C) = 0.007$ Å
 R factor = 0.035
 wR factor = 0.079
Data-to-parameter ratio = 14.6

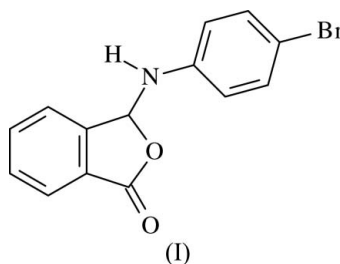
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

3-(4-Bromoanilino)isobenzofuran-1(3H)-one

Crystals of the title compound, $C_{14}H_{10}BrNO_2$, contain $N-H \cdots O$ hydrogen bond interactions that generate $C(6)$ chains; these chains are linked by $C-H \cdots O$ hydrogen bonds, generating an $R_4^3(21)$ ring motif.

Comment

We report here the structure of 3-(4-bromoanilino)-isobenzofuran-1(3H)-one, (I) (Fig. 1 and Table 1), and we briefly compare this with the structure of the chloro and fluoro analogues, which have been previously reported by us (Büyükgüngör & Odabaşoğlu, 2006; Odabaşoğlu & Büyükgüngör, 2006a). The dihedral angle between the *p*-bromophenyl ring and the mean plane of the phthalide group is $62.2(2)^\circ$; for comparison, this angle is $75.58(15)^\circ$ in 3-(4-chloroanilino)phthalide and $74.10(9)^\circ$ in 3-(4-fluoroanilino)phthalide.



The phthalide group (C1–C8/O2) is essentially planar, the largest deviation from the mean plane being $0.030(4)$ Å for atom C7. In (I), as in the chloro analogue, the crystal packing is stabilized by $N-H \cdots O$ intermolecular hydrogen bonds (Fig. 2 and Table 2), which generate a $C(6)$ chain. The $C(6)$ chains are linked by $C-H \cdots O$ interactions, generating an $R_4^3(21)$ ring motif (Etter, 1990). The chloro and fluoro analogues have $\pi-\pi$ stacking interactions but (I) does not.

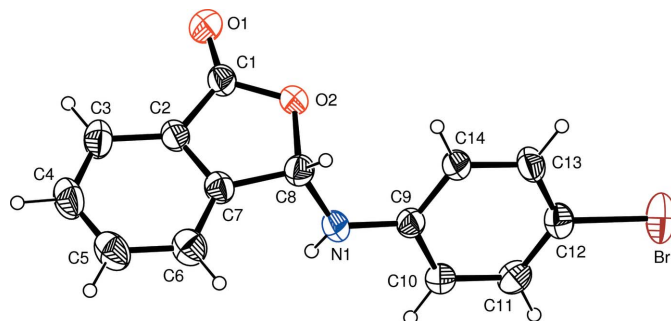


Figure 1

The molecular structure of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 30% probability level.

Received 18 July 2006
Accepted 4 September 2006
Substituted phthalides, Part XIV

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006*b*), using phthalaldehydic acid and 4-bromo-aniline as starting materials (yield 90%; m.p. 452–453 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

Crystal data

$C_{14}H_{10}BrNO_2$	$Z = 4$
$M_r = 304.14$	$D_x = 1.602 \text{ Mg m}^{-3}$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 8.1158 (8) \text{ \AA}$	$\mu = 3.25 \text{ mm}^{-1}$
$b = 27.3737 (18) \text{ \AA}$	$T = 296 \text{ K}$
$c = 5.6775 (4) \text{ \AA}$	Plate, colourless
$V = 1261.31 (17) \text{ \AA}^3$	$0.77 \times 0.31 \times 0.07 \text{ mm}$

Data collection

Stoe IPDS-2 diffractometer	11941 measured reflections
ω scans	2452 independent reflections
Absorption correction: integration (<i>X-RED</i> ; Stoe & Cie, 2002)	1446 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.298$, $T_{\max} = 0.810$	$R_{\text{int}} = 0.081$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.079$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 0.92$	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
2452 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$
168 parameters	Absolute structure: Flack (1983),
H atoms treated by a mixture of independent and constrained refinement	1089 Friedel pairs
	Flack parameter: 0.004 (15)

Table 1

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

C1–O1	1.193 (6)	C2–C7	1.360 (6)
C1–O2	1.354 (4)	C9–N1	1.397 (5)
O1–C1–O2	121.5 (4)	N1–C8–O2	112.2 (3)
O1–C1–C2	131.1 (4)		

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1 \cdots O1 ⁱ	0.78 (4)	2.35 (4)	3.083 (5)	156 (4)
C5–H5 \cdots O1 ⁱⁱ	0.93	2.42	3.254 (7)	149

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

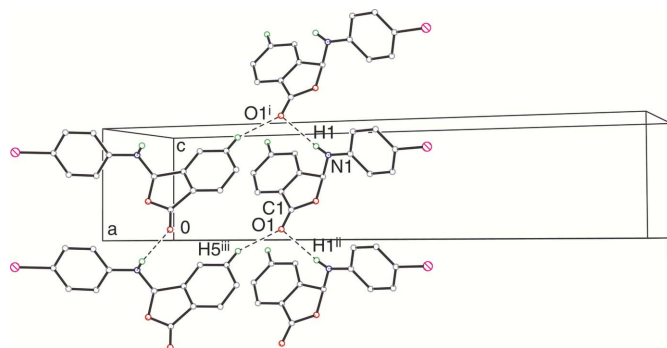


Figure 2

A partial packing diagram for (I), showing the N–H \cdots O and C–H \cdots O interactions (dashed lines). H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $x, y, 1 + z$; (ii) $x, y, z - 1$; (iii) $\frac{1}{2} + x, \frac{1}{2} - y, z - 1$].

All H atoms attached to C atoms were treated as riding on their parent atoms, with C–H = 0.93 \AA for aromatic and 0.98 \AA for methine H atoms, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom of the amino group was located in a Fourier difference map and freely refined.

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).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS2 diffractometer (purchased under grant F.279 of the University Research Fund).

References

- Büyükgüngör, O. & Odabaşoğlu, M. (2006). *Acta Cryst.* **E62**, o2003–o2004.
 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.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Odabaşoğlu, M. & Büyükgüngör, O. (2006*a*). *Acta Cryst.* **E62**, o4138–o4139.
 Odabaşoğlu, M. & Büyükgüngör, O. (2006*b*). *Acta Cryst.* **E62**, o1879–o1881.
 Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
 Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.