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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 = 0.055
 wR factor = 0.139
Data-to-parameter ratio = 14.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

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

The structure of the title compound, $\text{C}_{14}\text{H}_{10}\text{ClNO}_2$, is stabilized by $\text{N}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ interactions. The phthalide part of the molecule is planar and the dihedral angle between the phthalide group and the benzene ring is 75.58 (15)°.Received 10 April 2006
Accepted 20 April 2006
3-Substituted phthalides. Part IV.

Comment

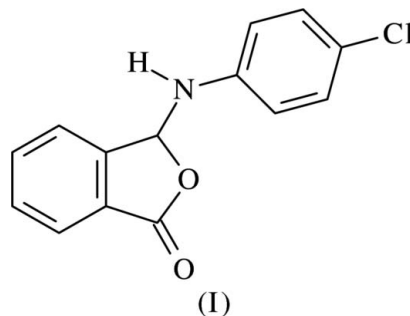
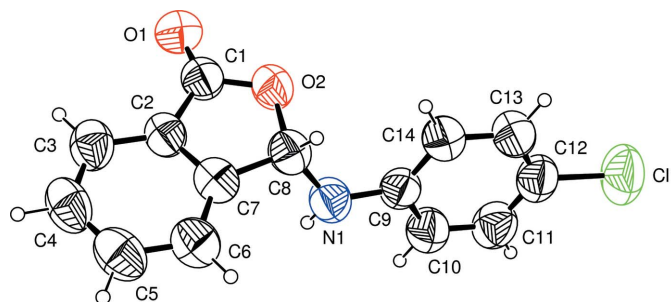
Phthalides are known to show diverse biological activities as hormones, pheromones and antibiotics (Aoki *et al.*, 1973; Kubota & Tatsuno, 1971; Tsi & Tan, 1997). As part of our ongoing research on 3-substituted phthalides, the title compound, (I), has been synthesized and its crystal structure is reported here.The molecule of (I) is built up from a phthalide unit connected to a chlorophenyl ring through an amino group (Fig. 1). The phthalide part (atoms C1–C8) is essentially planar, the largest deviation from the mean plane being 0.014 (3) Å for atom C1. The dihedral angle between the *p*-chlorophenyl ring and the mean plane of the phthalide group is 5.58 (15)°.

Figure 1

A view of (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

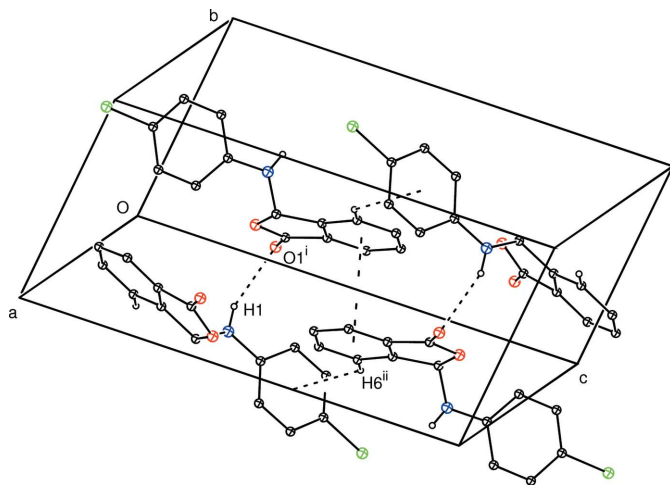


Figure 2
A packing diagram for (I), showing the N—H···O, C—H···π and π—π interactions represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$.]

The occurrence of N—H···O hydrogen bonds results in the formation of *C*(6) chains (Etter, 1990) developing parallel to the *a* axis (Table 1, Fig. 2). These *C*(6) chains are linked to each other by C—H···π and π—π interactions, resulting in the formation of a sheet parallel to the *bc* plane (Table 1, Fig. 2). The π—π interaction occurs between the C2—C7 six-membered ring and its symmetry-related counterpart at $(-x, -y + 1, -z)$, with a centroid-to-centroid distance of 3.618 Å and a plane-to-plane separation of 3.596 Å.

Experimental

The title compound was prepared according to the method described by Odabaşoğlu & Büyükgüngör (2006), using phthalaldehydic acid and 4-chloroaniline as starting materials (yield 90%; m.p. 454–455 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.

Crystal data

$C_{14}H_{10}ClNO_2$	$Z = 4$
$M_r = 259.68$	$D_x = 1.395 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.9256$ (14) Å	$\mu = 0.30 \text{ mm}^{-1}$
$b = 7.2383$ (10) Å	$T = 296 \text{ K}$
$c = 15.6115$ (16) Å	Prismatic plate, pale yellow
$\beta = 122.196$ (7)°	$0.60 \times 0.42 \times 0.16 \text{ mm}$
$V = 1236.0$ (3) Å ³	

Data collection

Stoe IPDS 2 diffractometer	16688 measured reflections
φ scans	2422 independent reflections
Absorption correction: integration (<i>X-RED32</i> ; Stoe & Cie, 2002)	1385 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.848, T_{\max} = 0.955$	$R_{\text{int}} = 0.090$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.139$
 $S = 1.05$
 2422 reflections
 167 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.036P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.213 (3)	C8—N1	1.404 (4)
C1—O2	1.347 (3)	C8—O2	1.505 (3)
C2—C7	1.375 (4)	C9—N1	1.400 (4)
C7—C8	1.492 (4)		
O1—C1—O2	121.5 (3)	N1—C8—C7	114.2 (2)
O1—C1—C2	130.0 (3)	N1—C8—O2	111.6 (2)

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

*Cg*1 is the centroid of ring C9—C14.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1···O1 ⁱ	0.82 (2)	2.29 (3)	3.046 (4)	155 (2)
C6—H6··· <i>Cg</i> 1 ⁱⁱ	0.93	3.29	3.987 (4)	134

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

All H atoms attached to C atoms were treated as riding on their parent atoms, with C—H = 0.93 Å for aromatic H and 0.98 Å for methine H, 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, 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).

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

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