

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 $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.040
 wR factor = 0.106
Data-to-parameter ratio = 14.4

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

3-(Thiazol-2-ylamino)isobenzofuran-1(3H)-one

The crystal structure of the title compound, $\text{C}_{11}\text{H}_8\text{N}_2\text{O}_2\text{S}$, is stabilized by one $\text{N}-\text{H}\cdots\text{N}$ and two $\text{C}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds and also by three $\text{C}-\text{H}\cdots\pi$ interactions. The $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds generate $R_4^4(26)$ ring motifs and the $\text{N}-\text{H}\cdots\text{N}$ and one of the $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds generate $R_3^3(26)$ ring motifs. The phthalide ring system of the molecule is almost planar and forms a dihedral angle of $74.84(9)^\circ$ with the thiazole ring.

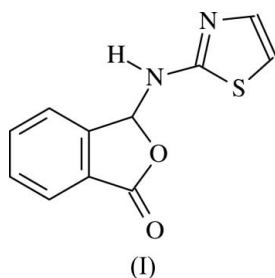
Received 11 May 2006

Accepted 13 June 2006

3-Substituted phthalides,
Part VIII

Comment

Phthalides (isobenzofuranones) are five-membered lactones found in plants and are known to show diverse biological activities as hormones, pheromones and antibiotics. These compounds possess several important properties, such as fungicidal (Aoki *et al.*, 1973; Lacova, 1974), bactericidal and herbicidal (Lacova, 1974), analgesic (Elderfield, 1951), and hypotensive and vasorelaxant activities (Tsi & Tan, 1997).



In earlier papers, we have reported the synthesis and crystal structures of some 3-hetero-substituted phthalides [3-(2-pyridylamino)phthalide (Odabaşoğlu & Büyükgüngör, 2006a), 3-(3-pyridylamino)phthalide (Odabaşoğlu & Büyükgüngör, 2006b) and 3-(4-methylpyridin-2-ylamino)isobenzofuran-1(3H)-one (Odabaşoğlu & Büyükgüngör, 2006c)]. We report here the structure of 3-(thiazol-2-ylamino)isobenzofuran-1(3H)-one, (I) (Fig. 1 and Table 1).

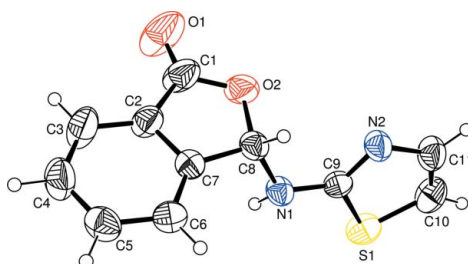
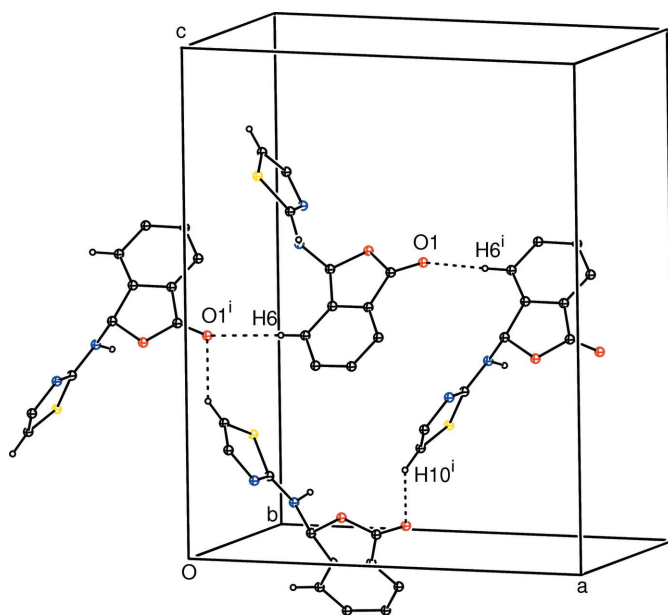
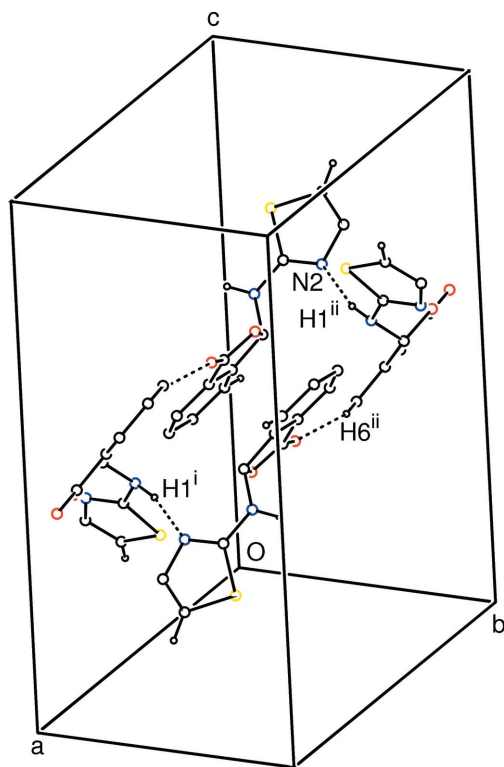


Figure 1

A view of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 40% probability level.

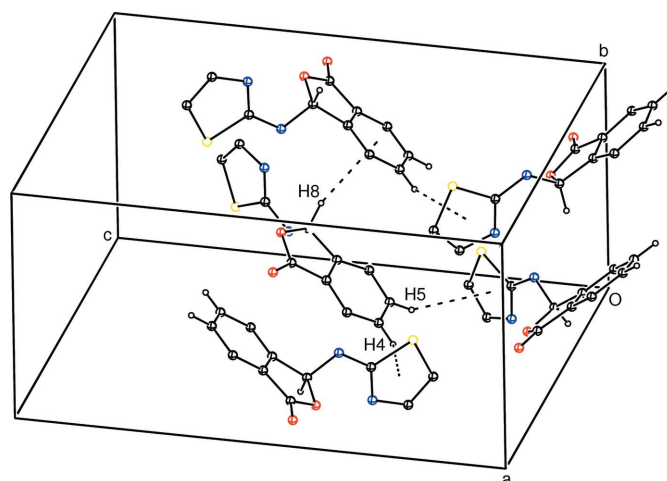
**Figure 2**

The packing of (I), showing the $R_4^3(26)$ ring motif, with hydrogen bonds drawn as dashed lines. H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, -z$.]

**Figure 3**

The packing of (I), showing the $R_4^1(26)$ ring motif, with hydrogen bonds drawn as dashed lines. H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, -z$; (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, z$.]

The phthalide group (C1–C8/O2) is planar, the largest deviation from the mean plane being 0.024 (2) Å for atom C8. The dihedral angle between the mean planes of the phthalide group and the thiazole ring is 74.84 (9)°.

**Figure 4**

The packing of (I), showing the C–H... π interactions as dashed lines. H atoms not involved in these interactions have been omitted.

The crystal packing is stabilized by N–H...N and C–H...O intermolecular hydrogen bonds and also by three C–H... π interactions (Table 2 and Figs. 2–4). The C–H...O intermolecular hydrogen bonds generate $R_4^3(26)$ ring motifs while the N1–H1...N1 and C–H...O intermolecular hydrogen bonds generate $R_4^1(26)$ ring motifs (Etter, 1990).

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006*d*), using *o*-phthalaldehydic acid and 2-aminothiazole as starting materials (yield 87%; m.p. 457–459 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.

Crystal data

$C_{11}H_8N_2O_2S$
 $M_r = 232.25$
 Orthorhombic, $Pbca$
 $a = 14.291$ (1) Å
 $b = 8.699$ (1) Å
 $c = 17.529$ (1) Å
 $V = 2179.2$ (3) Å³

$Z = 8$
 $D_x = 1.416$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.29$ mm⁻¹
 $T = 296$ K
 Prism, colorless
 $0.74 \times 0.42 \times 0.17$ mm

Data collection

Stoe IPDS-2 diffractometer
 ω scans
 Absorption correction: integration
 (X -RED32; Stoe, 2002)
 $T_{\min} = 0.853$, $T_{\max} = 0.960$

14575 measured reflections
 2145 independent reflections
 1579 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$
 $\theta_{\max} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.106$
 $S = 1.03$
 2145 reflections
 149 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.2248P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.21$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1—O1	1.200 (3)	C9—N2	1.295 (2)
C1—O2	1.344 (3)	C9—N1	1.370 (2)
C2—C7	1.364 (3)	C9—S1	1.7285 (18)
C7—C8	1.500 (2)	C10—S1	1.720 (3)
C8—N1	1.418 (2)		
O1—C1—O2	121.8 (2)	N1—C8—O2	111.09 (15)
O1—C1—C2	129.1 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

<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...N2 ⁱ	0.87 (2)	2.06 (2)	2.903 (2)	164 (2)
C6—H6...O1 ⁱⁱ	0.93	2.53	3.426 (3)	161
C10—H10...O1 ⁱⁱⁱ	0.93	2.40	3.140 (3)	137
C4—H4...Cg1 ^{iv}	0.93	3.12	3.749 (3)	127
C5—H5...Cg1 ^v	0.93	3.06	3.896 (2)	150
C8—H8...Cg2 ^{vi}	0.98	2.93	3.888 (2)	164

Symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, z$; (ii) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (iii) $x - \frac{1}{2}, y, -z + \frac{3}{2}$; (iv) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (v) $x, -y - \frac{1}{2}, z - \frac{3}{2}$; (vi) $-x - \frac{1}{2}, y - \frac{1}{2}, z$. Cg1 and Cg2 are the centroids of the S1/N2/C9—C11 and C2—C7 rings.

All C-bound H atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic H atoms and C—H = 0.98 Å for methine H atoms [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$]. 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, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe, 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 acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDSII diffractometer (purchased under grant F.279 of the University Research Fund).

References

- Aoki, K., Furusho, T., Kimura, T., Satake, K. & Funayama, S. (1973). Jpn Patent No. 7 324 724; (1974). *Chem. Abstr.* **80**, 129246.
- Elderfield, R. C. (1951). *Heterocyclic Compounds*, Vol. 2, ch. 2. New York: Wiley.
- 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.
- Lacova, M. (1974). *Chem. Abstr.* **80**, 59757.
- Odabaşoğlu, M. & Büyükgüngör, O. (2006a). *Acta Cryst.* **E62**, o2079–o2080.
- Odabaşoğlu, M. & Büyükgüngör, O. (2006b). *Acta Cryst.* **E62**, o2088–o2089.
- Odabaşoğlu, M. & Büyükgüngör, O. (2006c). *Acta Cryst.* **E62**, o2316–o2317.
- Odabaşoğlu, M. & Büyükgüngör, O. (2006d). *Acta Cryst.* **E62**, o1879–o1881.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Stoe (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
- Tsi, D. & Tan, B. K. H. (1997). *Phytother. Res.* **11**, 576–582.