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N-Benzylphthalimide

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Key indicators

Single-crystal X-ray study T = 298 K Mean σ (C–C) = 0.004 Å R factor = 0.073 wR factor = 0.142 Data-to-parameter ratio = 13.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e. In the title compound, $C_{15}H_{11}NO_2$, the benzene and phthalimide groups are planar and make a dihedral angle of 74.2 (1)° with one another. There are three weak $C-H\cdots O$ hydrogen bonds, forming a two-dimensional network structure.

Comment

Phthalimides exhibit various biological properties and have been reported as antipsychotics (Norman *et al.*, 1996), antiinflammatory agents (Collin *et al.*, 2001) and herbicides (Kawaguchi & Ikeda, 2001). In the study of phthalimides, some unconventional methods of synthesis have been adopted; for example, some substituted phthalimides have been obtained by a microwave-assisted synthesis (Martin *et al.*, 2003). Here, we report that the title compound, (I), has also been synthesized under microwave irradiation in our laboratory.



The molecular structure of (I) is shown in Fig. 1. The C8– N1, C9–N1, C8–O1 and C9–O2 bond lengths (Table 1) in the phthalimide system confirm the delocalization of the π electrons in this system. The benzene and phthalimide groups are planar and make a dihedral angle of 74.2 (1)° with each other.



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Figure 1 The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

organic papers



Figure 2

The two-dimensional network structure of (I), formed by intermolecular hydrogen-bonding interactions (shown as dashed lines).

In the crystal structure (Fig. 2 and Table 2), weak intermolecular hydrogen-bonding interactions exist, forming a twodimensional network structure.

Experimental

The synthesis of the title compound was carried out by mixing phthalimide (5 mmol) with benzyl bromide (7 mmol) and a catalytic amount of tetrabutylammonium bromide (TBAB). The mixture was adsorbed on potassium carbonate and irradiated in an open Erlenmeyer flask in a domestic microwave oven (300 W) for 5 min. The solid was recrystallized from ethanol to afford the pure product in 70% yield (m.p. 386–387 k). Single crystals of (I) suitable for X-ray data collection were obtained by slow evaporation of an acetone solution.

Crystal data

 $\begin{array}{l} C_{15}H_{11}NO_2\\ M_r = 237.25\\ Triclinic, P\overline{1}\\ a = 7.1840 \ (8) \ \text{\AA}\\ b = 8.5211 \ (9) \ \text{\AA}\\ c = 10.2370 \ (11) \ \text{\AA}\\ \alpha = 99.062 \ (2)^{\circ}\\ \beta = 97.578 \ (2)^{\circ}\\ \gamma = 106.848 \ (2)^{\circ} \end{array}$

Data collection

Bruker APEX area-detector diffractometer φ and ω scans Absorption correction: multi-scan (*SADABS*; Bruker 2002) $T_{\min} = 0.975, T_{\max} = 0.988$ $V = 581.74 (11) \text{ Å}^{3}$ Z = 2 $D_{x} = 1.354 \text{ Mg m}^{-3}$ Mo K\alpha radiation $\mu = 0.09 \text{ mm}^{-1}$ T = 298 (2) KBlock, colourless $0.23 \times 0.13 \times 0.11 \text{ mm}$

5772 measured reflections 2114 independent reflections 1800 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.025$ $\theta_{\text{max}} = 25.3^{\circ}$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.074$	+ 0.179P]
$wR(F^2) = 0.142$	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.25	$(\Delta/\sigma)_{\rm max} < 0.001$
2114 reflections	$\Delta \rho_{\rm max} = 0.15 \ {\rm e} \ {\rm \AA}^{-3}$
163 parameters	$\Delta \rho_{\rm min} = -0.19 \text{ e} \text{ \AA}^{-3}$
H-atom parameters constrained	

Table 1 Selected geometric parameters (Å, $^{\circ}$).

01-C8	1.205 (3)	N1-C7	1.460 (3)
O2-C9	1.205 (3)	C8-C11	1.480 (3)
N1-C9	1.386 (3)	C9-C10	1.486 (3)
N1-C8	1.388 (3)		
C9-N1-C8	112.0 (2)	O2-C9-N1	125.1 (2)
C9-N1-C7	123.6 (2)	O2-C9-C10	129.0 (2)
C8-N1-C7	124.3 (2)	N1-C9-C10	105.9 (2)
N1-C7-C1	111.9 (2)	C15-C10-C9	131.0 (2)
O1-C8-N1	125.2 (2)	C11-C10-C9	107.9 (2)
O1-C8-C11	128.9 (2)	C12-C11-C8	130.3 (2)
N1-C8-C11	105.9 (2)	C10-C11-C8	108.2 (2)

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

$D - H \cdots A$	D-H	$H \cdots A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$C13-H13\cdots O2^{i}$ $C7-H7B\cdots O1^{ii}$	0.93 0.97	2.62 2.70	3.468 (4) 3.514 (3)	151 142
C3−H3···O1 ⁱⁱⁱ	0.93	2.65	3.384 (4)	136

Symmetry codes: (i) x, y - 1, z; (ii) -x, -y + 1, -z + 1; (iii) -x + 1, -y + 1, -z + 1.

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C-H = 0.93 or 0.96 Å for aromatic and methylene H atoms, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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