Acta Crystallographica Section E

## Structure Reports

Online
ISSN 1600-5368

Yan-Wen Lü, ${ }^{\text {a }}$ Bo-Hua Wang, ${ }^{\text {b }}$ Ge-Dong Cai, ${ }^{\text {b,c }}$ Zhen-Hua Li ${ }^{\text {b }}$ and Ping Wang ${ }^{\text {b }}$ *

${ }^{\text {a }}$ Department of Chemistry and Pharmaceutical Engineering, West Branch of Zhejiang University of Technology, Quzhou 324006, People's Republic of China, ${ }^{\mathbf{b}}$ Zhejiang Key Laboratory of Pharmaceutical Engineering, College of Pharmaceutical Sciences, Zhejiang University of Technology, Hangzhou 310014, People's Republic of China, and ${ }^{\text {c }}$ Hangzhou Vanco Science and Technology Co. Ltd, Hangzhou 310012, People's Republic of China

Correspondence e-mail:
wangping45@zjut.edu.cn

## Key indicators

Single-crystal X-ray study
$T=298 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.004 \AA$
$R$ factor $=0.073$
$w R$ 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.

[^0]
## $N$-Benzylphthalimide

In the title compound, $\mathrm{C}_{15} \mathrm{H}_{11} \mathrm{NO}_{2}$, the benzene and phthalimide groups are planar and make a dihedral angle of 74.2 (1) ${ }^{\circ}$ with one another. There are three weak $\mathrm{C}-\mathrm{H} \cdots \mathrm{O}$ 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.

(I)

The molecular structure of (I) is shown in Fig. 1. The C8$\mathrm{N} 1, \mathrm{C} 9-\mathrm{N} 1, \mathrm{C} 8-\mathrm{O} 1$ and $\mathrm{C} 9-\mathrm{O} 2$ bond lengths (Table 1) in the phthalimide system confirm the delocalization of the $\pi$ electrons in this system. The benzene and phthalimide groups are planar and make a dihedral angle of $74.2(1)^{\circ}$ with each other.


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

Received 21 May 2006
Accepted 12 June 2006


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

$\mathrm{C}_{15} \mathrm{H}_{11} \mathrm{NO}_{2}$
$M_{r}=237.25$
Triclinic, $P \overline{1}$
$a=7.1840$ (8) Å
$b=8.5211$ (9) $\AA$
$c=10.2370(11) \AA$
$\alpha=99.062$ (2) ${ }^{\circ}$
$\beta=97.578$ (2) ${ }^{\circ}$
$\gamma=106.848(2)^{\circ}$

## Data collection

Bruker APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker 2002)

$$
T_{\min }=0.975, T_{\max }=0.988
$$

$V=581.74(11) \AA^{3}$
$Z=2$
$D_{x}=1.354 \mathrm{Mg} \mathrm{m}^{-3}$
Mo $K \alpha$ radiation
$\mu=0.09 \mathrm{~mm}^{-1}$
$T=298$ (2) K
Block, colourless
$0.23 \times 0.13 \times 0.11 \mathrm{~mm}$

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 $F^{2}$

$$
\begin{gathered}
w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}{ }^{2}\right)+(0.0417 P)^{2}\right. \\
\quad+0.179 P] \\
\text { where } P=\left(F_{\mathrm{o}}^{2}+2 F_{\mathrm{c}}^{2}\right) / 3 \\
(\Delta / \sigma)_{\max }<0.001 \\
\Delta \rho_{\max }=0.15 \mathrm{e}^{-3} \AA^{-3} \\
\Delta \rho_{\min }=-0.19 \mathrm{e}^{-3}
\end{gathered}
$$

$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.074$
$w R\left(F^{2}\right)=0.142$
$S=1.25$
2114 reflections
163 parameters
H -atom parameters constrained

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

| O1-C8 | $1.205(3)$ | $\mathrm{N} 1-\mathrm{C} 7$ | $1.460(3)$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{O} 2-\mathrm{C} 9$ | $1.205(3)$ | $\mathrm{C} 8-\mathrm{C} 11$ | $1.480(3)$ |
| N1-C9 | $1.386(3)$ | $\mathrm{C} 9-\mathrm{C} 10$ | $1.486(3)$ |
| N1-C8 | $1.388(3)$ |  |  |
| C9-N1-C8 | $112.0(2)$ | $\mathrm{O} 2-\mathrm{C} 9-\mathrm{N} 1$ | $125.1(2)$ |
| C9-N1-C7 | $123.6(2)$ | $\mathrm{O} 2-\mathrm{C} 9-\mathrm{C} 10$ | $129.0(2)$ |
| C8-N1-C7 | $124.3(2)$ | $\mathrm{N} 1-\mathrm{C} 9-\mathrm{C} 10$ | $105.9(2)$ |
| N1-C7-C1 | $111.9(2)$ | $\mathrm{C} 15-\mathrm{C} 10-\mathrm{C} 9$ | $131.0(2)$ |
| O1-C8-N1 | $125.2(2)$ | $\mathrm{C} 11-\mathrm{C} 10-\mathrm{C} 9$ | $107.9(2)$ |
| O1-C8-C11 | $128.9(2)$ | $\mathrm{C} 12-\mathrm{C} 11-\mathrm{C} 8$ | $130.3(2)$ |
| N1-C8-C11 | $105.9(2)$ | $\mathrm{C} 10-\mathrm{C} 11-\mathrm{C} 8$ | $108.2(2)$ |

Table 2
Hydrogen-bond geometry $\left(\AA,{ }^{\circ}\right)$.

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| C13-H13 $\cdots \mathrm{O} 2^{\mathrm{i}}$ | 0.93 | 2.62 | $3.468(4)$ | 151 |
| ${\text { C7-H7B }{ }^{\text {ii }}}^{\text {C3-H3 }}$ O1 |  |  |  |  |
| C3i $^{\text {C }}$ | 0.97 | 2.70 | $3.514(3)$ | 142 |

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 $\mathrm{C}-\mathrm{H}=0.93$ or $0.96 \AA$ for aromatic and methylene H atoms, respectively, and with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C})$.

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.

The authors are grateful to the Programme of Zhejiang Provincial Department of Science and Technology (grant No. 2004 C31039) for financial support.

## References

Bruker (2002). SADABS (Version 2.03), SAINT (Version 6.02), SMART (Version 5.62) and SHELXTL (Version 6.10). Bruker AXS Inc., Madison, Winsonsin, USA.
Collin, X., Robert, J.-M., Wielgosz, G., Le Baut, G., Bobin-Dubigeon, C., Grimaud, N. \& Petit, J.-Y. (2001). Eur. J. Med. Chem. 36, 639-649.
Kawaguchi, S. \& Ikeda, O. (2001). Jpn Pat. Appl. JP 2001328911.
Martin, B., Sekljic, H. \& Chassaing, C. (2003). Org. Lett. 5, 1851-1853.
Norman, M. H., Minick, D. J. \& Rigdon, G. C. (1996). J. Med. Chem. 39, 149157.

Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.


[^0]:    (C) 2006 International Union of Crystallography All rights reserved

