

**Xing-Guo Zhang,^{a*} Ping Zhong,^a
Mao-Lin Hu^a and Huanan Hu^b**^aSchool of Chemistry and Materials Science,
Wenzhou Normal College, 325027 Wenzhou,
People's Republic of China, and ^bDepartment of
Chemistry, Jiangxi Normal University, 330027
Nanchang, People's Republic of China

Correspondence e-mail: zyg7599@sohu.com

Key indicators

Single-crystal X-ray study

T = 298 K

Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$

R factor = 0.051

wR factor = 0.127

Data-to-parameter ratio = 12.9

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

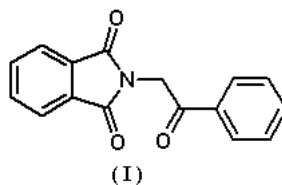
1-Phenyl-2-phthalimidoethanone

The title compound, $\text{C}_{16}\text{H}_{11}\text{NO}_3$, contains two planar ring systems and, in the crystal structure, the asymmetric unit is composed of two molecules. There are some intermolecular $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds and $\pi-\pi$ stacking interactions.

Comment

Phthalimides are of particular biological interest and have been reported as antipsychotics (Norman *et al.*, 1996), anti-inflammatory agents (Collin *et al.*, 2001), herbicides and insecticides. In addition, some phthalimide derivatives have been designed as electron acceptors in the formation of supramolecular assemblies (Barooh *et al.*, 2003). Some interesting crystal structures involving the phthalimide group have been reported (Barrett *et al.*, 1995).

In an earlier study, we reported the synthesis and crystal structure of 1-(2,4-dichlorophenyl)-2-phthalimidoethanone (Zhang *et al.*, 2004). Since then, we have prepared a new phthalimide derivative, *viz.* the title compound, (I), and its crystal structure is reported here.



In (I), all atoms of the phthalimide moiety are coplanar, as are all atoms of the phenyl group. The average deviation of the phthalimide ring system (C1–C8/N1) from planarity is 0.004 Å, and the dihedral angle between this plane and that of the phenyl ring (C11–C16) is 88.18 (1)°. For the other molecule of the asymmetric unit, the corresponding values are 0.007 Å and 83.29 (1)°, respectively.

As in other phthalimides (Barrett *et al.*, 1995), there are some intermolecular $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds (Table 1) and $\pi-\pi$ stacking interactions. The latter occur between the five-membered heterocyclic rings of the phthalimide moiety and the phenyl rings in adjacent molecules, with a face-to-face separation of $\sim 3.58 \text{ \AA}$.

Experimental

The title compound was synthesized from potassium phthalimide and 2-bromoacetophenone by the Gabriel (1887) reaction. Single crystals suitable for X-ray data collection were obtained on slow evaporation of a benzene/toluene (1:2) solution (m.p. 445–447 K). IR (KBr, cm^{-1}): ν 1771, 1700, 1425, 1226; ^1H NMR (CDCl_3 , p.p.m.): 8.02 (d, 2H, $J =$

Received 25 February 2004

Accepted 10 March 2004

Online 31 March 2004

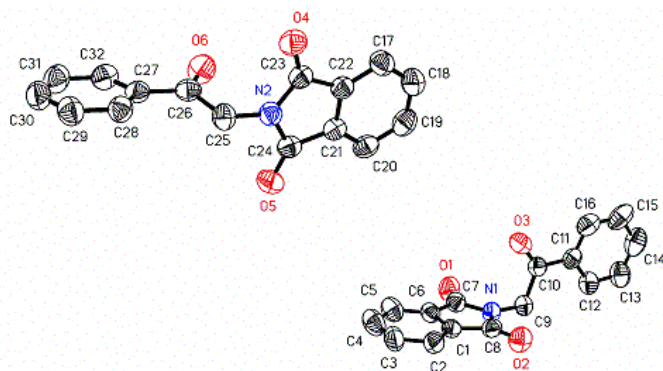


Figure 1
The structure of the asymmetric unit of (I), showing the atomic numbering scheme and displacement ellipsoids at the 50% probability level.

7.5 Hz), 7.95 (m, 2H), 7.75 (m, 2H), 7.70 (m, 1H), 7.48 (m, 2H), 5.10 (s, 2H).

Crystal data

$C_{16}H_{11}NO_3$
 $M_r = 265.26$
 Monoclinic, $P2_1/c$
 $a = 12.8670$ (5) Å
 $b = 14.2568$ (6) Å
 $c = 14.2196$ (6) Å
 $\beta = 94.728$ (2)°
 $V = 2599.60$ (18) Å³
 $Z = 8$

$D_x = 1.356$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 648 reflections
 $\theta = 2.5$ – 23.5 °
 $\mu = 0.10$ mm⁻¹
 $T = 298$ (2) K
 Block, colorless
 $0.39 \times 0.35 \times 0.32$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.963$, $T_{\max} = 0.974$
 13 485 measured reflections

4665 independent reflections
 3520 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\text{max}} = 25.2$ °
 $h = -15 \rightarrow 15$
 $k = -17 \rightarrow 12$
 $l = -17 \rightarrow 16$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.127$
 $S = 1.04$
 4665 reflections
 361 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.3423P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C9-H9A \cdots O1^i$	0.97	2.59	3.451 (2)	147
$C9-H9B \cdots O4$	0.97	2.56	3.506 (2)	165
$C14-H14 \cdots O6^{ii}$	0.93	2.59	3.206 (3)	124
$C15-H15 \cdots O1^{iii}$	0.93	2.57	3.438 (3)	155
$C20-H20 \cdots O4^{iv}$	0.93	2.54	3.447 (2)	166
$C30-H30 \cdots O3^v$	0.93	2.57	3.214 (3)	127

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

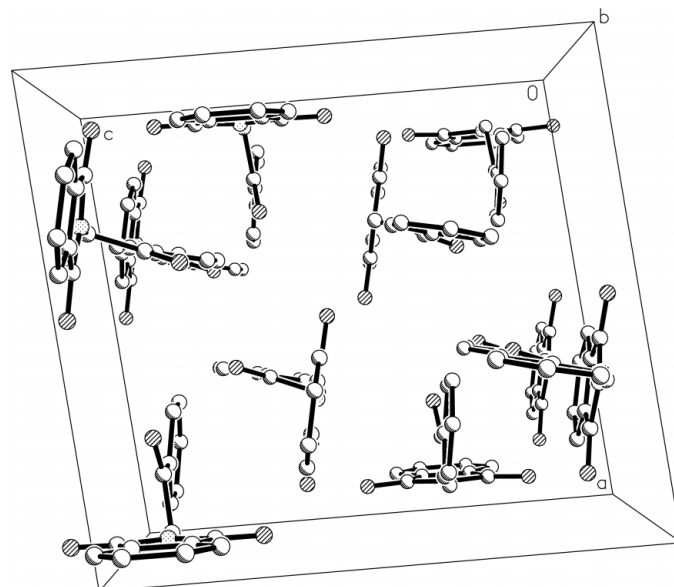


Figure 2

A packing diagram, viewed down the b axis. H atoms have been omitted.

All H atoms were initially located in a difference Fourier map; they were then placed in idealized positions and constrained to ride on their parent atoms, with $C_{\text{aromatic}}-H = 0.93$ Å, $C_{\text{methylene}}-H = 0.97$ Å and $U_{\text{iso}}(H) = 1.2_{\text{eq}}(C)$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXL97.

This work was supported by the National Natural Science Foundation of China (grant No. 20272043) and the Natural Science Foundation of Zhejiang Province (grant No. M203001).

References

- Barooah, N., Sarma, R. J. & Baruah, J. B. (2003). *Cryst. Growth Des.* **3**, 639–641.
- Barrett, D. M. Y., Kahwa, I. A., Mague, J. T. & McPherson, G. L. (1995). *J. Org. Chem.* **60**, 5946–5953.
- Bruker (2000). SMART, SAINT, SADABS and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, 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**, 639–650.
- Gabriel, S. (1887). *Ber. Dtsch. Chem. Ges.* **20**, 2224–2226.
- Norman, M. H., Minick, D. J. & Rigdon, G. C. (1996). *J. Med. Chem.* **39**, 149–157.
- Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.
- Zhang, X., Zhong, P., Hu, M. & Xiao, H. (2004). *Acta Cryst.* **E60**, o297–o298.