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## Key indicators

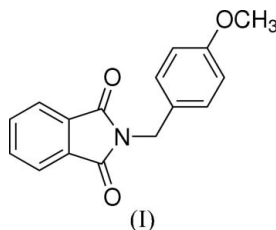
Single-crystal X-ray study  
 $T = 100\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.041  
 $wR$  factor = 0.095  
Data-to-parameter ratio = 12.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.***N*-(4-Methoxybenzyl)phthalimide: ribbons of  
alternating  $R(16)$  and  $R(22)$  ring motifs**

In the title compound [systematic name: 2-(4-methoxybenzyl)isoindoline-1,3-dione],  $\text{C}_{16}\text{H}_{13}\text{NO}_3$ , pairwise intermolecular  $\text{C}_{\text{aryl}}-\text{H}\cdots\text{O}=\text{C}$  bonds generate  $R_2^2(16)$  motifs. Additionally,  $\pi-\pi$  stacking of phthalimides in head-to-tail dimers, together with  $\text{C}_{\text{aryl}}-\text{H}\cdots\text{O}-\text{C}_{\text{aryl}}$  interactions, in which the O atom of an arylmethyl ether serves as a hydrogen bond acceptor, connect these rings into infinite ribbons *via*  $R(22)$  motifs.

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## Comment

The title compound, (I), was prepared in the context of a time-resolved spectroscopic study on the mechanism of photoinduced electron transfer reactions between *N*-substituted phthalimides and phenylacetates (Warzecha *et al.*, 2006).

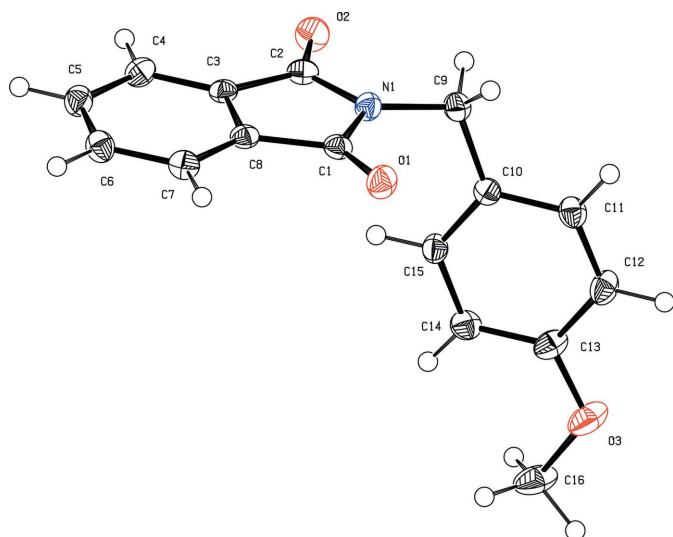


The compound (Fig. 1) contains two planar subunits, *viz.* the phthalimide chromophore and the 4-methoxyphenyl unit. The two units are linked by the methylene group C9.

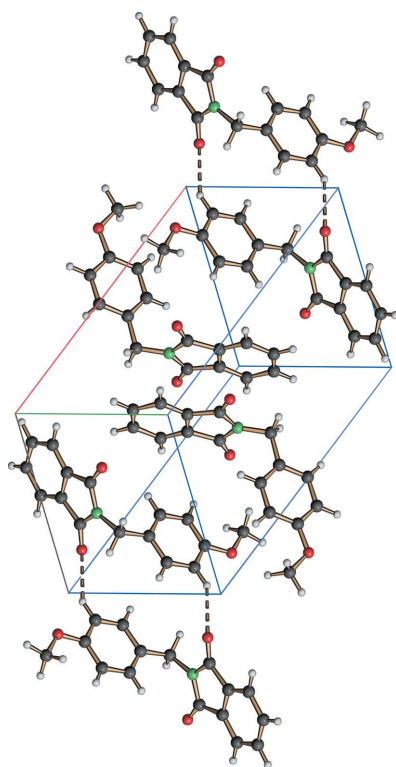
The  $\text{N1}-\text{C9}-\text{C10}$  bond angle is in good agreement with those in the parent *N*-benzylphthalimide (II) (Warzecha *et al.*, 2006a; Lü *et al.*, 2006), the regioisomeric *N*-(2-methoxybenzyl)phthalimide (Warzecha *et al.*, 2006b) and the 4-methylbenzyl derivative (Chen *et al.*, 2006). The methyl group C16 is coplanar with the benzene ring (Table 1).

Compared with *N*-(4-methylbenzyl)phthalimide, which shows the roof-shaped conformation of (II), the introduction of a methoxy group *para* to the  $\text{sp}^3$  linkage results in a significantly different conformation for the title compound. In (I), the torsion angles  $\text{C1}-\text{N1}-\text{C9}-\text{C10}$  and  $\text{C2}-\text{N1}-\text{C9}-\text{C10}$  differ significantly from  $90^\circ$  and the  $\text{C9}-\text{C10}$  bond is no longer orthogonal to the phthalimide ring plane. In addition, torsion angles  $\text{N1}-\text{C9}-\text{C10}-\text{C11}$  and  $\text{N1}-\text{C9}-\text{C10}-\text{C15}$ , involving the linkage of the imide N atom to the benzene ring, while virtually identical in the parent molecule, exhibit significantly different values in (I).

The packing of (I) features two different types of  $\text{C}-\text{H}\cdots\text{O}$  bonds (Desiraju, 1991; Steiner, 2002). On the one hand, two molecules related by symmetry code  $(2-x, -y, 1-z)$  form an  $R_2^2(16)$  motif (Etter, 1990; Etter *et al.*, 1990) by pairwise intermolecular  $\text{C}_{\text{aryl}}-\text{H}\cdots\text{O}=\text{C}$  hydrogen bonding between O1 and C12, the C atom *ortho* to the methoxy group (Table 2).

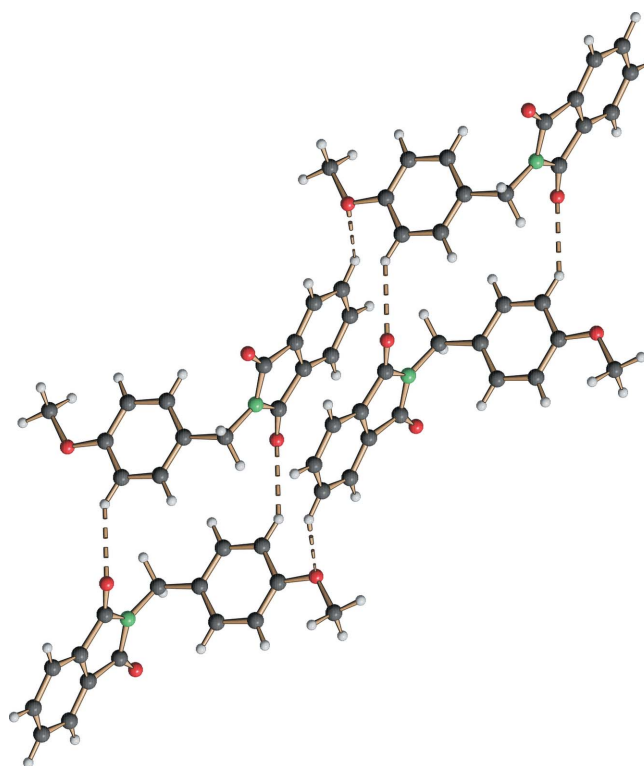


**Figure 1**  
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level; H atoms are shown as circles of arbitrary size.



**Figure 2**  
A view of the unit-cell contents of (I); pairwise  $C_{\text{aryl}}\text{—H}\cdots\text{O}=\text{C}$  bonds generate  $R_2^2(16)$  motifs. Dashed lines indicate hydrogen bonds.

Each molecule in such a motif also participates in  $\pi$ - $\pi$ -stacking where two phthalimide groups related by an inversion centre are oriented in head-to-tail fashion with an interplanar distance of 3.487 (1) Å. This  $\pi$ - $\pi$  interaction can also be described in terms of two centroid-to-centroid distances, where  $Cg1$  is the centroid of the five-membered imide and  $Cg2$  is the centroid of the six-membered ring of the phthalimide



**Figure 3**  
In the packing of (I), the combination of  $C_{\text{aryl}}\text{—H}\cdots\text{O}=\text{C}$  bonds,  $\pi$ - $\pi$ -stacking and  $C_{\text{aryl}}\text{—H}\cdots\text{O}—C_{\text{aryl}}$  bonds features ribbons of alternating  $R_2^2(16)$  and  $R_4^4(22)$  motifs. Dashed lines indicate hydrogen bonds.

$[Cg1\cdots Cg1(1-x, 1-y, -z)] = 3.615(1)$  Å and  $Cg1\cdots Cg2(1-x, 1-y, -z) = 3.682(1)$  Å.

Each molecule in a  $\pi$ - $\pi$ -dimer also features a second, weaker, set of  $C_{\text{aryl}}\text{—H}\cdots\text{O}—C_{\text{aryl}}$  interactions to a neighbouring molecule (Table 2). In the crystal structure, the interplay of  $\pi$ - $\pi$  stacking and two types of  $C\text{—H}\cdots\text{O}—C$  bonds results in infinite ribbons of alternating  $R_2^2(16)$  and  $R_4^4(22)$  motifs running along the crystallographic  $b$  axis.

## Experimental

Phthalic anhydride (Acros) and 4-methoxybenzylamine (Acros) were used as received. A mixture of well ground phthalic anhydride (5.92 g, 40 mmol) and 4-methoxybenzylamine (5.48 g, 40 mmol) was fused in an open beaker by heating in a domestic microwave oven (800 W) in four cycles of 1 min heating and subsequent cooling. Recrystallization of the resulting crude material from ethanol furnished colourless prisms of the title compound (9.62 g, 36 mmol, 90%, m. p. 404 K) suitable for X-ray diffraction.

### Crystal data

$C_{16}H_{13}NO_3$   
 $M_r = 267.27$   
Monoclinic,  $P2_1/c$   
 $a = 10.1225(4)$  Å  
 $b = 15.8036(6)$  Å  
 $c = 8.2249(3)$  Å  
 $\beta = 99.562(1)^\circ$   
 $V = 1297.47(9)$  Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.368$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 100(2)$  K  
Prism, colourless  
 $0.48 \times 0.32 \times 0.25$  mm

Data collection

Nonius KappaCCD diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: none  
 6586 measured reflections

2826 independent reflections  
 1806 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.045$   
 $\theta_{\text{max}} = 27.0^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.095$   
 $S = 0.97$   
 2826 reflections  
 234 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.002$   
 $\Delta\rho_{\text{max}} = 0.21 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{Å}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.015 (2)

Table 1

Selected bond and torsion angles ( $^\circ$ ).

N1—C9—C10	113.25 (12)	C1—N1—C9	122.52 (13)
C2—N1—C9	125.32 (12)	C13—O3—C16	117.65 (14)
C10—C9—N1—C1	73.01 (18)	N1—C9—C10—C15	28.9 (2)
C10—C9—N1—C2	-102.95 (18)	C12—C13—O3—C16	179.67 (16)
N1—C9—C10—C11	-153.41 (14)	C14—C13—O3—C16	0.9 (2)

Table 2

Hydrogen-bond geometry ( $\text{Å}, ^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C5—H5 $\cdots$ O3 <sup>i</sup>	0.99 (2)	2.48 (2)	3.231 (2)	133 (1)
C12—H12 $\cdots$ O1 <sup>ii</sup>	0.99 (2)	2.51 (2)	3.360 (2)	145 (1)

Symmetry codes: (i)  $x - 1, y, z - 1$ ; (ii)  $-x + 2, -y, -z + 1$ .

All H atoms were refined isotropically [range of refined C—H distances = 0.93 (2)–1.06 (2)  $\text{Å}$ ].

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SCHAKAL99* (Keller, 1999); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *enCIFer* (Allen *et al.*, 2004).

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