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2-(4-Hydroxyphenyl)isoindoline-1,3-dione

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Key indicators

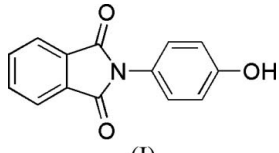
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.140
Data-to-parameter ratio = 13.7

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

In the title compound, $C_{14}H_9NO_3$, the dihedral angle between the phthalimide ring system and the hydroxybenzene ring is 64.77 (5)°. O—H···O hydrogen bonds link the molecules into zigzag chains along the b axis.

Comment

Phthalimides and *N*-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002; Orzeszka *et al.*, 2000; Bailleux *et al.*, 1993). Phthalimides have also served as starting materials and intermediates for the syntheses of alkaloids (Couture *et al.*, 1998) and pharmacophores (Couture *et al.*, 1997). In this paper, the structure of the title compound, (I), is reported.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The phthalimide moiety is essentially planar, with a mean deviation of 0.015 (2) Å. Considering the different substitution patterns, the geometry of the phthalimide ring system compares favourably with that in the related compounds 4-(1,3-dioxoisoindolin-2-yl)benzaldehyde (Liu *et al.*, 2004) and 5-amino-2-methylisoindoline-1,3-dione (Liang *et al.*, 2006). The hydroxybenzene ring (atoms C9–C14) is planar to within 0.009 (2) Å. The dihedral angle between the N1/O1/O2/C1–C8 and C9–C14 planes is 64.77 (5)°.

Symmetry-related molecules are linked *via* O3—H3···O2^{i} hydrogen bonds (the symmetry code is given in Table 1), forming a zigzag chain along the b axis. In addition, the molecular packing is stabilized by π–π interactions between the

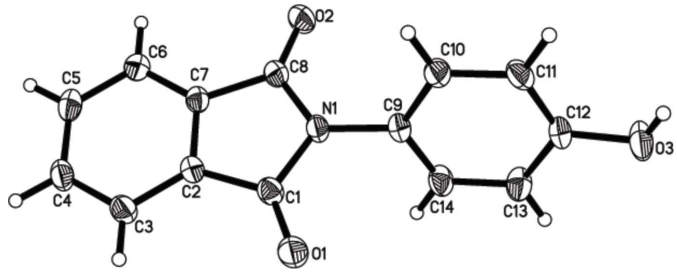


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

phthalimide ring systems of the molecules at (x, y, z) and ($1-x$, $-y$, $1-z$); their centroids are separated by 3.519 (2) Å.

Experimental

A solution of phthalimide (0.1 mol), 4-aminophenol (0.1 mol) and triethylamine (0.01 ml) in xylene (100 ml) was refluxed for 3 h. After cooling, filtration and drying, the title compound was obtained. 10 mg of (I) was dissolved in 15 ml acetone, the solution was allowed to evaporate at room temperature and colourless single crystals formed after 10 d.

Crystal data

$C_{14}H_9NO_3$
$M_r = 239.22$
Orthorhombic, *Pbca*
$a = 11.524$ (3) Å
$b = 7.7133$ (19) Å
$c = 24.890$ (6) Å
$V = 2212.4$ (10) Å^3
$Z = 8$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.32 × 0.22 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.968$, $T_{max} = 0.986$
11576 measured reflections
2265 independent reflections
1300 reflections with $I > 2\sigma(I)$
$R_{int} = 0.073$
$\theta_{max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.140$
$S = 0.92$
2265 reflections
165 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0843P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.031 (3)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{i}	0.82	1.95	2.723 (2)	156

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined in a riding model, with U_{iso}(H) = 1.5U_{eq}(carrier) for methyl H atoms and 1.2U_{eq}(carrier) for all other H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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