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

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The crystal structure of the title compound, $C_{14}H_9NO_3$, is stabilized by a weak O—H···O hydrogen bond. The dihedral angle between the phthalimide and hydroxyphenyl planes is 71.8 (2)°.

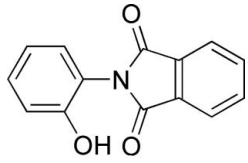
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.146
Data-to-parameter ratio = 13.6

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

Comment

Phthalimides and N-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002). We report here the structure of the title compound, (I) (Fig. 1).



(I)

The phthalimide and hydroxyphenyl units are essentially planar, with mean deviations of 0.007 (4) and 0.006 (2) Å, respectively. The dihedral angle between these planes is 71.8 (2)°. The geometry of the molecule is close to that of the related compound 2-(4-hydroxyphenyl)isoindoline-1,3-dione (Liang & Li, 2006). The crystal structure is stabilized by a weak O—H···O hydrogen bond (Table 1).

Experimental

A mixture of phthalimide (0.1 mol), 2-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. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetone solution for 8 d at room temperature.

Crystal data

$C_{14}H_9NO_3$
M_r = 239.22
Monoclinic, $P2_1/c$
a = 11.584 (2) Å
b = 13.704 (3) Å
c = 7.0359 (13) Å
β = 103.877 (3)°
V = 1084.4 (4) Å^3
Z = 4
D_x = 1.465 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, yellow
0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.969, T_{max} = 0.979
6010 measured reflections
2225 independent reflections
1674 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.146$
$S = 1.05$
2225 reflections
164 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2 + 0.4133P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{i}	0.82	2.00	2.798 (2)	163

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

H atoms were positioned geometrically (C—H = 0.93 Å and O—H = 0.82 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

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*.

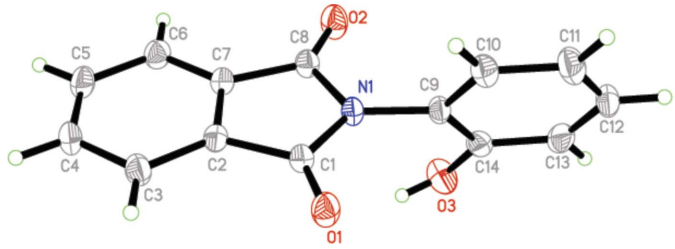


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

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