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

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.096
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, $C_{13}H_8N_2O_2$, the phthalimide unit and the pyridine ring are each essentially planar. The dihedral angle between these two planar ring systems is 62.1 (3)°.

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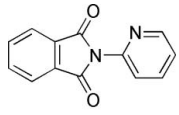
Comment

Phthalimides and *N*-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002). As a part of our study of substituted phthalimides (Liang & Li., 2006*a*,*b*), we have synthesized the title compound, (I) (Fig. 1). The phthalimide unit is planar with a mean deviation of 0.012 (2) Å. The pyridine ring is also planar, with a mean deviation of 0.005 (1) Å. The dihedral angle between the pyridine ring and the phthalimide unit is 62.1 (3)°.



(I)

Experimental

A mixture of phthalic anhydride (0.1 mol) and 2-aminopyridine (0.1 mol) in acetic acid (100 ml) was refluxed for 4 h. After cooling, filtration and drying, the title compound was obtained. 10 mg of (I) were dissolved in 15 ml acetone, and the solution was allowed to stand at room temperature for 7 days, yielding colourless single crystals suitable for X-ray analysis.

Crystal data

$C_{13}H_8N_2O_2$
M_r = 224.21
Orthorhombic, *Pbca*
a = 11.410 (5) Å
b = 7.846 (3) Å
c = 23.167 (9) Å
V = 2073.9 (14) Å^3
Z = 8
D_x = 1.436 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.20 × 0.16 mm

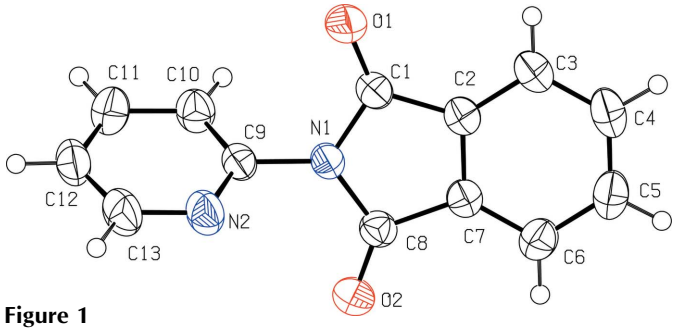


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.976, T_{max} = 0.984
10729 measured reflections
2124 independent reflections
1511 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.06
2124 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.3809P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0122 (11)

H atoms were initially located in difference maps and then refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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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