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4-(1,3-Dioxoisoindolin-2-yl)benzaldehyde

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.091
Data-to-parameter ratio = 7.1

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

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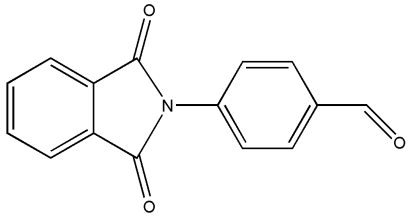
The title compound, $C_{15}H_9NO_3$, was synthesized from phthalic anhydride and 4-aminobenzaldehyde. The dihedral angle between the planes of the phthalimide moiety and the benzene ring is 56.22 (2)°.

Comment

N-Phthalyl derivatization is one of the most frequently used methods of protection in synthesis involving compounds with primary amino groups (Falck *et al.*, 1995). Phthalimides have also served as starting materials and intermediates for the syntheses of alkaloids (Couture *et al.*, 1998) and pharmacophores (Couture *et al.*, 1997). Moreover, they have cytotoxicity (Hall *et al.*, 1995) and anti-HIV activity (Van Derpoorten *et al.*, 1997). In this paper, the structure of the title compound, 4-(1,3-dioxoisoindolin-2-yl)benzaldehyde, (I), is reported (Fig. 1).



(I)

The structure of (I) comprises a conventional phthalimide unit with the benzene ring of the *p*-benzaldehyde moiety bound to the imide N atom. The phthalimide unit is effectively planar, with a mean deviation of 0.015 (2) Å. The dihedral angle between this plane and that of the benzene ring of the benzaldehyde moiety is 56.22 (3)°.

Experimental

A solution of phthalic anhydride (10 mmol) and 4-aminobenzaldehyde (10 mmol) in acetic acid (40 ml) was heated at reflux until

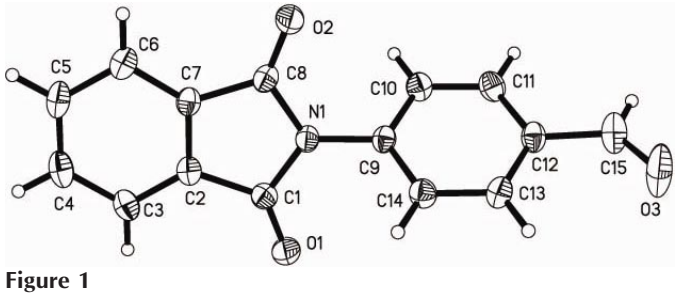


Figure 1
The molecular structure of (I), atoms are drawn with 30% probability ellipsoids. H atoms aare drawn as spheres of arbitrary radius.

the disappearance of the starting materials, as evidenced by thin-layer chromatography. The resulting yellow precipitate was filtered off and washed with a minimum amount of water to give the title compound, (I). ^{1}H NMR ($CDCl_3$, p.p.m.): 7.26–8.05 (*m*, 8H), 10.07 (*s*, 1H). Recrystallization from $CHCl_3$ over 12 d at ambient temperature gave colorless single crystals of (I) suitable for X-ray analysis.

Crystal data

$C_{15}H_9NO_3$	Mo $K\alpha$ radiation
M_r = 251.23	Cell parameters from 1004 reflections
Orthorhombic, $Pna2_1$	θ = 2.4–24.1°
a = 7.646 (3) Å	μ = 0.10 mm^{-1}
b = 11.070 (4) Å	T = 293 (2) K
c = 13.815 (4) Å	Block, colorless
V = 1169.3 (7) Å^3	0.20 × 0.18 × 0.14 mm
Z = 4	
D_x = 1.427 Mg m^{-3}	

Data collection

Bruker SMART CCD area-detector diffractometer	1227 independent reflections
φ and ω scans	947 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	R_{int} = 0.046
T_{min} = 0.960, T_{max} = 0.986	θ_{max} = 26.3°
6256 measured reflections	$h = -9 \rightarrow 9$
	$k = -11 \rightarrow 13$
	$l = -17 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.1003P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	
$wR(F^2)$ = 0.092	
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.001
1227 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
H-atom parameters constrained	

In the absence of significant anomalous scattering effects, Friedel pairs in the data set were merged. H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(carrier).

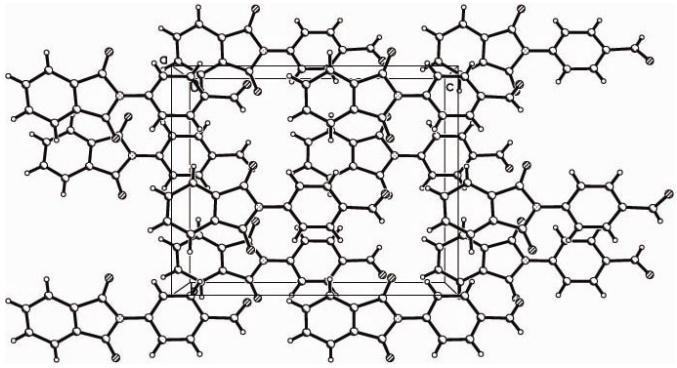


Figure 2
The crystal structure of (I), viewed down the *a* axis.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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