Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(Hydroxymethyl)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 = 0.107
Data-to-parameter ratio = 13.3

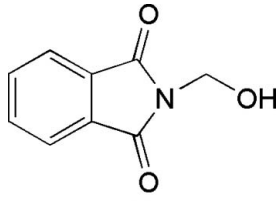
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 August 2006
Accepted 30 August 2006

The title compound, $C_9H_7NO_3$, was synthesized by mixing phthalimide with a solution of formaldehyde. Apart from the hydroxy group, the molecule is essentially planar. The crystal structure is stabilized by weak O—H···O hydrogen bonds.

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. Apart from the hydroxy group, the molecule is essentially planar to within 0.005 (1) Å. Atom O3 is displaced by 1.517 (2) Å from the plane through atoms C1–C8/N1/O1/O2. The bond lengths and angles have normal values. The crystal structure is stabilized by weak O—H···O hydrogen bonds (Fig. 2 and Table 1).

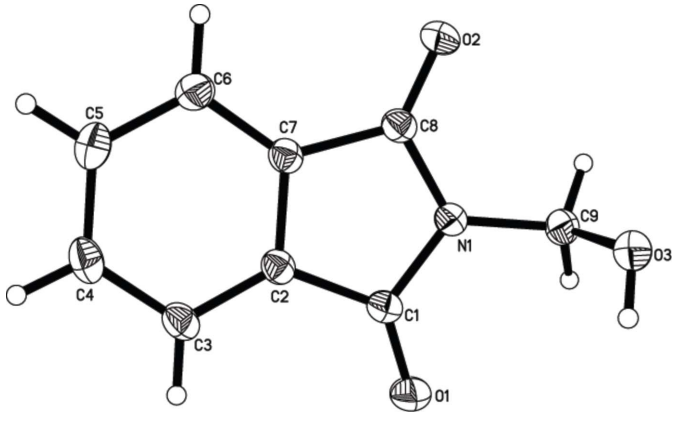


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

Experimental

A mixture of phthalimide (0.15 mol), formaldehyde (36%, 20 ml) and distilled water (40 ml) was refluxed for 4 h. After cooling and filtration, the title compound was recrystallized from ethyl acetate (m.p. 415–416 K). 10 mg of (I) were dissolved in 12 ml ethyl acetate and the solution was allowed to evaporate at room temperature, yielding colourless single crystals after 6 d.

Crystal data

$C_9H_7NO_3$
M_r = 177.16
Monoclinic, $P2_1/c$
a = 11.324 (2) Å
b = 6.6040 (14) Å
c = 11.862 (2) Å
β = 117.066 (3)°
V = 789.9 (3) Å^3
Z = 4
D_x = 1.490 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, colourless
0.30 × 0.24 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.967, T_{max} = 0.984
4040 measured reflections
1596 independent reflections
1234 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.107
S = 1.00
1596 reflections
120 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.1081P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.048 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{i}	0.82	2.03	2.8497 (16)	175

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

H atoms were positioned geometrically, with C—H = 0.93–0.97 Å and O—H = 0.82 Å, and refined using a riding model, with U_{iso}(H) = 1.5U_{eq}(O) and 1.2U_{eq}(C).

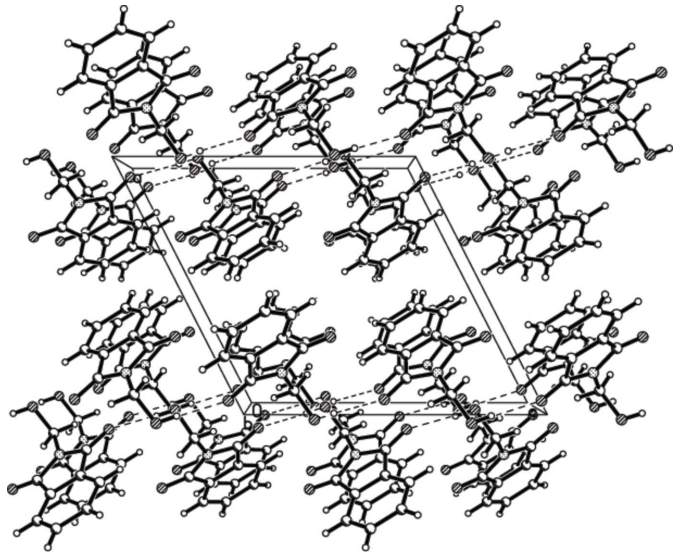


Figure 2
The crystal packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

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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