Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-Methylphthalimide

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Received 9 August 2006
Accepted 30 August 2006

The title compound [systematic name: 2-methylisoindoline-1,3-dione], $C_9H_7NO_2$, was synthesized by mixing phthalic anhydride, a methanamine solution and triethylamine in toluene. The molecule is approximately planar for all non-H atoms.

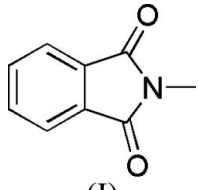
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.049
wR factor = 0.132
Data-to-parameter ratio = 6.8

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

Comment

The molecular structure of the title compound, (I), is illustrated in Fig. 1. The isoindoline ring system is essentially planar, with a mean deviation of 0.009 (1) Å. The geometry of the isoindoline ring system compares favourably with that in the related compounds phthalimide (Ng, 1992) and *N*-(2-phenethyl)phthalimide (Warzecha *et al.*, 2006). The molecule is approximately planar, with a mean deviation of 0.025 (2) Å for all non-H atoms.



(I)

Experimental

A mixture of phthalic anhydride (0.1 mol), methanamine solution (40% in water, 13 ml) and triethylamine (0.01 mol) was stirred under reflux in toluene (30 ml) for 5 h. After cooling, filtration and drying, the title compound was obtained (m.p. 509–511 K). 15 mg of (I) were dissolved in 20 ml acetonitrile, and the solution was kept at room temperature for 7 d. Natural evaporation gave colourless single crystals of the title compound suitable for X-ray analysis.

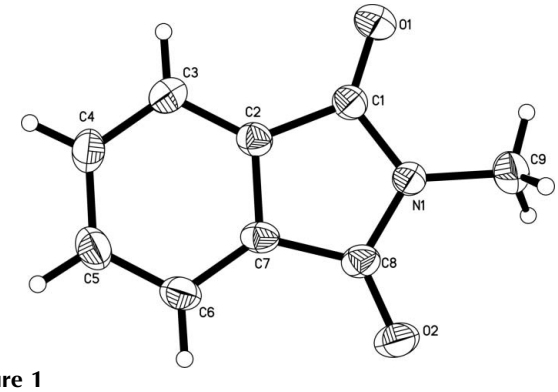


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

Crystal data

$C_9H_7NO_2$	$Z = 2$
$M_r = 161.16$	$D_x = 1.347$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 4.023$ (4) Å	$\mu = 0.10$ mm^{-1}
$b = 7.948$ (8) Å	$T = 294$ (2) K
$c = 12.445$ (12) Å	Plate, colourless
$\beta = 92.803$ (18)°	0.28 × 0.22 × 0.08 mm
$V = 397.5$ (7) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	1977 measured reflections
	760 independent reflections
φ and ω scans	495 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	$R_{int} = 0.088$
	$\theta_{max} = 25.0°$
$T_{min} = 0.973$, $T_{max} = 0.992$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.049$	
$wR(F^2) = 0.132$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.04$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
760 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
111 parameters	Extinction correction: *SHELXL97*
H-atom parameters constrained	Extinction coefficient: 0.22 (4)

In the absence of significant anomalous scattering effects, Friedel pairs were merged. H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined as riding, with $U_{iso}(H) = 1.5U_{eq}$(methyl C) or $1.2U_{eq}$(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*.

References

Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Ng, S. W. (1992). *Acta Cryst.* C**48**, 1694–1695.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Warzecha, K.-D., Lex, J., Neudörfl, J. M. & Griesbeck, A. G. (2006). *Acta Cryst.* E**62**, o1580–o1581.