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

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.012 Å
R factor = 0.059
wR factor = 0.185
Data-to-parameter ratio = 6.7

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

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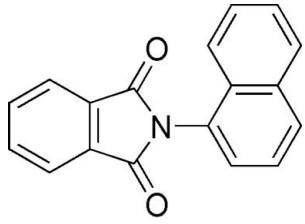
The asymmetric unit of the title compound, $C_{18}H_{11}NO_2$, comprises three independent molecules, which differ in the dihedral angle between the phthalimide unit and the naphthalene ring system. In the asymmetric unit, two molecules lie on either side of the phthalimide plane of the third molecule.

Comment

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



(I)

The asymmetric unit of (I) (Fig. 1) consists of three independent molecules, which differ in their dihedral angle between the phthalimide group and naphthalene ring system (see below). The geometric parameters of the phthalimide groups are close to those in the related compounds 2-(4-hydroxyphenyl)isoindoline-1,3-dione and 2-ethylisoindoline-1,3-dione (Liang *et al.*, 2006*a*,*b*). In molecules *A* (N1/O1/O2/C1–C18), *B* (N2/O3/O4/C19–C36) and *C* (N3/O5/O6/C37–C54), the dihedral angles between the phthalimide unit and the naphthalene ring system are 37.0 (2), 66.8 (2) and 82.2 (2)°, respectively. The dihedral angles between the phthalimide groups of molecules *A* and *B* and that of molecule *C* are 37.0 (1) and 50.0 (1)°, respectively. Related torsion angles listed in Table 1.

Experimental

A mixture of phthalic anhydride (0.1 mol) and 2-aminonaphthalene (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) was dissolved in 13 ml acetone, and the solution was allowed to stand at room temperature for 6 d. Natural evaporation gave colourless single crystals of the title compound suitable for X-ray analysis.

Crystal data

$C_{18}H_{11}NO_2$
M_r = 273.28
Orthorhombic, $Pna2_1$
a = 16.029 (13) Å
b = 8.709 (7) Å
c = 29.04 (2) Å
V = 4055 (6) Å^3
Z = 12
D_x = 1.343 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
Plate, colourless
0.26 × 0.24 × 0.12 mm

Data collection

Bruker SMART 1000 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.977, T_{max} = 0.990
19648 measured reflections
3660 independent reflections
1981 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.185
S = 1.15
3660 reflections
544 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0822P)^2 + 0.621P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected torsion angles (°).

N1—C9—C18—C17	−2.6 (12)	N3—C45—C50—C51	2.2 (4)
N2—C27—C36—C35	4.6 (11)		

In the absence of significant anomalous dispersion effects, Freidel pairs were merged. H atoms were initially located in difference maps and then refined in a riding model, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(methyl 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*.

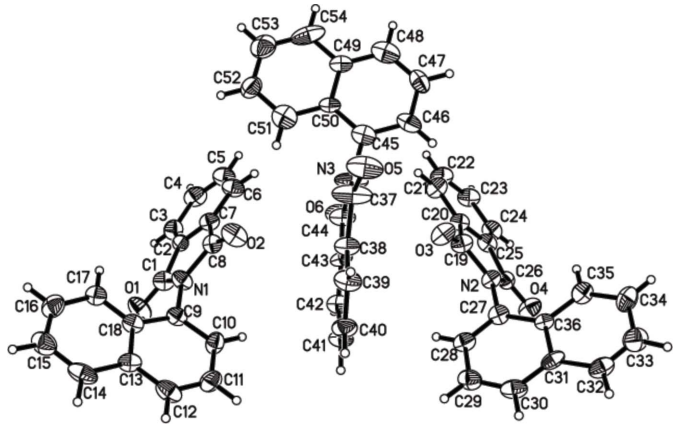


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level.

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