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N-(3-Methoxypropyl)-1,8-naphthalimide

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Key indicators

Single-crystal X-ray study
T = 90 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.100
Data-to-parameter ratio = 14.0

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

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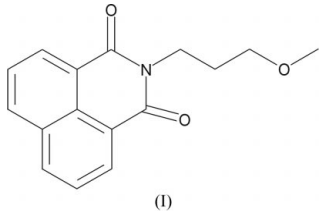
In the title compound, $C_{16}H_{15}NO_3$, the 1,8-naphthalenodicarboximide group is nearly planar and, in the naphthalimide ring system, the characteristic alternating pattern of bond lengths is observed. In the crystal, the molecules are connected by a weak C—H···O hydrogen bond and extend in the direction parallel to the *b* axis.

Comment

N-Substituted 1,8-naphthalimide derivatives have fluorescence properties, which are interesting in view of their use as laser active media (Pardo *et al.*, 1987), and they are excellent fluorescent cell markers (Stewert, 1981; Marling *et al.*, 1974). Substituent effects on the photophysical properties of these compounds have been investigated widely (Demeter *et al.*, 1994). With the aim of studying the relationship between the molecular structure and the photophysical properties of *N*-substituted 1,8-naphthalimide derivatives, the crystal structure of *N*-(3-methoxypropyl)-1,8-naphthalimide, (I), was investigated.



(I)

In (I), the 1,8-naphthalenodicarboximide group is nearly planar. The torsion angles which most significantly deviate from 0° are C8—C11—N1—C12 [5.3 (2)°] and C1—C12—N1—C11 [−4.5 (2)°] (Table 1). In the naphthalimide ring system, the characteristic pattern of bond lengths is observed. Specifically, bonds C7—C8, C5—C6, C3—C4 and C1—C2 are shorter (average value 1.380 Å) than the expected aromatic bond length, whereas all other bonds in the aromatic rings are longer than expected (average value 1.420 Å). This pattern of bond lengths has been observed previously in other *N*-substituted naphthalimide molecules (Clark & Hall, 1989). The C1—C12—N1 and C8—C11—N1 bond angles are 3.2 (1)° smaller, and the C1—C12—O2 and C8—C11—O1 bond angles are 2.5 (1)° larger than 120°. The two neighboring angles O1—C11—N1 and O2—C12—N1 differ from 120° by only 0.5 (1) and 0.6 (1)°, respectively. The bond lengths and angles of the 3-methoxypropyl group are normal and in accordance with the anticipated values (Hädicke & Graser, 1986).

In the crystal structure, the molecules are linked by a C—H···O hydrogen bond between the naphthalene ring and the carbonyl group (Table 2), and form a hydrogen-bonded polymer extending in the *b* direction.

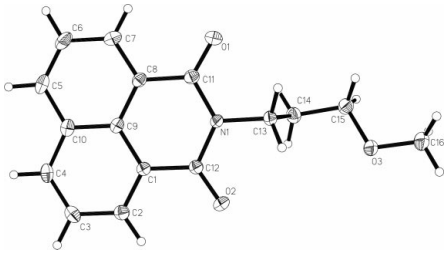


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

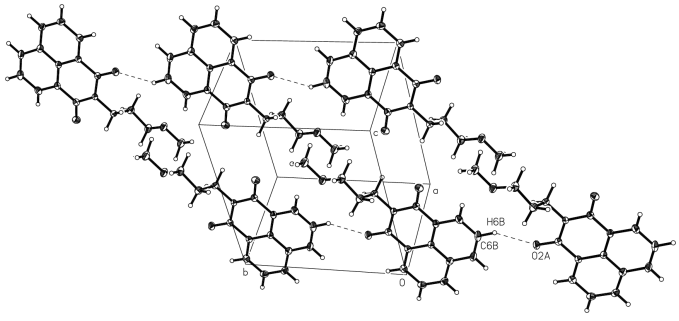


Figure 2
The crystal structure of (I). Displacement ellipsoids are drawn at the 50% probability level [symetry codes: (*A*) $x, -1+y, z$ (*B*) $1-x, -y, 1-z$].

Experimental

The title compound was synthesized by refluxing 1,8-naphthalic anhydride (1.98 g, 0.01 mol) and 3-methoxy-1-aminopropane (0.89 g, 0.01 mol) in concentrated acetic acid (50 ml). The reaction mixture was refluxed for 8 h, then poured into cold water and the resulting solid was then filtered off. This solid product was boiled with an aqueous solution of sodium bicarbonate (10%, 50 ml) for 20 min and the insoluble solid residue was then dried *in vacuo*. Column chromatography on aluminium oxide with C_6H_6 as eluant gave the product as a light-brown solution. The resulting solution was evaporated to obtain brown crystals (78% yield; m.p. 369–370 K).

Crystal data

$C_{16}H_{15}NO_3$
$M_r = 269.29$
Triclinic, $P\overline{1}$
$a = 7.154$ (1) Å
$b = 9.554$ (2) Å
$c = 9.866$ (2) Å
$\alpha = 85.27$ (3)°
$\beta = 82.88$ (3)°
$\gamma = 89.57$ (3)°
$V = 666.9$ (2) Å^3
$Z = 2$
$D_x = 1.341$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3178 reflections
$\theta = 4.2$–28°
$\mu = 0.09$ mm^{-1}
$T = 90.0$ (1) K
Block, colourless
0.6 × 0.5 × 0.5 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
ω scans
5193 measured reflections
3174 independent reflections
1793 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 28°$
$h = -8 \rightarrow 9$
$k = -13 \rightarrow 12$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.100$
$S = 0.81$
3174 reflections
226 parameters
All H-atom parameters refined.
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.385 (2)	C6—C7	1.407 (2)
C1—C9	1.425 (2)	C7—C8	1.390 (2)
C2—C3	1.410 (2)	C8—C9	1.422 (2)
C3—C4	1.375 (2)	C8—C11	1.474 (2)
C4—C10	1.422 (2)	C9—C10	1.424 (2)
C5—C6	1.372 (2)	C11—N1	1.413 (2)
C5—C10	1.429 (2)	C12—N1	1.407 (2)
O1—C11—N1	120.5 (1)	O2—C12—N1	120.6 (1)
O1—C11—C8	122.5 (1)	O2—C12—C1	122.4 (1)
N1—C11—C8	116.8 (1)	N1—C12—C1	116.9 (1)
C1—C12—N1—C11	−4.5 (2)	C8—C11—N1—C12	5.3 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O2^{i}	0.99 (1)	2.37 (1)	3.235 (2)	145 (1)

Symmetry code: (i) $x, y-1, z$.

Refined C—H distances were in the range 0.928 (17)–1.054 (18) Å.

Data collection: *CrysAlisCCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlisRED* (Oxford Diffraction, 2002); data reduction: *CrysAlisRED*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL*97.

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