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N-Benzyl-8-nitroquinolin-2-amine

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.119
Data-to-parameter ratio = 6.6

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

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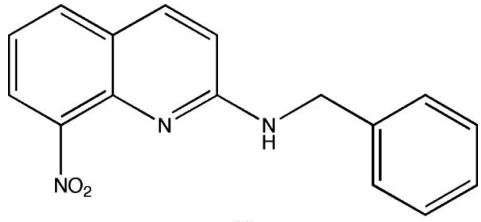
In the crystal structure of the title compound, $C_{16}H_{13}N_3O_2$, there are two independent L-shaped molecules in the asymmetric unit. No classical hydrogen bonds were found in the crystal structure.

Comment

The investigation of the structure of the title compound, (I), is part of our search for good fluorescent materials that could be used to detect and measure available metals within cells (Pearce *et al.*, 2001).



(I)

Compound (I) crystallizes in the monoclinic space group *Pc* with two independent molecules (*A* and *B*) in the asymmetric unit (Fig. 1). The dihedral angle between the planes of the benzene ring and the quinoline group is 74.3 (1)° for molecule

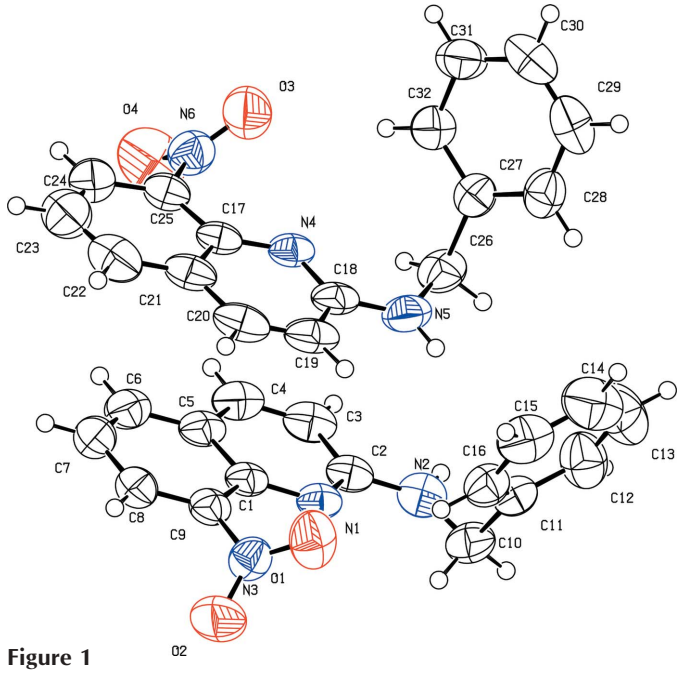


Figure 1
The structure of the asymmetric unit of (I), showing the atom labeling (molecule *A* is below molecule *B*) and displacement ellipsoids drawn at the 50% probability level.

A and 80.83 (9)° for molecule *B*. The quinoline system is essentially planar, but the O atoms of the nitro group deviate from the mean planes, *viz*. −0.877 (5) and 0.842 (5) Å for atoms O1 and O2, respectively, in molecule *A*, and −0.908 (5) and 0.822 (6) Å for atoms O3 and O4, respectively, in molecule *B*. The torsion angles in the two molecules are C2—N2—C10—C11 = −86.1 (4)° and C18—N5—C26—C27 = 79.1 (4)° (Fig. 1). No classical hydrogen bonds were found in the crystal structure.

Experimental

The title compound, (I), was prepared according to the literature procedure of Fox & Wenner (1951). Crystals suitable for X-ray data collection were obtained by recrystallization from dichloromethane–hexane (1:1 *v*/*v*).

Crystal data

$C_{16}H_{13}N_3O_2$
M_r = 279.29
Monoclinic, *Pc*
a = 7.439 (1) Å
b = 11.215 (1) Å
c = 16.541 (1) Å
β = 93.96 (1)°
V = 1376.7 (2) Å^3
Z = 4
D_x = 1.348 Mg m^{-3}
Cu *Kα* radiation
Cell parameters from 25 reflections
θ = 3.9–19.4°
μ = 0.75 mm^{-1}
T = 299 (2) K
Needle, orange
0.68 × 0.20 × 0.10 mm

Data collection

Nonius CAD-4 diffractometer
ω/2θ scans
Absorption correction: none
2913 measured reflections
2497 independent reflections
2233 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 67.9°
h = −8 → 0
k = −13 → 1
l = −19 → 19
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.119
S = 1.08
2497 reflections
379 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0853P)^2 + 0.028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

The H atoms were positioned with idealized geometry and refined with isotropic displacement parameters set at 1.2 times U_{eq} of the parent atom using a riding model, with N—H = 0.86 Å and C—H = 0.93 Å. In the absence of significant anomalous dispersion effects, Friedel pairs were merged and the f′ term set to zero.

Data collection: *CAD-4/PC Software* (Nonius, 1996); cell refinement: *CAD-4/PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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