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4-Benzyloxy-2-nitroaniline

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.132
Data-to-parameter ratio = 15.0

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

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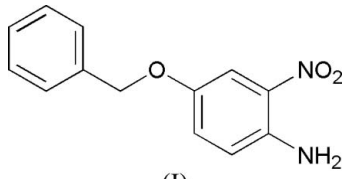
In the title compound, $C_{13}H_{12}N_2O_3$, the dihedral angle between the benzene rings is 65.8 (2)°. The crystal structure is stabilized by N—H···O hydrogen bonds and C—H···π interactions.

Comment

The benzothiazole system is a common component of many compounds with a wide range of biological activities (Huang & Yang, 2006). Substituted amines are important intermediates in the synthesis of benzothiazole derivatives. We present here the structure of one such amine derivative, the title compound, (I) (Fig. 1).



(I)

The aromatic ring C1–C6 of the nitrophenylamine group is twisted with respect to the benzyl ring system, with a dihedral angle of 65.8 (2)° between the ring planes.

The crystal packing is consolidated by N—H···O hydrogen bonds and intermolecular C—H···π stacking interactions (Table 1 and Fig. 2). N—H···O hydrogen bonds link the molecules into rows along the a axis. Additional C—H···π interactions link adjacent rows to give a network structure.

Experimental

The title compound was synthesized according to a literature procedure (Garcia & Schultz, 2006). Crystals of (I) suitable for X-ray analysis were grown from acetone at 277 K.

Crystal data

$C_{13}H_{12}N_2O_3$
M_r = 244.25
Monoclinic, $P2_1/c$
a = 5.7578 (12) Å
b = 26.192 (6) Å
c = 7.7338 (16) Å
β = 90.159 (4)°
V = 1166.3 (4) Å^3
Z = 4
D_x = 1.391 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 297 (2) K
Plate, red
0.30 × 0.20 × 0.06 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
8532 measured reflections
2532 independent reflections
2065 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.0°

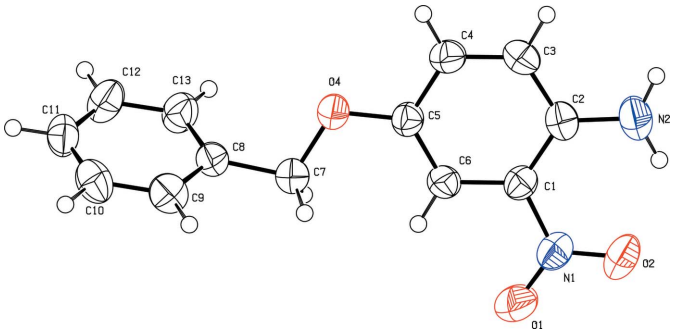


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.132$
$S = 1.14$
2532 reflections
169 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.2514P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O2	0.92 (2)	1.94 (3)	2.636 (3)	130 (2)
N2—H2A···O1^{i}	0.88 (3)	2.11 (3)	2.983 (3)	171 (2)
C4—H4···Cg^{ii}	0.93	2.94	3.751 (3)	141 (2)
C7—H7B···Cg^{iii}	0.97	2.74	3.573 (3)	144 (2)

Symmetry codes: (i) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x, -y+1, -z$. *Cg* is the centroid of the C8–C13 benzene ring.

The H atoms on N2 were located in a difference Fourier map and refined freely with isotropic displacement parameters. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H, and C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2 atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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*.

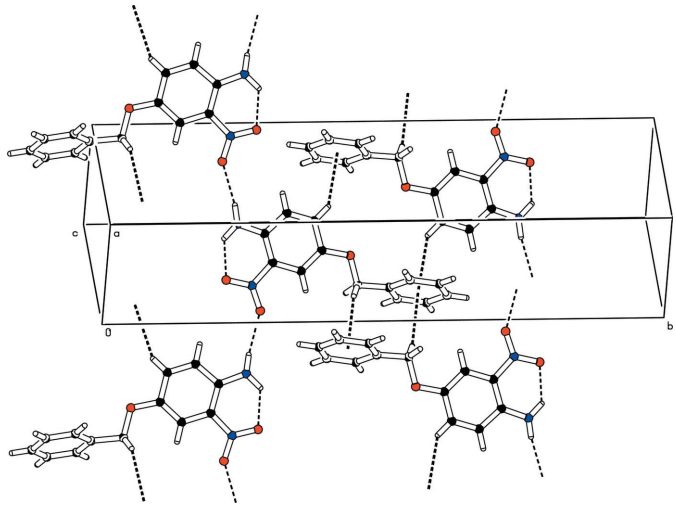


Figure 2
The packing of (I), with hydrogen bonds and C—H···π interactions drawn as dashed lines.

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