Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-Nitro-1-(2-phenylethyl)-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.113
Data-to-parameter ratio = 14.1

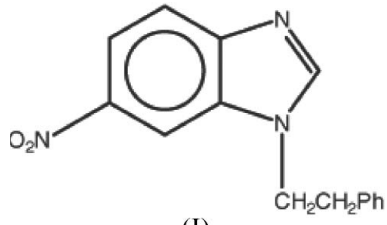
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 18 May 2005
Accepted 2 June 2005
Online 10 June 2005

The title compound, $C_{15}H_{13}N_3O_2$, was synthesized from 5-nitrobenzimidazole, 2-bromoethylbenzene and KOH in ethanol. The phenyl and benzimidazole ring systems are each planar and make a dihedral angle of 43.9 (1)°. The crystal structure is stabilized by weak intermolecular C—H···N hydrogen-bond interactions.

Comment

In recent years, considerable attention has been given to the synthesis of nitrobenzimidazole compounds because of their pharmacological properties (Sarlauskas *et al.*, 1997). We have synthesized and investigated the crystal structures of some benzimidazole and nitrobenzimidazole derivatives (Akkurt *et al.*, 2005). We now report the synthesis of a biologically interesting nitrobenzimidazole compound, its crystal structure and a comparison of the results with our previous studies related to heterocycles (Akkurt, Öztürk, Küçükbay *et al.*, 2004; Akkurt, Öztürk, Şireci *et al.*, 2004).



(I)

A molecular view of (I) is shown in Fig. 1. The geometric parameters agree with those previously reported (Akkurt, Öztürk, Küçükbay *et al.*, 2004; Akkurt, Öztürk, Şireci *et al.*, 2004; Akkurt *et al.*, 2005). The conformation of the phenyl ring with respect to the benzimidazole ring is described by the N2—C8—C9—C10 torsion angle of −60.6 (2)°. The dihedral angle between the planes of the phenyl and benzimidazole ring systems is 43.9 (1)°. Weak C—H···N interactions generate a chain parallel to the *a* axis (Table 1 and Fig. 2).

Experimental

5-Nitrobenzimidazole (2.0 g, 12.26 mmol) and 2-bromoethylbenzene (1.7 ml, 12.27 mmol) were added to a solution of KOH (1.02 g, 18.39 mmol) in ethanol (25 ml) and the mixture was refluxed for 5 h. The precipitated KBr was then filtered off while the solution was still hot. The solution was cooled to room temperature, and the crude product was precipitated and then crystallized from ethanol (10 ml) (yield 2.58 g, 79%; m.p. 409–410 K). ^{1}H NMR ($CDCl_3$): δ 3.2 (*t*, NCH_2CH_2, 2H), 4.5 (*t*, N—CH_2CH_2, 2H), 7.0–8.3 (*m*, Ar—H, 8H), 8.7 (*s*, benzimidazole-C2—H, 1H). Analysis calculated for $C_{15}H_{13}N_3O_2$: C 67.42, H 4.85, N 15.73%; found: C 67.25, H 4.83, N 15.67%.

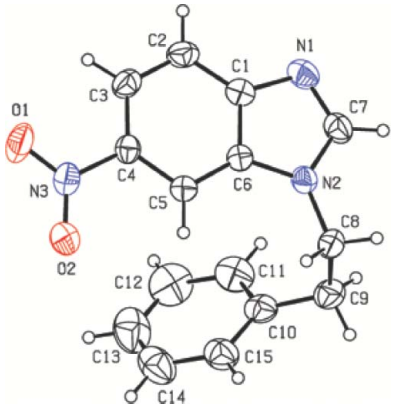


Figure 1
An *ORTEP-3* (Farrugia, 1997) drawing of (I), with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

Crystal data

$C_{15}H_{13}N_3O_2$	D_x = 1.340 Mg m^{-3}
M_r = 267.28	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 11275 reflections
a = 6.6382 (6) Å	θ = 2.1–28.0°
b = 11.4258 (6) Å	μ = 0.09 mm^{-1}
c = 18.2702 (16) Å	T = 296 K
β = 107.039 (7)°	Prism, colourless
V = 1324.91 (19) Å^3	0.40 × 0.26 × 0.09 mm
Z = 4	

Data collection

Stoe IPDS-II diffractometer	1674 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.089
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	θ_{max} = 26.0°
T_{min} = 0.971, T_{max} = 0.992	$h = -8 \rightarrow 7$
14688 measured reflections	$k = -14 \rightarrow 14$
2570 independent reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.113	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
S = 0.93	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
2570 reflections	Extinction correction: *SHELXL97*
182 parameters	Extinction coefficient: 0.008 (2)
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···N1^{i}	0.97	2.60	3.509 (2)	156

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

H atoms were positioned geometrically and refined with a riding model, with C—H = 0.93–0.97 Å, and with U_{iso}(H) constrained to be 1.2 times U_{eq} of the carrier atom.

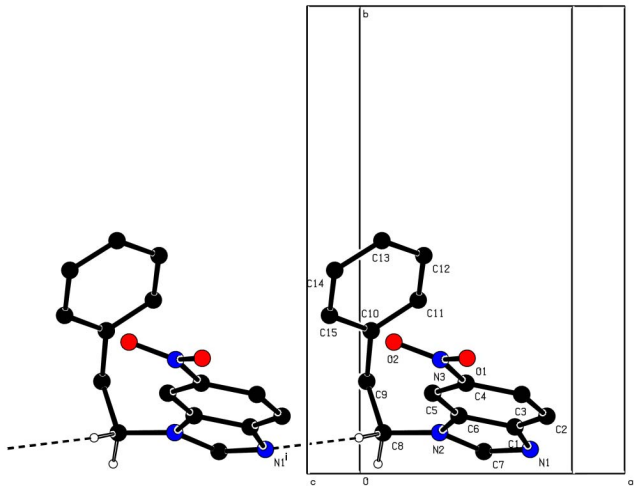


Figure 2
Part of the crystal packing of (I). Hydrogen bonds are shown as dashed lines, and H atoms on atoms not involved in the motifs shown have been omitted. [Symmetry code: (i) $x-1, y, z$.]

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the diffractometer (purchased under grant F.279 of the University Research Fund). HK and EO thank İnönü University Scientific Research Unit (BAPB-2005/36) for financial support for this study.

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