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1-Methoxyethyl-5-nitrobenzimidazole

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.124
Data-to-parameter ratio = 13.7

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

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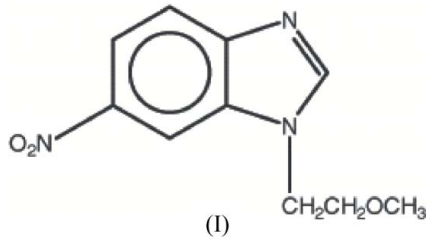
The title compound, $C_{10}H_{11}N_3O_3$, was synthesized by the reaction of 5-nitrobenzimidazole, 2-chloroethyl methyl ether and KOH in ethanol. The bond lengths and angles are unexceptional.

Comment

Nitrobenzimidazoles have attracted considerable interest due to their presence in a number of therapeutically and biologically active compounds. Nitrobenzimidazoles represent a group of nitro compounds that have seldom been characterized, although some of them possess antitrychomonal and other types of antimicrobial activities. Some nitrobenzimidazoles are relatively efficient substrates for DT-diaphorase and this enzyme is partly responsible for their cytotoxicity to bovine leukemia virus-transformed fibroblast culture (Sarlauskas *et al.*, 1997). We have also synthesized and investigated the crystal structures of some benzimidazole and nitrobenzimidazole derivatives (Öztürk *et al.*, 2003). We report here the synthesis of a biologically interesting nitrobenzimidazole compound; the results may be compared with those of a related heterocycle (Akkurt *et al.*, 2004).



(I)

The molecular structure with the atom-numbering scheme is shown in Fig. 1. The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The results agree with those for the benzimidazole and nitrobenzimidazole compounds (Akkurt, Karaca *et al.*, 2005; Akkurt, Türktekin *et al.*, 2005; Akkurt, Yıldırım Öztürk *et al.*, 2005). The benzimidazole ring is planar. The dihedral angle between the benzene and the fused five-membered ring system is 0.88 (11)°. The molecular packing is shown in Fig. 2.

Experimental

5-Nitrobenzimidazole (2.0 g, 12.26 mmol) and 2-chloroethyl methyl ether (2.3 ml, 25.18 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 KCl was then filtered off while the solution was hot. The solution was cooled to room temperature and a crude product precipitated. The precipitate was crystallized from ethanol (10 ml)

(yield: 2.32 g, 77%; m.p. 351–352 K). ^{1}H NMR ($CDCl_3$): δ 3.4 (*s*, OCH_3, 3H), 3.8 (*t*, N–CH_2CH_2O, 2H), 4.4 (*t*, N–CH_2CH_2O, 2H), 7.2–8.4 (*m*, Ar—H, 3H), 8.7 (*s*, benzimidazole-C^2—H, 1 H). Elemental analysis calculated for $C_{10}H_{11}N_3O_3$: C 54.29, H 4.98, N 19.00%; found: C 54.25, H 4.95, N 18.87%.

Crystal data

$C_{10}H_{11}N_3O_3$	$Z = 2$
$M_r = 221.22$	$D_x = 1.399$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 4.7940$ (7) Å	Cell parameters from 7061 reflections
$b = 8.4531$ (13) Å	$\theta = 2.7$–$27.9°$
$c = 13.411$ (2) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 97.350$ (12)°	$T = 296$ K
$\beta = 94.854$ (12)°	Plate, colorless
$\gamma = 101.266$ (12)°	0.80 × 0.37 × 0.05 mm
$V = 525.25$ (14) Å^3	

Data collection

Stoe IPDS-II diffractometer	1327 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.049$
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	$\theta_{max} = 27.7°$
$T_{min} = 0.920$, $T_{max} = 0.995$	$h = -6 \rightarrow 6$
8616 measured reflections	$k = -11 \rightarrow 11$
2443 independent reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.124$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.98$	$\Delta\rho_{max} = 0.14$ e Å^{-3}
2443 reflections	$\Delta\rho_{min} = -0.20$ e Å^{-3}
178 parameters	

H atoms were located in a difference synthesis and refined isotropically [C—H = 0.92 (3)–1.02 (4) Å]. The U_{iso}(H) values were set at 1.2 (1.5 for methyl group) times U_{eq} of the carrier atom.

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: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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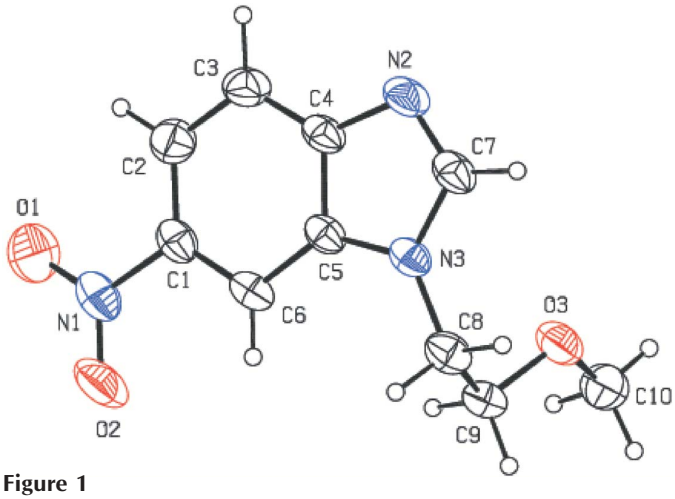

Figure 1
An *ORTEP3* drawing of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

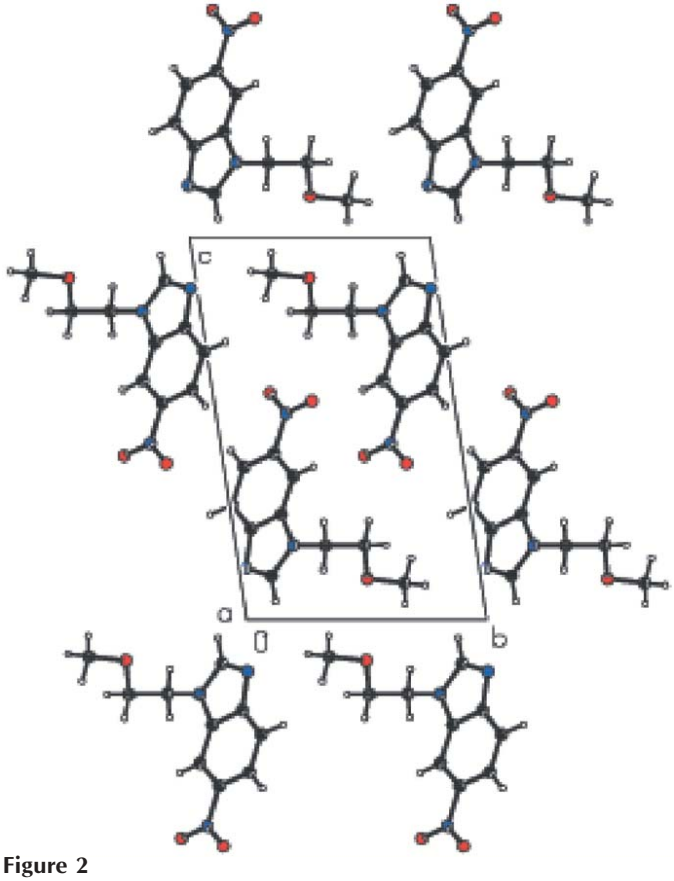

Figure 2
The packing of molecules of (I) in the crystal structure.

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