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2-(2-Nitrophenyl)-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.113
Data-to-parameter ratio = 13.8

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

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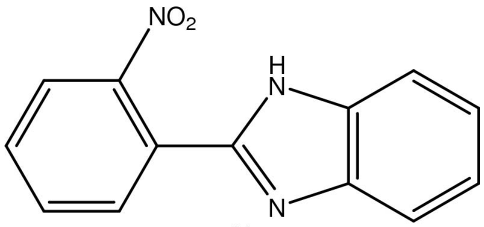
In the title compound, $C_{13}H_9N_3O_2$, the dihedral angle between the benzimidazole moiety and the benzene ring is 40.08 (6)°. The molecules are linked into chains along the *b* axis by intermolecular N—H···N hydrogen bonds. The chains are interlinked into a two-dimensional network by C—H···O hydrogen bonds.

Comment

We have reported the synthesis and crystal structure of 6-methoxycarbonyl-2-methyl-1*H*-benzimidazol-3-ium nitrate hemihydrate (Ding *et al.*, 2004). In our ongoing studies of benzimidazole derivatives, the title compound, (I), was obtained in the reaction of *o*-diaminobenzene and 2-nitrobenzoyl chloride.



(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and comparable with those in the related compound *N*-methyl-2-(*o*-nitrophenyl)benzimidazole (Das *et al.*, 2003). The benzimidazole moiety is essentially planar, with a dihedral angle of 1.7 (1)° between the planes of the benzene ring and its fused imidazole ring. The whole molecule is non-planar; the benzimidazole ring makes an angle of 40.08 (6)° with the C8–C13 benzene ring. In the crystal structure, the molecules of (I) are linked into chains along the *b* axis by N1—H1N···N2^{i} intermolecular hydrogen bonds. The chains are interlinked into a two-dimensional network by C12—H12···O1^{ii} hydrogen bonds (Fig. 2; symmetry codes as in Table 2). The packing is further stabilized by van der Waals forces.

Experimental

Compound (I) was synthesized according to the method of Fekner *et al.* (2004). A solution of 2-nitrobenzoyl chloride (3.71 g, 20 mmol) in CH_2Cl_2 (40 ml) was added dropwise over 2 h to a solution of *o*-diaminobenzene (2.16 g, 20 mmol) and Et_3N (3.6 ml) in CH_2Cl_2 (20 ml). After the addition was complete, the reaction mixture was stirred at 273 K for 1 h and at room temperature for 3 h. The volatiles were removed *in vacuo* to give an off-white solid. The solid was refluxed in glacial AcOH (50 ml) in the presence of AcONa (1.64 g,

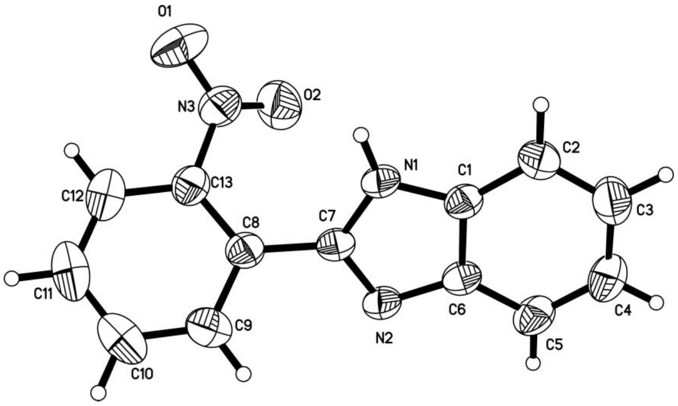


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

20 mmol) for 15 h. The resulting brown oil was partitioned between CH_2Cl_2 and water. The organic extracts were evaporated *in vacuo* to give a yellow solid. Single crystals of (I) were obtained from a CH_2Cl_2 solution over a period of 2 d.

Crystal data

$C_{13}H_9N_3O_2$
$M_r = 239.23$
Orthorhombic, *Pbca*
$a = 7.806$ (2) Å
$b = 9.901$ (3) Å
$c = 29.307$ (8) Å
$V = 2265.1$ (11) Å^3
$Z = 8$
$D_x = 1.403$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2718 reflections
$\theta = 2.8$–23.4°
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Needle, yellow
0.43 × 0.17 × 0.12 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.959$, $T_{\max} = 0.988$
11735 measured reflections
2256 independent reflections
1808 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 26.2°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 10$
$l = -36 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.113$
$S = 1.06$
2256 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.6337P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 1
Selected interatomic distances (Å).

N1—C7	1.3509 (19)	N2—C6	1.388 (2)
N1—C1	1.3713 (19)	N3—C13	1.469 (2)
N2—C7	1.3236 (19)		

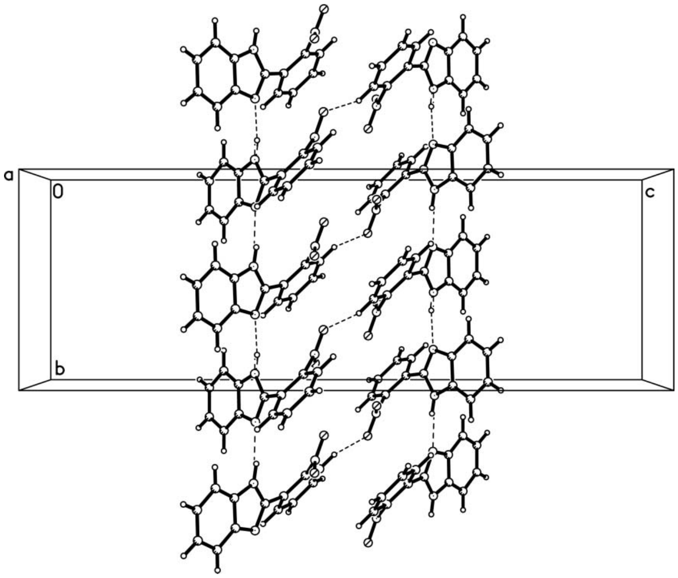


Figure 2
Part of the two-dimensional network in (I), viewed down the *a* axis. Hydrogen bonds are indicated by dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···N2$^{\rm i}$	0.86	1.99	2.823 (2)	163
C12—H12···O1$^{\rm ii}$	0.93	2.54	3.285 (3)	137

Symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, z$; (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, -z$.

After their location in a difference Fourier map, all H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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