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2-(3-Methyl-2-nitrophenyl)-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.158
Data-to-parameter ratio = 14.3

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

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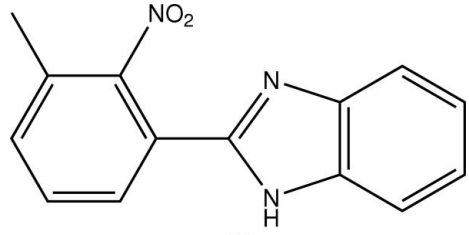
In the title compound, $C_{14}H_{11}N_3O_2$, the dihedral angle between the benzimidazole group and the other benzene ring is 39.8 (1)°. The molecules are linked into chains along the *c* axis by N—H···N hydrogen bonds. The packing is further stabilized by C—H···π interactions.

Comment

We have reported the structure of 2-(2-nitrophenyl)-1*H*-benzimidazole, (II) (Li *et al.*, 2005). In order to investigate the effect of the substituent on the molecular conformation, the title compound, (I), was synthesized from the reaction of *o*-diaminobenzene and 3-methyl-2-nitrobenzoyl chloride.



(I)

All bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are in good agreement with those in (II). The benzimidazole group is essentially planar, with a dihedral angle of 1.0 (1)° between the planes of the benzene ring and its fused imidazole ring. The benzimidazole group makes a dihedral angle of 39.8 (1)° with the C8–C13 benzene ring. There is an intramolecular hydrogen bond, *viz*. C14—H14*A*···O1, forming a six-membered ring. In the crystal structure, molecules are linked into chains along the *c* axis (Fig. 2) by N—H···N interactions (Table 2). The packing is further stabilized by C—H···π interactions (Table 2).

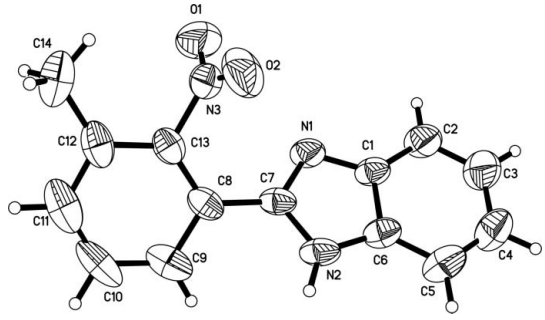


Figure 1
The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

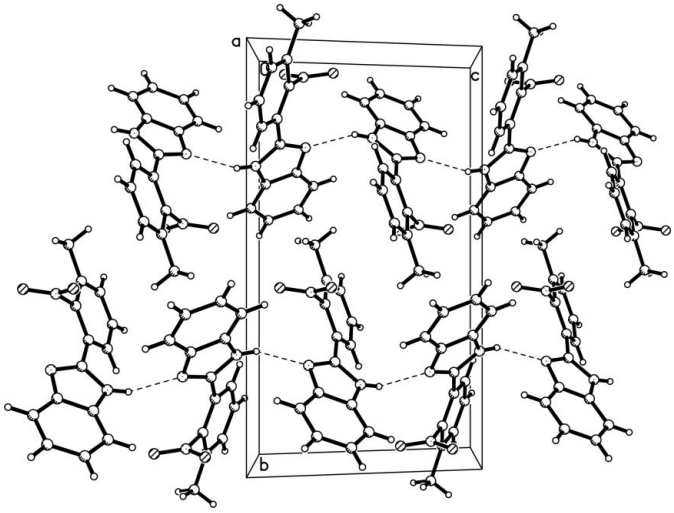


Figure 2
A view down the *a* axis of (I), showing the chains. Hydrogen bonds are indicated by dashed lines.

Experimental

A solution of 3-methyl-2-nitrobenzoyl chloride (4.0 g, 20 mmol) in CH_2Cl_2 (40 ml) was added dropwise over 2 h to a solution of *o*-diaminobenzene (2.2 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 (1.6 g, 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 were obtained from a tetrahydrofuran solution over a period of one week.

Crystal data

$C_{14}H_{11}N_3O_2$
M_r = 253.26
Monoclinic, $P2_1/c$
a = 7.755 (1) Å
b = 17.229 (2) Å
c = 9.7792 (12) Å
β = 105.598 (2)°
V = 1258.5 (3) Å^3
Z = 4
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1276 reflections
θ = 2.5–22.4°
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, yellow
0.37 × 0.13 × 0.06 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.995
6830 measured reflections
2464 independent reflections
1705 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.1°
$h = -4 \rightarrow 9$
$k = -20 \rightarrow 21$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.158
S = 1.03
2464 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 0.2947P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected bond lengths (Å).

N1—C7	1.317 (3)	N2—C6	1.373 (3)
N1—C1	1.392 (3)	N3—C13	1.468 (3)
N2—C7	1.352 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.86	2.09	2.850 (3)	146
C14—H14A···O1	0.96	2.48	3.112 (4)	123
C14—H14C···$Cg2^{ii}$	0.96	2.74	3.536	141

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$. $Cg2$ denotes the centroid of the C1–C6 benzene ring

After their location in a difference Fourier map, all H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2 or 1.5 times U_{iso}(C,*N*).

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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