Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Methoxyphenyl)-1*H*-benzimidazole

Hermenegilda Moreno-Diaz,[a] Gabriel Navarrete-Vázquez,[a] Samuel Estrada-Soto[a] and Hugo Tlahuext[b]*

[a]Facultad de Farmacia, Universidad Autónoma del Estado de Morelos, Avenida Universidad 1001 Col Chamilpa, CP 62100, Cuernavaca Mor., Mexico, and [b]Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos, Avenida Universidad 1001 Col Chamilpa, CP 62100, Cuernavaca Mor., Mexico

Correspondence e-mail: tlahuext@ciq.uaem.mx

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.117
Data-to-parameter ratio = 14.4

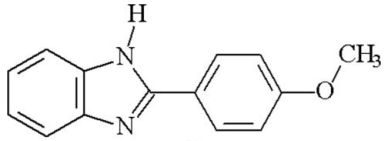
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 18 May 2006
Accepted 30 May 2006

In the title compound, $C_{14}H_{12}N_2O$, the dihedral angle between the benzimidazole ring system and the 4-methoxyphenyl substituent is 34.12 (6)°. The molecules are linked by intermolecular N—H···N hydrogen bonds, forming chains running along the c axis.

Comment

Benzimidazole and its derivatives are important heterocyclic compounds with versatile pharmacological activities (Bali *et al.*, 2005). They have been used as antiparasitic (Navarrete-Vázquez *et al.*, 2003), antimicrobial (Özden *et al.*, 2005), antitumoural (Andrzejewska *et al.*, 2002) and antifungal agents (Küçükbay *et al.*, 2003). In our ongoing studies of benzimidazole derivatives as vasorelaxant agents, the title compound, (I) (Fig. 1), was obtained by the reaction of 1,2-phenylenediamine, *p*-anisaldehyde and sodium metabisulfite.



(I)

The 4-methoxyphenyl substituent of (I) is planar. The plane through atoms C7–C13,O1 makes a dihedral angle of −32.9 (6)° with the benzimidazole system (Table 1).

An intermolecular N1—H1···N2^{i} hydrogen bond [symmetry code: (i) $x, \frac{3}{2} - y, -\frac{1}{2} + z$] links the molecules into chains running along the c axis (Fig. 2), with H1···N2^{i} = 2.15 Å, N1···N2^{i} = 3.005 (2) Å and N1···H1—N2^{i} = 173°.

Experimental

A mixture of 1,2-phenylenediamine (3.38 g, 31 mmol), *p*-anisaldehyde (4.62 g, 34 mmol) and sodium metabisulfite (6.46 g, 34 mmol) was stirred and placed in an open Erlenmeyer Pyrex flask. The mixture was irradiated in a household microwave oven (1000 W) for 40–50 s. After irradiation, the mixture was poured into cold water. The precipitate which formed was collected by filtration, washed with water and dried to give a white solid (m.p. 501.6–503 K). Single crystals of (I) were obtained from a solution in a methanol–water mixture (9:1) (yield 6.31 g, 90%).

Crystal data

$C_{14}H_{12}N_2O$
M_r = 224.26
Monoclinic, $P2_1/c$
a = 11.354 (2) Å
b = 10.562 (2) Å
c = 9.868 (2) Å
β = 112.22 (3)°
V = 1095.5 (4) Å^3
Z = 4
D_x = 1.360 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
Block, colourless
0.28 × 0.23 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
5998 measured reflections
2245 independent reflections
2033 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 26.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.117$
$S = 1.14$
2245 reflections
156 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.5933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.380 (2)	C7—N1	1.363 (2)
C6—N2	1.397 (2)	C11—O1	1.363 (2)
C7—N2	1.328 (2)		
N1—C7—C8—C9	−32.9 (2)	C10—C11—O1—C14	11.6 (2)

The amino H atom was located in a difference Fourier map and then refined as riding, with N—H = 0.86 Å; the isotropic displacement parameter was freely refined. All remaining H atoms were treated as riding, with methyl C—H distances of 0.96 Å and aromatic C—H distances of 0.93 Å. The U_{iso}(H) values were fixed by the riding-model technique, at $1.2U_{eq}$(C) for aromatic H atoms and $1.5U_{eq}$(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Consejo Nacional de Ciencia y Tecnología (CONACyT) under grant Nos. 3562P-E and PROMEP-SEP (GNV). The manuscript was prepared using the beta test version 1.0.0 of the program publCIF to be released by the IUCr.

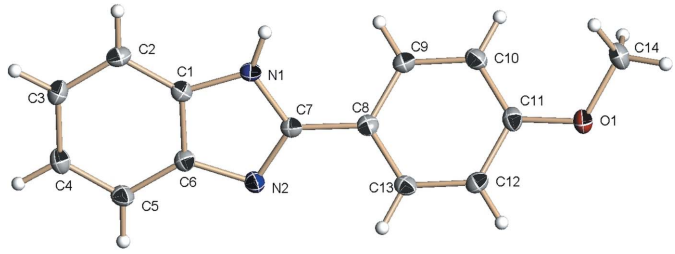


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

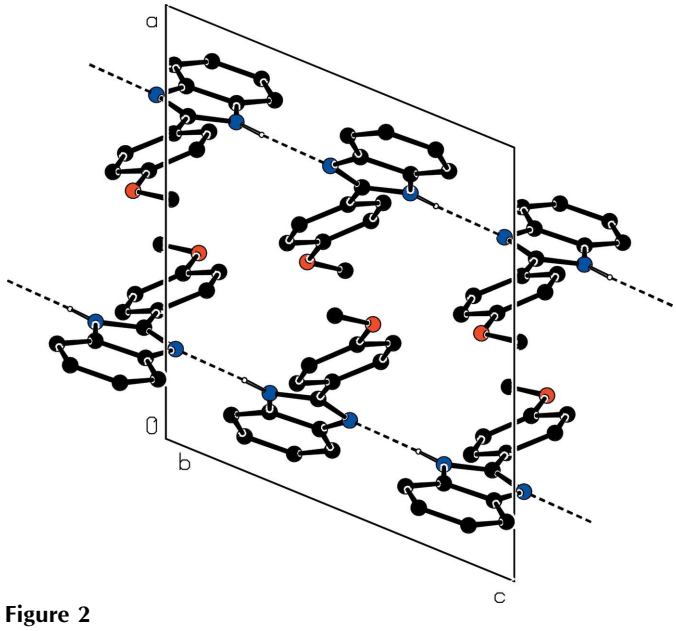


Figure 2
The crystal packing of (I), showing the formation of chains. Hydrogen bonds are represented by dashed lines and H atoms not involved in hydrogen bonding have been omitted for clarity.

References

Andrzejewska, M., Yépez-Mulia, L., Cedillo-Rivera, R., Tapia, A., Vilpo, L., Vilpo, J. & Kazimierczuk, Z. (2002). *Eur. J. Med. Chem.* **37**, 973–978.
Bali, A., Bansal, Y., Sugumaran, M., Singh Saggu, J., Balakumar, P., Kaur, G., Bansal, G., Sharma, A. & Singh, M. (2005). *Bioorg. Med. Chem. Lett.* **15**, 3962–3965.
Bruker (2000). *SMART* (Version 5.618), *SAINT-Plus-NT* (Version 6.04) and *SHELXTL-NT* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Küçükbay, H., Durmaz, R., Orhan, E. & Günal, S. (2003). *Farmaco*, **58**, 431–437.
Navarrete-Vázquez, G., Yepez-Mulia, L., Hernández-Campos, A., Tapia, A., Hernández-Luis, F., Cedillo, R., González, J., Martínez-Fernández, M., Martínez-Grueiro, M. & Castillo, R. (2003). *Bioorg. Med. Chem.* **11**, 4615–4622.
Özden, S., Atabey, D., Yıldız, S. & Göker, H. (2005). *Bioorg. Med. Chem.* **13**, 1587–1597.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.