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

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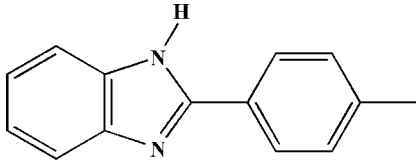
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.135; data-to-parameter ratio = 14.6.

In the title compound, $C_{14}H_{12}N_2$, the benzimidazole and tolyl groups are not coplanar, exibiting a dihedral angle of 27.5 (3)°. The structure is held intact through N—H···N hydrogen bonds and π–π stacking interactions [perpendicular distance 3.504 Å and centroid-to-centroid distance 4.080 Å], displaying a two-dimensional supramolecular array.

Related literature

For related literature, see: Johnson (1976); Ma *et al.* (2006); Migawa *et al.* (1998); Porcari *et al.* (1998); Roth *et al.* (1997); Tamm (1957); Tamm & Seghal (1978).



Experimental

Crystal data

$C_{14}H_{12}N_2$
M_r = 208.26
Orthorhombic, *Pbca*
a = 9.0763 (10) Å
b = 9.8053 (11) Å
c = 24.628 (3) Å
V = 2191.8 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.40 × 0.20 × 0.16 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.988
9605 measured reflections
2133 independent reflections
1850 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.135
S = 1.10
2133 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.85	2.07	2.9151 (19)	171

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RT2008).

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supplementary materials

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

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Comment

2-Substituted benzimidazoles have attracted considerable interest as intermediates in the development of molecules of pharmaceutical interest. Benzimidazole derivatives exhibit significant activity against several viruses such as HIV, herpes (HSV-1), RNA, influenza, and human cytomegalovirus (HCMV) (Tamm, 1957; Tamm & Seghal, 1978; Roth *et al.*, 1997; Migawa *et al.*, 1998; Porcari *et al.*, 1998). The objective of this study therefore was to synthesize and elucidate the crystal structure of a new benzimidazole compound.

A view of the molecule of (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. The dihedral angle between the benzimidazole and tolyl portions of the title compound, (I), is 27.5 °. The molecules are linked into a linear chain through N—H···N hydrogen bonds interactions (N2···H1 2.072 Å, N1—H1···N2 170.8 °), as shown in Fig. 2. There exist π–π stacking interactions in adjacent linear chains, adjacent tolyl rings are exactly parallel, the perpendicular spacing of the rings is 3.504 Å, and the ring centroid-to-centroid distance is 4.080 Å. These π–π stacking interactions form a two dimensional supramolecular array.

Experimental

The title compound was synthesized according to the reported procedure (Ma *et al.*, 2006). *o*-Phenylenediamine (10 mmol) and *p*-Tolualdehyde (10 mmol) were mixed in DMF (30 ml) thoroughly, followed by the addition of $KHSO_4$ (3.4 mmol), heating and stirring for one hour. When the reaction was finished, the solution was cooled to room temperature. The reaction mixture was added dropwise with vigorous stirring into a mixture of Na_2CO_3 (3.4 mmol) and H_2O (250 ml). The precipitate was collected by filtration, and recrystalized from ethanol to form the brown block crystals of the title compound. Yield: 416.5 mg (20%).

Refinement

The H atoms were placed in calculated positions (aromatic C—H 0.93 Å and methyl C—H 0.96 Å; U 1.2U_{eq}C) and were included in the refinement in the riding model approximation. The nitrogen-bound H atom was located and refined with an N—H distance restraint of 0.85 Å.

Figures

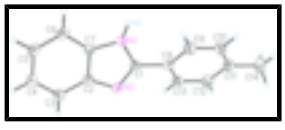

Fig. 1. *ORTEP*II (Johnson, 1976) plot of the title compound, with displacement ellipsoids drawn at the 30% probability level, and H atoms given as spheres of arbitrary radii.

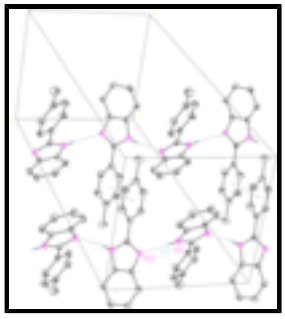

Fig. 2. A view of title compound, showing the extended two-dimensional structure linked by N—H···N hydrogen interactions and π–π stacking interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level, and H atoms given as spheres of arbitrary radii.

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

Crystal data

$C_{14}H_{12}N_2$	F_{000} = 880
M_r = 208.26	D_x = 1.262 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2911 reflections
a = 9.0763 (10) Å	θ = 2.8–24.9º
b = 9.8053 (11) Å	μ = 0.08 mm^{-1}
c = 24.628 (3) Å	*T* = 295 (2) K
V = 2191.8 (4) Å^3	Block, brown
Z = 8	0.40 × 0.20 × 0.16 mm

Data collection

Bruker APEX area-detector diffractometer	2133 independent reflections
Radiation source: fine-focus sealed tube	1850 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 295(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −11→11
T_{min} = 0.970, T_{max} = 0.988	*k* = −11→4
9605 measured reflections	*l* = −30→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.052	H-atom parameters constrained
$wR(F^2)$ = 0.135	$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 0.6749P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max} < 0.001$

2133 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
146 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.21900 (15)	0.85838 (14)	0.35353 (6)	0.0377 (4)
N2	0.16814 (14)	1.08050 (14)	0.35983 (6)	0.0386 (4)
C1	0.26414 (18)	0.98288 (16)	0.37105 (6)	0.0352 (4)
C2	0.05379 (17)	1.01519 (17)	0.33254 (7)	0.0363 (4)
C3	−0.0747 (2)	1.06679 (19)	0.30950 (8)	0.0477 (5)
H3	−0.0977	1.1590	0.3120	0.057*
C4	−0.1665 (2)	0.9773 (2)	0.28295 (8)	0.0523 (5)
H4	−0.2523	1.0100	0.2670	0.063*
C5	−0.1337 (2)	0.8385 (2)	0.27942 (8)	0.0494 (5)
H5	−0.1980	0.7810	0.2610	0.059*
C6	−0.00918 (19)	0.78515 (18)	0.30242 (7)	0.0445 (4)
H6	0.0118	0.6924	0.3006	0.053*
C7	0.08437 (17)	0.87557 (17)	0.32862 (7)	0.0349 (4)
C8	0.40695 (17)	1.00359 (17)	0.39761 (7)	0.0369 (4)
C9	0.5242 (2)	0.9178 (2)	0.38676 (8)	0.0514 (5)
H9	0.5111	0.8441	0.3635	0.062*
C10	0.6605 (2)	0.9398 (2)	0.40998 (9)	0.0557 (5)
H10	0.7378	0.8810	0.4019	0.067*
C11	0.68392 (19)	1.0476 (2)	0.44493 (8)	0.0478 (5)
C12	0.5668 (2)	1.1330 (2)	0.45579 (8)	0.0497 (5)
H12	0.5803	1.2065	0.4791	0.060*
C13	0.42976 (19)	1.11181 (18)	0.43277 (7)	0.0429 (4)
H13	0.3524	1.1706	0.4409	0.052*
C14	0.8329 (2)	1.0698 (3)	0.47036 (11)	0.0714 (7)
H14A	0.8284	1.0475	0.5083	0.107*
H14B	0.8612	1.1635	0.4662	0.107*
H14C	0.9042	1.0124	0.4528	0.107*
H1	0.2595	0.7809	0.3577	0.086*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0392 (8)	0.0252 (7)	0.0488 (8)	0.0010 (6)	−0.0021 (6)	−0.0011 (6)
N2	0.0376 (7)	0.0267 (7)	0.0513 (8)	−0.0004 (5)	−0.0035 (6)	−0.0013 (6)
C1	0.0384 (8)	0.0263 (8)	0.0410 (9)	−0.0015 (6)	0.0025 (7)	−0.0005 (7)
C2	0.0364 (8)	0.0285 (9)	0.0440 (9)	−0.0025 (6)	0.0002 (7)	0.0011 (7)
C3	0.0463 (10)	0.0342 (10)	0.0625 (12)	0.0031 (7)	−0.0092 (9)	0.0020 (9)
C4	0.0447 (10)	0.0510 (12)	0.0610 (12)	−0.0014 (8)	−0.0150 (9)	0.0056 (10)
C5	0.0501 (10)	0.0454 (11)	0.0528 (11)	−0.0134 (8)	−0.0090 (8)	−0.0005 (9)
C6	0.0501 (10)	0.0315 (9)	0.0518 (10)	−0.0063 (7)	−0.0021 (8)	−0.0016 (8)

C7	0.0365 (8)	0.0282 (9)	0.0399 (9)	−0.0025 (6)	0.0026 (7)	0.0019 (7)
C8	0.0382 (8)	0.0295 (9)	0.0430 (9)	−0.0020 (7)	−0.0007 (7)	0.0021 (7)
C9	0.0449 (10)	0.0441 (11)	0.0651 (12)	0.0054 (8)	−0.0048 (9)	−0.0164 (9)
C10	0.0394 (10)	0.0581 (13)	0.0697 (13)	0.0092 (8)	−0.0020 (9)	−0.0072 (11)
C11	0.0430 (10)	0.0499 (12)	0.0506 (11)	−0.0057 (8)	−0.0054 (8)	0.0060 (9)
C12	0.0532 (11)	0.0434 (11)	0.0525 (11)	−0.0043 (8)	−0.0098 (9)	−0.0067 (9)
C13	0.0439 (9)	0.0347 (10)	0.0502 (10)	0.0030 (7)	−0.0031 (8)	−0.0036 (8)
C14	0.0489 (12)	0.0831 (18)	0.0821 (16)	−0.0062 (11)	−0.0174 (11)	0.0000 (14)

Geometric parameters (Å, °)

N1—C1	1.358 (2)	C6—H6	0.9300
N1—C7	1.378 (2)	C8—C9	1.383 (2)
N1—H1	0.8500	C8—C13	1.385 (2)
N2—C1	1.323 (2)	C9—C10	1.379 (3)
N2—C2	1.392 (2)	C9—H9	0.9300
C1—C8	1.466 (2)	C10—C11	1.380 (3)
C2—C3	1.392 (2)	C10—H10	0.9300
C2—C7	1.400 (2)	C11—C12	1.379 (3)
C3—C4	1.375 (3)	C11—C14	1.506 (3)
C3—H3	0.9300	C12—C13	1.382 (2)
C4—C5	1.396 (3)	C12—H12	0.9300
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.368 (3)	C14—H14A	0.9600
C5—H5	0.9300	C14—H14B	0.9600
C6—C7	1.387 (2)	C14—H14C	0.9600
C1—N1—C7	107.41 (13)	C9—C8—C13	118.16 (16)
C1—N1—H1	129.3	C9—C8—C1	120.67 (15)
C7—N1—H1	123.2	C13—C8—C1	121.14 (15)
C1—N2—C2	105.01 (13)	C10—C9—C8	120.97 (18)
N2—C1—N1	112.65 (14)	C10—C9—H9	119.5
N2—C1—C8	125.11 (14)	C8—C9—H9	119.5
N1—C1—C8	122.21 (14)	C9—C10—C11	121.14 (18)
C3—C2—N2	130.84 (16)	C9—C10—H10	119.4
C3—C2—C7	119.56 (15)	C11—C10—H10	119.4
N2—C2—C7	109.59 (14)	C12—C11—C10	117.83 (17)
C4—C3—C2	118.00 (17)	C12—C11—C14	121.60 (19)
C4—C3—H3	121.0	C10—C11—C14	120.57 (19)
C2—C3—H3	121.0	C11—C12—C13	121.52 (18)
C3—C4—C5	121.50 (17)	C11—C12—H12	119.2
C3—C4—H4	119.3	C13—C12—H12	119.2
C5—C4—H4	119.3	C12—C13—C8	120.39 (16)
C6—C5—C4	121.55 (17)	C12—C13—H13	119.8
C6—C5—H5	119.2	C8—C13—H13	119.8
C4—C5—H5	119.2	C11—C14—H14A	109.5
C5—C6—C7	116.98 (17)	C11—C14—H14B	109.5
C5—C6—H6	121.5	H14A—C14—H14B	109.5
C7—C6—H6	121.5	C11—C14—H14C	109.5
N1—C7—C6	132.22 (15)	H14A—C14—H14C	109.5

N1—C7—C2	105.35 (14)	H14B—C14—H14C	109.5
C6—C7—C2	122.40 (15)		
C2—N2—C1—N1	−0.80 (18)	C3—C2—C7—C6	0.0 (3)
C2—N2—C1—C8	177.07 (15)	N2—C2—C7—C6	−178.71 (15)
C7—N1—C1—N2	0.53 (19)	N2—C1—C8—C9	−150.60 (19)
C7—N1—C1—C8	−177.40 (14)	N1—C1—C8—C9	27.1 (2)
C1—N2—C2—C3	−177.71 (18)	N2—C1—C8—C13	27.3 (3)
C1—N2—C2—C7	0.76 (18)	N1—C1—C8—C13	−155.08 (17)
N2—C2—C3—C4	177.59 (18)	C13—C8—C9—C10	−0.5 (3)
C7—C2—C3—C4	−0.8 (3)	C1—C8—C9—C10	177.46 (18)
C2—C3—C4—C5	0.6 (3)	C8—C9—C10—C11	0.3 (3)
C3—C4—C5—C6	0.3 (3)	C9—C10—C11—C12	−0.2 (3)
C4—C5—C6—C7	−1.1 (3)	C9—C10—C11—C14	179.5 (2)
C1—N1—C7—C6	177.98 (18)	C10—C11—C12—C13	0.2 (3)
C1—N1—C7—C2	−0.02 (18)	C14—C11—C12—C13	−179.46 (19)
C5—C6—C7—N1	−176.77 (17)	C11—C12—C13—C8	−0.4 (3)
C5—C6—C7—C2	0.9 (3)	C9—C8—C13—C12	0.5 (3)
C3—C2—C7—N1	178.21 (15)	C1—C8—C13—C12	−177.42 (16)
N2—C2—C7—N1	−0.46 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.85	2.07	2.9151 (19)	171

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*.

Fig. 1

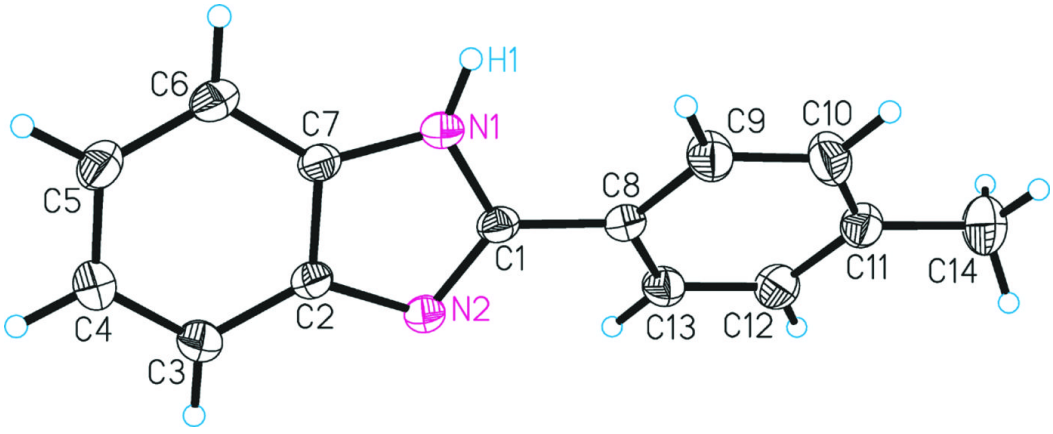

Fig. 2