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2-(1-Naphthylmethyl)-1*H*-benzo[*d*]-imidazole

Ming-Wu Ding,[a,b]* Yang-Gen Hu[c] and Ming-Guo Liu[d]

[a]Hubei Key Laboratory of Native Compounds and Chemical Biology, College of Chemistry and Life Science, China Three Gorges University, Yichang 443002, People's Republic of China, [b]Key Laboratory of Pesticide & Chemical Biology of Ministry of Education, Central China Normal University, Wuhan 430079, People's Republic of China, [c]Department of Medicinal Chemistry, Yunyang Medical College, Shiyan 442000, People's Republic of China, and [d]College of Chemistry & Life Science, China Three Gorges University, Yichang 443002, People's Republic of China
Correspondence e-mail: huyangg111@yahoo.com.cn

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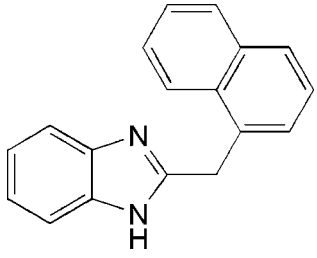
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.044; wR factor = 0.098; data-to-parameter ratio = 9.0.

In the title compound, $C_{18}H_{14}N_2$, the benzimidazole and naphthalene ring systems are planar, making a dihedral angle of 78.71 (1)° with each other. The packing of the molecules in the crystal structure is mainly due to an intermolecular N—H···N hydrogen bond.

Related literature

Many derivatives of benzimidazole have been prepared and their biological and pharmaceutical activities have ben studied by Matsuno *et al.* (2000) and Garuti *et al.* (1999).



Experimental

Crystal data

$C_{18}H_{14}N_2$
M_r = 258.31
Monoclinic, *Pc*
a = 8.4578 (16) Å
b = 9.0329 (17) Å
c = 9.6474 (18) Å
β = 108.932 (3)°
V = 697.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.13 × 0.06 × 0.05 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
5884 measured reflections
1651 independent reflections
1176 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.098
S = 1.03
1651 reflections
184 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1^{i}	0.87 (3)	2.03 (3)	2.855 (3)	160 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2176).

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Matsuno, T., Kato, M., Sasahara, H., Watanabe, T., Inaba, M., Takahashi, M., Yaguchi, S. I., Yoshioka, K., Sakato, M. & Kawashima, S. (2000). *Chem. Pharm. Bull.* **48**, 1778–1781.
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  doi:10.1107/S1600536807028449

supplementary materials

Acta Cryst. (2007). E**63**, o3184 [**doi:10.1107/S1600536807028449**]

2-(1-Naphthylmethyl)-1*H*-benzo[*d*]imidazole

M.-W. Ding, Y.-G. Hu and M.-G. Liu

Comment

Benzimidazoles are important heterocycles which exhibite good biological and pharmaceutical activities, such as antitumor activity (Matsuno *et al.*, 2000). Many derivatives of benzimidazole have been prepared and their biological activities were studied (Garuti *et al.*, 1999). In our work of preparing potentially active heterocycles, we obtained the title compound, (I). The benzimidazole ring is planar. The naphthalene ring C1—C10 is twisted with respect to this benzimidazole ring, with a dihedral angle of 78.71 (1)° (Fig. 1). In the crystal structure, intermolecular N—H···N hydrogen bonds form zigzag tapes running along the *c* axis (Fig. 2 and Table 1). There are no marked π-π interactions.

Experimental

A solution of 1,2-benzenediamine (10.8 g, 0.1 mol) and 2-(1-naphthalenyl) acetic acid (18.6 g, 0.1 mol) in ethane-1,2-diol (30 ml) was refluxed for 8 h. After the reaction mixture was cooled to room temperature, it was poured into water (200 ml) and the precipitate was filtered and recrystallized from DMF/ethanol (1:8) to give the title compound, (I), in yield of 83% (m.p. 523 K). Suitable crystals were obtained by vapor diffusion of ethanol and dichloromethane at room temperature.

Refinement

The N-bound H atom was refined isotropically, with U_{iso}(H) = 1.2U_{eq}(N). Other H atoms were treated as riding atoms, with C—H distances 0.93 Å (aromatic) and 0.97 Å (CH_2), and with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs have been merged.

Figures

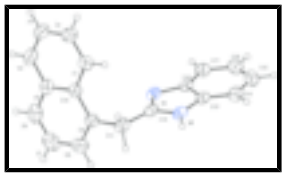

Fig. 1. The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

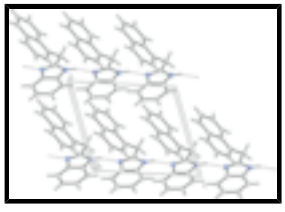

Fig. 2. A crystal packing diagram, viewed along the *b* axis. Hydrogen bonds are indicated by dashed lines.

2-(1-Naphthylmethyl)-1*H*-benzo[*d*]imidazole

Crystal data

$C_{18}H_{14}N_2$	F_{000} = 272
M_r = 258.31	D_x = 1.231 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 1373 reflections
a = 8.4578 (16) Å	θ = 2.3–21.6º
b = 9.0329 (17) Å	μ = 0.07 mm^{-1}
c = 9.6474 (18) Å	*T* = 298 (2) K
β = 108.932 (3)º	Plate, colorless
V = 697.2 (2) Å^3	0.13 × 0.06 × 0.05 mm
Z = 2	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	1176 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.035
Monochromator: graphite	θ_{max} = 28.0º
T = 298(2) K	θ_{min} = 2.3º
φ and ω scans	*h* = −11→10
Absorption correction: none	*k* = −11→11
5884 measured reflections	*l* = −12→12
1651 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.098	$(\Delta/\sigma)_{max} < 0.001$
S = 1.03	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
1651 reflections	$\Delta\rho_{min}$ = −0.10 e Å^{-3}
184 parameters	Extinction correction: none
2 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5318 (3)	0.5708 (3)	0.8424 (3)	0.0601 (8)
H1	0.5074	0.5024	0.9046	0.072*
C2	0.6502 (4)	0.5376 (4)	0.7806 (4)	0.0729 (9)
H2	0.7065	0.4477	0.8017	0.087*
C3	0.6881 (4)	0.6359 (5)	0.6866 (4)	0.0806 (10)
H3	0.7701	0.6124	0.6452	0.097*
C4	0.6063 (4)	0.7663 (4)	0.6546 (4)	0.0771 (10)
H4	0.6316	0.8311	0.5899	0.093*
C5	0.4828 (3)	0.8063 (4)	0.7175 (3)	0.0581 (7)
C6	0.4001 (5)	0.9432 (4)	0.6883 (4)	0.0820 (10)
H6	0.4275	1.0105	0.6268	0.098*
C7	0.2818 (5)	0.9784 (4)	0.7480 (5)	0.0912 (11)
H7	0.2274	1.0691	0.7268	0.109*
C8	0.2403 (4)	0.8782 (4)	0.8424 (4)	0.0763 (9)
H8	0.1569	0.9032	0.8816	0.092*
C9	0.3195 (3)	0.7456 (3)	0.8776 (3)	0.0535 (7)
C10	0.4441 (3)	0.7073 (3)	0.8147 (3)	0.0489 (7)
C11	0.2779 (4)	0.6426 (3)	0.9853 (3)	0.0632 (8)
H11A	0.3815	0.6068	1.0547	0.076*
H11B	0.2202	0.6990	1.0398	0.076*
C12	0.1730 (3)	0.5134 (3)	0.9175 (3)	0.0489 (7)
C13	0.0257 (3)	0.3107 (3)	0.9082 (3)	0.0479 (6)
C14	−0.0602 (4)	0.1883 (3)	0.9324 (3)	0.0638 (8)
H14	−0.0532	0.1591	1.0267	0.077*
C15	−0.1564 (4)	0.1118 (3)	0.8113 (4)	0.0731 (9)
H15	−0.2157	0.0290	0.8237	0.088*
C16	−0.1667 (4)	0.1559 (4)	0.6702 (4)	0.0717 (9)
H16	−0.2347	0.1030	0.5903	0.086*
C17	−0.0787 (4)	0.2758 (3)	0.6463 (3)	0.0581 (7)
H17	−0.0845	0.3037	0.5520	0.070*
C18	0.0192 (3)	0.3537 (3)	0.7677 (3)	0.0452 (6)
N1	0.1148 (3)	0.4813 (3)	0.7772 (2)	0.0509 (6)
N2	0.1247 (3)	0.4135 (3)	1.0011 (2)	0.0519 (6)

H2A	0.142 (4)	0.430 (3)	1.093 (3)	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0574 (17)	0.0615 (19)	0.0588 (18)	0.0032 (15)	0.0151 (14)	0.0005 (14)
C2	0.0534 (18)	0.077 (2)	0.088 (2)	0.0037 (16)	0.0223 (18)	−0.0165 (19)
C3	0.061 (2)	0.099 (3)	0.093 (3)	−0.012 (2)	0.0403 (19)	−0.023 (2)
C4	0.073 (2)	0.095 (3)	0.073 (2)	−0.021 (2)	0.0381 (18)	−0.0052 (19)
C5	0.0572 (18)	0.0603 (19)	0.0554 (17)	−0.0093 (14)	0.0163 (14)	0.0017 (13)
C6	0.081 (2)	0.078 (2)	0.085 (3)	−0.0061 (19)	0.024 (2)	0.0206 (19)
C7	0.089 (3)	0.059 (2)	0.117 (3)	0.019 (2)	0.021 (2)	0.019 (2)
C8	0.070 (2)	0.074 (2)	0.085 (2)	0.0127 (18)	0.0263 (18)	−0.0128 (19)
C9	0.0543 (17)	0.0585 (18)	0.0474 (15)	−0.0023 (14)	0.0160 (13)	−0.0078 (13)
C10	0.0478 (15)	0.0545 (17)	0.0416 (15)	−0.0067 (13)	0.0109 (12)	−0.0058 (12)
C11	0.0685 (19)	0.083 (2)	0.0419 (14)	−0.0090 (16)	0.0234 (13)	−0.0129 (14)
C12	0.0512 (15)	0.0670 (18)	0.0332 (14)	0.0059 (13)	0.0200 (11)	0.0005 (13)
C13	0.0496 (15)	0.0592 (17)	0.0390 (13)	0.0084 (13)	0.0201 (11)	0.0002 (12)
C14	0.078 (2)	0.063 (2)	0.0555 (17)	0.0067 (16)	0.0297 (15)	0.0087 (14)
C15	0.087 (2)	0.0592 (19)	0.080 (2)	−0.0094 (18)	0.0360 (18)	−0.0006 (17)
C16	0.078 (2)	0.071 (2)	0.066 (2)	−0.0070 (18)	0.0233 (16)	−0.0150 (18)
C17	0.0671 (18)	0.0673 (19)	0.0415 (15)	0.0035 (16)	0.0201 (14)	−0.0034 (13)
C18	0.0467 (14)	0.0549 (16)	0.0392 (14)	0.0094 (13)	0.0210 (11)	0.0011 (12)
N1	0.0556 (13)	0.0660 (15)	0.0346 (11)	0.0004 (11)	0.0196 (9)	−0.0011 (10)
N2	0.0606 (14)	0.0695 (15)	0.0291 (10)	0.0046 (12)	0.0193 (10)	0.0032 (11)

Geometric parameters (Å, °)

C1—C2	1.356 (4)	C11—C12	1.484 (4)
C1—C10	1.419 (4)	C11—H11A	0.9700
C1—H1	0.9300	C11—H11B	0.9700
C2—C3	1.379 (5)	C12—N1	1.314 (3)
C2—H2	0.9300	C12—N2	1.358 (3)
C3—C4	1.350 (5)	C13—N2	1.371 (3)
C3—H3	0.9300	C13—C14	1.383 (4)
C4—C5	1.414 (4)	C13—C18	1.394 (3)
C4—H4	0.9300	C14—C15	1.374 (4)
C5—C6	1.403 (5)	C14—H14	0.9300
C5—C10	1.409 (4)	C15—C16	1.393 (4)
C6—C7	1.344 (5)	C15—H15	0.9300
C6—H6	0.9300	C16—C17	1.375 (4)
C7—C8	1.407 (5)	C16—H16	0.9300
C7—H7	0.9300	C17—C18	1.387 (4)
C8—C9	1.361 (4)	C17—H17	0.9300
C8—H8	0.9300	C18—N1	1.394 (3)
C9—C10	1.418 (4)	N2—H2A	0.87 (3)
C9—C11	1.519 (4)		
C2—C1—C10	121.7 (3)	C12—C11—H11A	108.6

C2—C1—H1	119.2	C9—C11—H11A	108.6
C10—C1—H1	119.2	C12—C11—H11B	108.6
C1—C2—C3	120.6 (3)	C9—C11—H11B	108.6
C1—C2—H2	119.7	H11A—C11—H11B	107.6
C3—C2—H2	119.7	N1—C12—N2	112.4 (2)
C4—C3—C2	120.1 (3)	N1—C12—C11	126.7 (2)
C4—C3—H3	120.0	N2—C12—C11	120.9 (2)
C2—C3—H3	120.0	N2—C13—C14	132.4 (2)
C3—C4—C5	121.3 (3)	N2—C13—C18	105.6 (2)
C3—C4—H4	119.3	C14—C13—C18	122.0 (3)
C5—C4—H4	119.3	C15—C14—C13	117.2 (3)
C6—C5—C10	119.0 (3)	C15—C14—H14	121.4
C6—C5—C4	121.9 (3)	C13—C14—H14	121.4
C10—C5—C4	119.1 (3)	C14—C15—C16	121.3 (3)
C7—C6—C5	120.9 (3)	C14—C15—H15	119.3
C7—C6—H6	119.5	C16—C15—H15	119.3
C5—C6—H6	119.5	C17—C16—C15	121.5 (3)
C6—C7—C8	120.1 (3)	C17—C16—H16	119.3
C6—C7—H7	119.9	C15—C16—H16	119.3
C8—C7—H7	119.9	C16—C17—C18	117.7 (3)
C9—C8—C7	121.4 (3)	C16—C17—H17	121.1
C9—C8—H8	119.3	C18—C17—H17	121.1
C7—C8—H8	119.3	C17—C18—C13	120.3 (2)
C8—C9—C10	118.8 (3)	C17—C18—N1	130.5 (2)
C8—C9—C11	120.3 (3)	C13—C18—N1	109.2 (2)
C10—C9—C11	120.8 (2)	C12—N1—C18	105.4 (2)
C5—C10—C9	119.7 (2)	C12—N2—C13	107.4 (2)
C5—C10—C1	117.2 (3)	C12—N2—H2A	120.6 (18)
C9—C10—C1	123.1 (2)	C13—N2—H2A	130.8 (19)
C12—C11—C9	114.8 (2)		
C10—C1—C2—C3	−0.7 (5)	C10—C9—C11—C12	−77.1 (3)
C1—C2—C3—C4	−0.4 (5)	C9—C11—C12—N1	−0.1 (4)
C2—C3—C4—C5	1.0 (5)	C9—C11—C12—N2	−179.1 (2)
C3—C4—C5—C6	178.2 (3)	N2—C13—C14—C15	176.7 (3)
C3—C4—C5—C10	−0.4 (5)	C18—C13—C14—C15	−1.5 (4)
C10—C5—C6—C7	−2.1 (5)	C13—C14—C15—C16	0.0 (4)
C4—C5—C6—C7	179.3 (3)	C14—C15—C16—C17	1.3 (5)
C5—C6—C7—C8	0.6 (6)	C15—C16—C17—C18	−1.1 (4)
C6—C7—C8—C9	1.1 (5)	C16—C17—C18—C13	−0.3 (4)
C7—C8—C9—C10	−1.3 (4)	C16—C17—C18—N1	−176.9 (2)
C7—C8—C9—C11	177.2 (3)	N2—C13—C18—C17	−176.9 (2)
C6—C5—C10—C9	1.9 (4)	C14—C13—C18—C17	1.7 (4)
C4—C5—C10—C9	−179.5 (3)	N2—C13—C18—N1	0.3 (3)
C6—C5—C10—C1	−179.4 (3)	C14—C13—C18—N1	178.9 (2)
C4—C5—C10—C1	−0.7 (4)	N2—C12—N1—C18	1.2 (3)
C8—C9—C10—C5	−0.2 (4)	C11—C12—N1—C18	−177.8 (3)
C11—C9—C10—C5	−178.7 (2)	C17—C18—N1—C12	175.9 (3)
C8—C9—C10—C1	−178.9 (3)	C13—C18—N1—C12	−0.9 (2)
C11—C9—C10—C1	2.6 (4)	N1—C12—N2—C13	−1.1 (3)

C2—C1—C10—C5	1.3 (4)	C11—C12—N2—C13	178.1 (2)
C2—C1—C10—C9	180.0 (3)	C14—C13—N2—C12	−178.0 (3)
C8—C9—C11—C12	104.5 (3)	C18—C13—N2—C12	0.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N1^{i}	0.87 (3)	2.03 (3)	2.855 (3)	160 (3)

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

Fig. 1

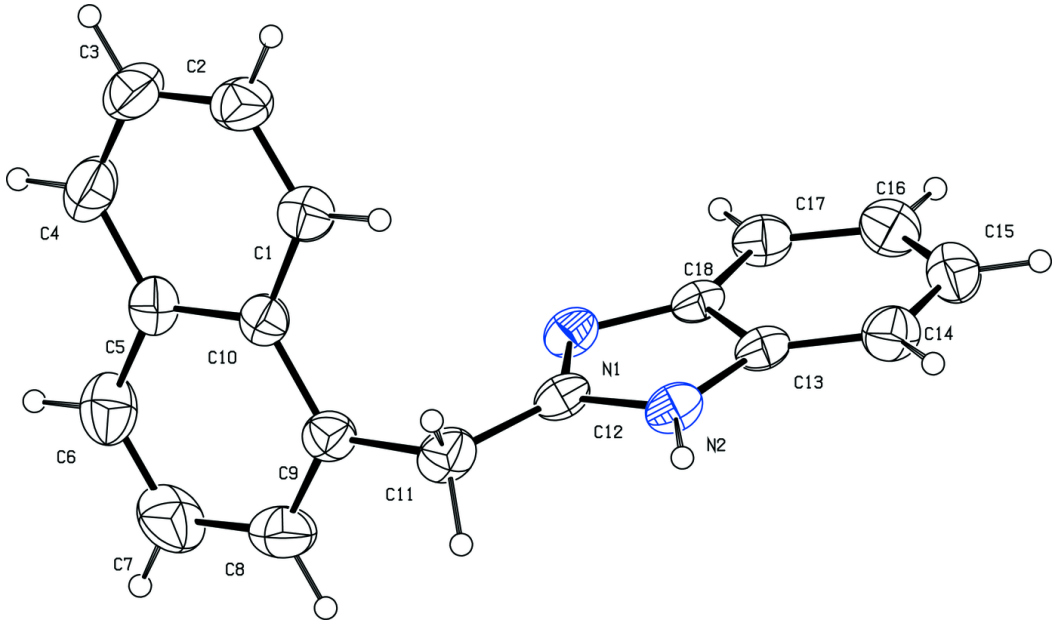

Fig. 2