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An orthorhombic polymorph of 1-benzyl-1*H*-benzimidazole

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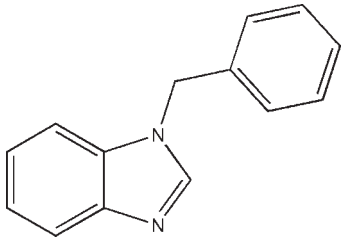
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.068; wR factor = 0.148; data-to-parameter ratio = 12.2.

The title compound, $C_{14}H_{12}N_2$, in contrast to the previously reported monoclinic polymorph [Lei *et al.* (2009). *Acta Cryst.* E**65**, o2613], crystallizes in the orthorhombic crystal system. The dihedral angle between the imidazole ring system and the phenyl ring is 76.78 (16)°. Weak C—H···N and C—H···π interactions are observed in the crystal structure.

Related literature

For the synthesis, see: Lionel *et al.* (1996). For the monoclinic polymorph, see: Lei & Zhou (2009).



Experimental

Crystal data

$C_{14}H_{12}N_2$ M_r = 208.26
Orthorhombic, $P2_12_12_1$
a = 6.124 (3) Å
b = 7.443 (4) Å
c = 23.860 (8) Å
V = 1087.6 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
3168 measured reflections
1886 independent reflections
892 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.148
S = 0.98
1886 reflections
154 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*2 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8*B*···N2^{i}	1.03 (5)	2.55 (5)	3.570 (8)	171 (4)
C12—H12···*Cg*2^{ii}	0.93	2.66	3.559 (5)	162

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, y+\frac{5}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2008); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank Hu Min of Zhengzhou University of Light Industry for the X-ray analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5418).

References

Lei, G. & Zhou, L. (2009). *Acta Cryst.* E**65**, o2613.
Lionel, R. M., Philip, J. F. D. & Gokhan, Y. (1996). *Tetrahedron,* **52**, 9877–9890
Oxford Diffraction (2008). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, o1208 [**doi:10.1107/S1600536810015114**]

An orthorhombic polymorph of 1-benzyl-1*H*-benzimidazole

Y. Zhang, X. Zhu, H. Qian, Z. Yin and C. Zhang

Comment

The title compound, 1-benzyl-1*H*-benzimidazole was first synthesized by Lionel (Lionel *et al.* 1996) using DMF as solvent.

The structure reported here is an orthorhombic form polymorph of the title compound, ($C_{14}H_{12}N_2$), which has been characterized previously in a monoclinic form (Lei & Zhou, 2009). The bond lengths and angles are closely similar to those previously described . The dihedral angle between the imidazole ring and the benzyl ring is 76.78 (16)°, indicated that those two rings are not mutually perpendicular. In the crystal structure, molecules are linked *via* weak intermolecular C—H···N interactions, forming a chain along the *b*-axis direction. The structure is further stabilized by C—H···π contacts involving both of the aromatic rings. This arrangement is similar to that observed in the monoclinic polymorph.

Experimental

The title compound was obtained by reacting benzimidazole (1.18 g, 0.01 mol) with benzyl chloride (1.25 g, 0.01 mol) and potassium carbonate (1.38 g, 0.01 mol) in acetone (50 ml). The reaction mixture was refluxed for 10 h. After removal of the solvents, the residue was dispersed in water to obtain an oil layer. Then the oil was dissolved in hot ethanol/water (2:1) and colourless blocks of (I) arose.

Refinement

The absolute sturcture of (I) is indeterminate in the present refinement. The methylene H atoms were freely refined. The other H atoms were positioned geometrically (C—H = 0.93Å) and refined as riding with *U*iso(H) = 1.2*U*eq(C).

Figures

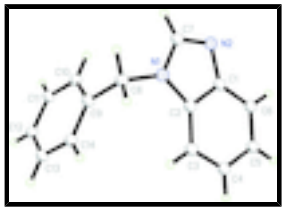


Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids.

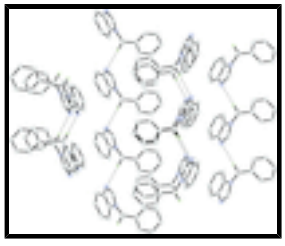


Fig. 2. The crystal packing of (I), showing the hydrogen-bonded (dashed lines) network. H atoms not involved in the hydrogen bond interactions have been omitted for clarity.

1-benzyl-1*H*-benzimidazole

Crystal data

$C_{14}H_{12}N_2$	$D_x = 1.272$ Mg m^{-3}
$M_r = 208.26$	Melting point: 387 K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 500 reflections
$a = 6.124$ (3) Å	$\theta = 3.2$–$26.2°$
$b = 7.443$ (4) Å	$\mu = 0.08$ mm^{-1}
$c = 23.860$ (8) Å	$T = 293$ K
$V = 1087.6$ (8) Å^3	Block, colorless
$Z = 4$	0.25 × 0.20 × 0.18 mm
$F(000) = 440$	

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer	$R_{int} = 0.069$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.2°$, $\theta_{min} = 3.2°$
graphite	$h = -7 \rightarrow 7$
φ and ω scans	$k = -9 \rightarrow 6$
3168 measured reflections	$l = -22 \rightarrow 29$
1886 independent reflections	1886 standard reflections every 0 min
892 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.068$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
1886 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
0 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.022 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > \sigma(F^2)$ 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}
N1	0.9512 (6)	0.9532 (5)	0.13981 (13)	0.0379 (9)
C2	0.9503 (7)	1.1255 (6)	0.16196 (16)	0.0376 (11)
C7	0.7567 (8)	0.8802 (8)	0.15157 (18)	0.0515 (13)
H7	0.7190	0.7639	0.1411	0.062*
N2	0.6248 (7)	0.9861 (7)	0.17888 (16)	0.0614 (13)
C3	1.1077 (8)	1.2581 (7)	0.16401 (18)	0.0524 (14)
H3	1.2438	1.2429	0.1474	0.063*
C10	0.9963 (8)	0.9160 (6)	0.01210 (18)	0.0463 (13)
H10	0.8689	0.8567	0.0224	0.056*
C9	1.1566 (7)	0.9393 (6)	0.05047 (16)	0.0379 (11)
C14	1.3448 (8)	1.0270 (7)	0.03496 (18)	0.0478 (13)
H14	1.4553	1.0447	0.0611	0.057*
C8	1.1293 (10)	0.8674 (8)	0.1093 (2)	0.0502 (13)
C13	1.3702 (9)	1.0881 (7)	−0.0187 (2)	0.0567 (15)
H13	1.4984	1.1465	−0.0290	0.068*
C11	1.0182 (9)	0.9782 (7)	−0.04190 (18)	0.0564 (14)
H11	0.9057	0.9624	−0.0676	0.068*
C1	0.7441 (8)	1.1405 (8)	0.18669 (18)	0.0484 (14)
C5	0.8491 (14)	1.4320 (9)	0.2169 (2)	0.0766 (19)
H5	0.8180	1.5377	0.2362	0.092*
C4	1.0542 (12)	1.4117 (8)	0.1914 (2)	0.0692 (17)
H4	1.1550	1.5049	0.1934	0.083*
C12	1.2063 (9)	1.0635 (6)	−0.05752 (19)	0.0570 (15)
H12	1.2236	1.1045	−0.0941	0.068*
C6	0.6953 (10)	1.3013 (9)	0.21424 (19)	0.0647 (17)
H6	0.5588	1.3184	0.2305	0.078*
H8B	1.274 (8)	0.887 (6)	0.1303 (18)	0.058 (15)*
H8A	1.078 (7)	0.746 (6)	0.1111 (16)	0.046 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

N1	0.037 (2)	0.043 (2)	0.0343 (18)	−0.002 (2)	0.0042 (18)	0.0001 (19)
C2	0.043 (3)	0.047 (3)	0.023 (2)	0.001 (3)	−0.011 (2)	0.000 (2)
C7	0.045 (3)	0.057 (3)	0.052 (3)	−0.010 (3)	0.000 (3)	0.009 (3)
N2	0.051 (3)	0.081 (3)	0.052 (3)	0.001 (3)	0.008 (2)	−0.001 (3)
C3	0.059 (3)	0.051 (3)	0.048 (3)	−0.005 (3)	−0.017 (3)	0.004 (3)
C10	0.051 (3)	0.046 (3)	0.042 (2)	−0.013 (3)	0.005 (3)	−0.007 (2)
C9	0.039 (3)	0.038 (3)	0.037 (2)	0.003 (3)	−0.001 (3)	−0.011 (2)
C14	0.041 (3)	0.054 (3)	0.049 (3)	−0.003 (3)	−0.002 (3)	−0.007 (3)
C8	0.053 (3)	0.052 (3)	0.045 (3)	0.007 (3)	0.004 (3)	0.005 (3)
C13	0.054 (3)	0.053 (4)	0.063 (3)	−0.007 (3)	0.022 (3)	−0.006 (3)
C11	0.064 (3)	0.061 (3)	0.044 (3)	−0.004 (3)	−0.008 (3)	−0.003 (3)
C1	0.048 (3)	0.072 (4)	0.025 (2)	0.021 (3)	0.007 (3)	0.006 (3)
C5	0.119 (6)	0.069 (4)	0.042 (3)	0.032 (5)	−0.038 (4)	−0.026 (3)
C4	0.095 (5)	0.053 (4)	0.060 (3)	0.003 (3)	−0.025 (4)	−0.006 (3)
C12	0.078 (4)	0.048 (3)	0.045 (3)	0.003 (3)	0.016 (3)	−0.003 (3)
C6	0.072 (4)	0.090 (5)	0.032 (3)	0.029 (4)	0.002 (3)	−0.010 (3)

Geometric parameters (Å, °)

N1—C7	1.339 (6)	C14—C13	1.367 (6)
N1—C2	1.387 (5)	C14—H14	0.9300
N1—C8	1.459 (6)	C8—H8B	1.03 (5)
C2—C3	1.380 (6)	C8—H8A	0.96 (5)
C2—C1	1.398 (6)	C13—C12	1.379 (6)
C7—N2	1.303 (6)	C13—H13	0.9300
C7—H7	0.9300	C11—C12	1.367 (6)
N2—C1	1.374 (6)	C11—H11	0.9300
C3—C4	1.358 (7)	C1—C6	1.398 (7)
C3—H3	0.9300	C5—C6	1.356 (8)
C10—C9	1.354 (5)	C5—C4	1.404 (8)
C10—C11	1.376 (6)	C5—H5	0.9300
C10—H10	0.9300	C4—H4	0.9300
C9—C14	1.375 (6)	C12—H12	0.9300
C9—C8	1.511 (6)	C6—H6	0.9300
C7—N1—C2	107.0 (4)	N1—C8—H8A	98 (3)
C7—N1—C8	126.3 (4)	C9—C8—H8A	114 (2)
C2—N1—C8	126.7 (4)	H8B—C8—H8A	113 (4)
C3—C2—N1	132.2 (4)	C14—C13—C12	120.1 (5)
C3—C2—C1	124.0 (5)	C14—C13—H13	119.9
N1—C2—C1	103.8 (4)	C12—C13—H13	119.9
N2—C7—N1	114.3 (5)	C12—C11—C10	119.6 (5)
N2—C7—H7	122.9	C12—C11—H11	120.2
N1—C7—H7	122.9	C10—C11—H11	120.2
C7—N2—C1	104.1 (4)	N2—C1—C6	131.7 (5)
C4—C3—C2	116.8 (5)	N2—C1—C2	110.9 (4)
C4—C3—H3	121.6	C6—C1—C2	117.4 (6)
C2—C3—H3	121.6	C6—C5—C4	121.6 (5)
C9—C10—C11	121.3 (5)	C6—C5—H5	119.2
C9—C10—H10	119.4	C4—C5—H5	119.2

C11—C10—H10	119.4	C3—C4—C5	121.1 (6)
C10—C9—C14	119.1 (4)	C3—C4—H4	119.5
C10—C9—C8	120.2 (5)	C5—C4—H4	119.5
C14—C9—C8	120.7 (4)	C11—C12—C13	119.5 (4)
C13—C14—C9	120.4 (5)	C11—C12—H12	120.3
C13—C14—H14	119.8	C13—C12—H12	120.3
C9—C14—H14	119.8	C5—C6—C1	119.2 (6)
N1—C8—C9	113.0 (4)	C5—C6—H6	120.4
N1—C8—H8B	110 (2)	C1—C6—H6	120.4
C9—C8—H8B	108 (2)		
C7—N1—C2—C3	177.5 (5)	C14—C9—C8—N1	116.5 (6)
C8—N1—C2—C3	−2.7 (7)	C9—C14—C13—C12	0.5 (8)
C7—N1—C2—C1	0.4 (4)	C9—C10—C11—C12	0.8 (7)
C8—N1—C2—C1	−179.8 (4)	C7—N2—C1—C6	−178.1 (4)
C2—N1—C7—N2	0.5 (5)	C7—N2—C1—C2	1.5 (5)
C8—N1—C7—N2	−179.2 (4)	C3—C2—C1—N2	−178.6 (4)
N1—C7—N2—C1	−1.2 (5)	N1—C2—C1—N2	−1.2 (5)
N1—C2—C3—C4	−177.3 (4)	C3—C2—C1—C6	1.1 (6)
C1—C2—C3—C4	−0.7 (7)	N1—C2—C1—C6	178.5 (4)
C11—C10—C9—C14	0.0 (7)	C2—C3—C4—C5	0.8 (7)
C11—C10—C9—C8	−179.2 (5)	C6—C5—C4—C3	−1.4 (8)
C10—C9—C14—C13	−0.6 (7)	C10—C11—C12—C13	−0.9 (7)
C8—C9—C14—C13	178.5 (5)	C14—C13—C12—C11	0.3 (7)
C7—N1—C8—C9	106.1 (5)	C4—C5—C6—C1	1.8 (8)
C2—N1—C8—C9	−73.7 (6)	N2—C1—C6—C5	178.0 (5)
C10—C9—C8—N1	−64.3 (6)	C2—C1—C6—C5	−1.6 (7)

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8B···N2^{i}	1.03 (5)	2.55 (5)	3.570 (8)	171 (4)
C12—H12···Cg2^{ii}	0.93	2.66	3.559 (5)	162

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*, *y*+5/2, −*z*+1/2.

Fig. 1

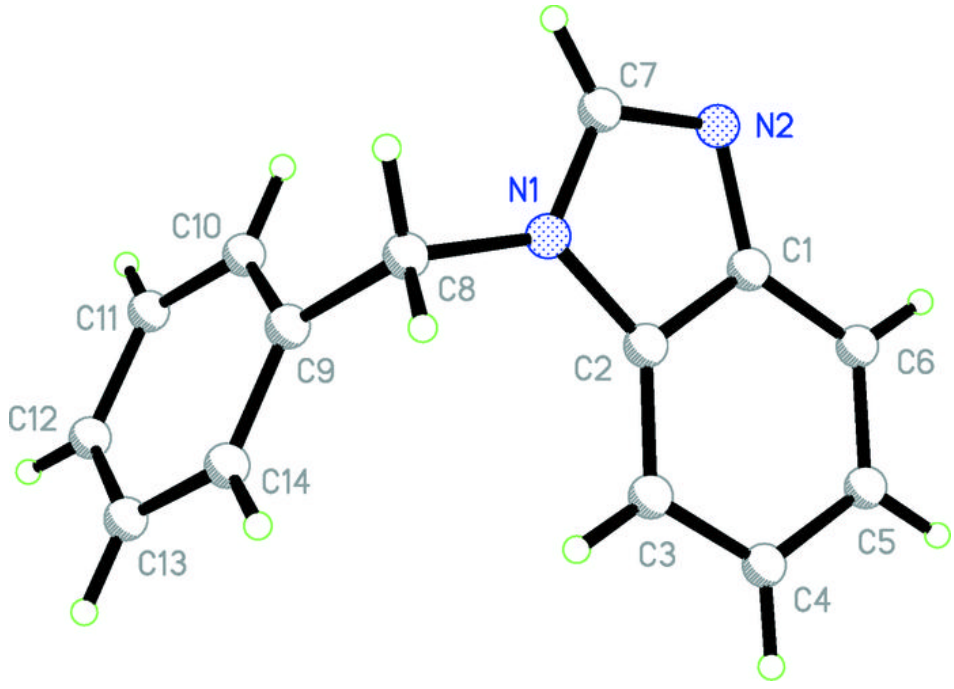


Fig. 2