organic compounds

1,3-Dibenzyl-1H-benzimidazol-2(3H)-one

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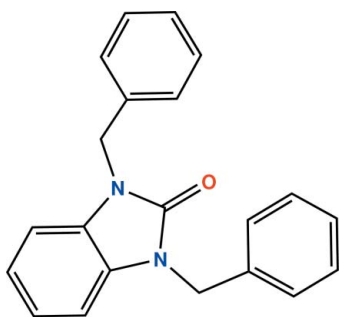Correspondence e-mail: ouazzani_chahid@yahoo.fr

In the molecular structure of the title compound, $C_{21}H_{18}N_2O$, the fused-ring system is essentially planar, the largest deviation from the mean plane being 0.0121 (9) Å. The O atom and adjacent C atom are located in Wyckoff position 4e on a twofold axis (0, y, 1/4). The two benzyl groups are almost perpendicular to the benzimidazole plane, but point in opposite directions. The dihedral angle between the benzimidazole mean plane and the phenyl ring is 81.95 (5)°, whereas that between the two benzyl groups is 60.96 (7)°.

Related literature

For pharmacological and biochemical properties of benzimidazoles, see: Gravatt *et al.* (1994); Horton *et al.* (2003); Kim *et al.* (1996); Roth *et al.* (1997). Ouzidan *et al.* (2011a,b,c).

Experimental

Crystal data

$C_{21}H_{18}N_2O$	V = 1613.98 (10) Å^3
M_r = 314.37	Z = 4
Monoclinic, $C2/c$	Cu $K\alpha$ radiation
a = 19.5983 (7) Å	μ = 0.63 mm^{-1}
b = 9.0882 (2) Å	T = 200 K
c = 10.0473 (3) Å	0.37 × 0.21 × 0.15 mm
β = 115.593 (4)°	

Data collection

Agilent SuperNova Dual Cu at zero Atlas diffractometer	(1995)]
	T_{min} = 0.950, T_{max} = 1.000
Absorption correction: multi-scan [*CrysAlis PRO* (Agilent, 2011), using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm (Clark & Reid	7837 measured reflections
	1611 independent reflections
	1397 reflections with $I > 2\sigma(I)$
	R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037	111 parameters
$wR(F^2)$ = 0.106	H-atom parameters constrained
S = 1.07	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
1611 reflections	$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *CrysAlis PRO* (Agilent, 2011); 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* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2334).

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supporting information

1,3-Dibenzyl-1*H*-benzimidazol-2(3*H*)-one

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S1. Comment

Benzimidazoles are very useful intermediates/subunits for the development of molecules of pharmaceutical or biological interest. Benzimidazole and its derivatives are an important class of bioactive molecules in the field of drugs and pharmaceuticals. Benzimidazole derivatives have found applications in diverse therapeutic areas including anti-ulcers, anti-hypertensives, anti-virals, anti-fungals, anti-cancers, (Gravatt *et al.* 1994; Horton *et al.* 2003; Kim *et al.* 1996; Roth *et al.* 1997).

As a continuation of our research work devoted to the development of substituted benzimidazol-2-one derivatives (Ouzidan *et al.*, 2011*a*, 2011*b*), we reported the synthesis of new benzimidazol-2-one derivative by action of benzyl chloride with 1*H*-benzimidazol-2(3*H*)-one in the presence of a catalytic quantity of tetra-n-butylammonium bromide under mild conditions to furnish two compounds: mono-substituted (Ouzidan *et al.*, 2011*c*) and the title compound (Scheme 1).

The title compound $C_{21}H_{18}N_2O$ is a new heterocyclic system deriving from benzimidazole. The crystal structure of this molecule is built up from two fused six and five-membered rings linked to two benzyl groups. The oxygen and the adjacent carbon atom are located in the Wyckoff position 4 e on the twofold axis (0, *y*, 1/4). The fused-ring system is essentially planar, with the maximum deviation of 0.0121 (9) Å for N1 as shown in Fig.1. The benzyl groups are almost perpendicular to the benzimidazole plane but oriented in opposite directions, with a dihedral angle of 81.95 (7). The dihedral angle between the two benzyl rings is abut 60.965 (7)°.

S2. Experimental

To a mxture of 1*H*-benzimidazol-2(3*H*)-one (0.2 g, 1.5 mmol), potassium carbonate (0.41 g, 3 mmol) and tetra-n-butyl-ammonium bromide (0.05 g, 0.15 mmol) in DMF (15 ml) was added benzyl chloride (0.34 ml, 3 mmol). Stirring was continued at room temperature for 6 h. The salt was removed by filtration and the filtrate concentrated under reduced pressure. The residue was separated by chromatography on a column of silica gel with ethyl acetate/hexane (1/2) as eluent. The compound was recrystallized from ethanol to give colourless crystals (yield: 75%).

S3. Refinement

H atoms were located in a difference map and treated as riding with C—H = 0.93 Å for all H atoms with $U_{iso}(H) = 1.2$ U_{eq} for aromatic and methylene.
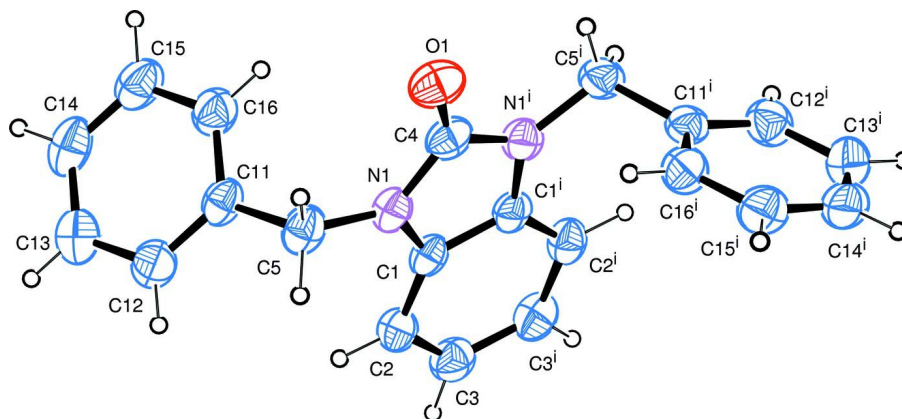
Figure 1

Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

1,3-Dibenzyl-1H-benzimidazol-2(3H)-one

Crystal data

$C_{21}H_{18}N_2O$	$F(000) = 664$
$M_r = 314.37$	$D_x = 1.294$ Mg m^{-3}
Monoclinic, $C2/c$	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Hall symbol: -C 2yc	Cell parameters from 5000 reflections
$a = 19.5983$ (7) Å	$\theta = 5$–50°
$b = 9.0882$ (2) Å	$\mu = 0.63$ mm^{-1}
$c = 10.0473$ (3) Å	$T = 200$ K
$\beta = 115.593$ (4)°	Block, colourless
$V = 1613.98$ (10) Å^3	$0.37 \times 0.21 \times 0.15$ mm
$Z = 4$	

Data collection

Agilent SuperNova Dual Cu at zero Atlas diffractometer	Absorption correction: multi-scan [*CrysAlis PRO* (Agilent, 2011), using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm (Clark & Reid (1995)]
Radiation source: SuperNova (Cu) X-ray Source	
Mirror monochromator	$T_{min} = 0.950$, $T_{max} = 1.000$
Detector resolution: 10.4051 pixels mm^{-1}	7837 measured reflections
ω scans	1611 independent reflections
	1397 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.028$
	$\theta_{max} = 73.4°$, $\theta_{min} = 5.0°$
	$h = -23 \rightarrow 18$
	$k = -11 \rightarrow 11$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	111 parameters
Least-squares matrix: full	0 restraints
$R[F^2 > 2\sigma(F^2)] = 0.037$	Primary atom site location: structure-invariant direct methods
$wR(F^2) = 0.106$	Secondary atom site location: difference Fourier map
$S = 1.07$	
1611 reflections	

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.4305P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.0010 (2)

Special details

Experimental. CrysAlisPro, Agilent Technologies, Version 1.171.35.11 (release 16-05-2011 CrysAlis171 .NET) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm (Clark & Reid (1995)).

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5000	0.58201 (13)	0.2500	0.0492 (4)
N1	0.53746 (5)	0.35600 (11)	0.19370 (10)	0.0366 (3)
C1	0.52407 (6)	0.20943 (12)	0.21516 (11)	0.0333 (3)
C2	0.54925 (7)	0.08014 (14)	0.17958 (13)	0.0390 (3)
H2	0.5835	0.0806	0.1346	0.047*
C3	0.52422 (7)	−0.05071 (14)	0.21593 (14)	0.0432 (3)
H3	0.5402	−0.1444	0.1907	0.052*
C4	0.5000	0.44731 (19)	0.2500	0.0378 (4)
C5	0.58741 (7)	0.40758 (14)	0.13068 (13)	0.0412 (3)
H5A	0.5785	0.5117	0.1088	0.049*
H5B	0.5751	0.3564	0.0384	0.049*
C11	0.67024 (7)	0.38418 (13)	0.23142 (12)	0.0376 (3)
C12	0.71696 (8)	0.30976 (15)	0.18389 (14)	0.0459 (3)
H12	0.6970	0.2694	0.0896	0.055*
C13	0.79366 (8)	0.29464 (16)	0.27566 (17)	0.0522 (4)
H13	0.8249	0.2450	0.2425	0.063*
C14	0.82333 (8)	0.35325 (17)	0.41560 (16)	0.0518 (4)
H14	0.8748	0.3445	0.4765	0.062*
C15	0.77703 (8)	0.42476 (16)	0.46569 (14)	0.0507 (4)
H15	0.7970	0.4626	0.5610	0.061*
C16	0.70099 (8)	0.44026 (15)	0.37424 (14)	0.0450 (3)
H16	0.6699	0.4888	0.4085	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0546 (8)	0.0361 (7)	0.0477 (7)	0.000	0.0136 (6)	0.000

N1	0.0302 (5)	0.0396 (6)	0.0357 (5)	−0.0023 (4)	0.0103 (4)	0.0015 (4)
C1	0.0233 (5)	0.0391 (6)	0.0293 (5)	−0.0018 (4)	0.0036 (4)	0.0003 (4)
C2	0.0295 (6)	0.0461 (7)	0.0374 (6)	0.0012 (5)	0.0107 (5)	−0.0031 (5)
C3	0.0371 (7)	0.0390 (6)	0.0469 (7)	0.0015 (5)	0.0120 (6)	−0.0036 (5)
C4	0.0329 (9)	0.0390 (9)	0.0311 (8)	0.000	0.0038 (7)	0.000
C5	0.0356 (7)	0.0493 (7)	0.0337 (6)	−0.0049 (5)	0.0101 (5)	0.0064 (5)
C11	0.0331 (6)	0.0406 (6)	0.0349 (6)	−0.0063 (5)	0.0106 (5)	0.0064 (5)
C12	0.0424 (7)	0.0531 (8)	0.0415 (6)	−0.0052 (6)	0.0174 (6)	0.0003 (6)
C13	0.0403 (8)	0.0581 (9)	0.0592 (8)	0.0011 (6)	0.0224 (7)	0.0053 (7)
C14	0.0336 (7)	0.0607 (9)	0.0511 (8)	−0.0050 (6)	0.0088 (6)	0.0129 (6)
C15	0.0412 (7)	0.0618 (9)	0.0377 (7)	−0.0089 (6)	0.0065 (6)	0.0011 (6)
C16	0.0393 (7)	0.0527 (7)	0.0397 (7)	−0.0028 (6)	0.0139 (6)	0.0000 (6)

Geometric parameters (Å, º)

O1—C4	1.224 (2)	C5—H5B	0.9700
N1—C4	1.3807 (14)	C11—C12	1.3790 (19)
N1—C1	1.3924 (15)	C11—C16	1.3910 (18)
N1—C5	1.4541 (15)	C12—C13	1.3896 (19)
C1—C2	1.3801 (17)	C12—H12	0.9300
C1—C1[i]	1.397 (2)	C13—C14	1.376 (2)
C2—C3	1.3939 (18)	C13—H13	0.9300
C2—H2	0.9576	C14—C15	1.376 (2)
C3—C3[i]	1.390 (3)	C14—H14	0.9300
C3—H3	0.9773	C15—C16	1.3790 (18)
C4—N1[i]	1.3807 (14)	C15—H15	0.9300
C5—C11	1.5118 (17)	C16—H16	0.9300
C5—H5A	0.9700		
C4—N1—C1	110.02 (10)	H5A—C5—H5B	107.8
C4—N1—C5	124.18 (11)	C12—C11—C16	118.71 (12)
C1—N1—C5	125.68 (10)	C12—C11—C5	121.24 (11)
C2—C1—N1	131.45 (11)	C16—C11—C5	120.04 (12)
C2—C1—C1[i]	121.63 (7)	C11—C12—C13	120.56 (12)
N1—C1—C1[i]	106.92 (6)	C11—C12—H12	119.7
C1—C2—C3	116.92 (12)	C13—C12—H12	119.7
C1—C2—H2	121.4	C14—C13—C12	119.89 (14)
C3—C2—H2	121.7	C14—C13—H13	120.1
C3[i]—C3—C2	121.44 (8)	C12—C13—H13	120.1
C3[i]—C3—H3	119.4	C13—C14—C15	120.15 (13)
C2—C3—H3	119.1	C13—C14—H14	119.9
O1—C4—N1[i]	126.94 (7)	C15—C14—H14	119.9
O1—C4—N1	126.94 (7)	C14—C15—C16	119.88 (13)
N1[i]—C4—N1	106.12 (14)	C14—C15—H15	120.1
N1—C5—C11	113.16 (9)	C16—C15—H15	120.1
N1—C5—H5A	108.9	C15—C16—C11	120.78 (13)
C11—C5—H5A	108.9	C15—C16—H16	119.6

| N1—C5—H5B | 108.9 | C11—C16—H16 | 119.6 |
| C11—C5—H5B | 108.9 | | |

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