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1-Benzyl-3-(2-phenethyl)benzimidazolium bromide monohydrate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.100
Data-to-parameter ratio = 16.5

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

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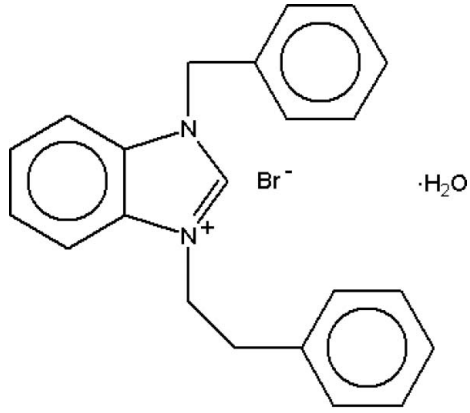
The title compound, $C_{22}H_{20}N_2^+\cdot Br^-\cdot H_2O$, was synthesized from 1-benzylbenzimidazole and 2-bromoethylbenzene in dimethylformamide. The dihedral angle between the two phenyl rings is 70.6 (1)°. These phenyl rings make dihedral angles of 52.99 (9) and 83.03 (8)° with the benzimidazole ring system. The crystal structure is stabilized by intermolecular C—H···Br and O—H···Br hydrogen-bond interactions.

Comment

Considerable attention has been given to the synthesis of benzimidazole derivatives because of their therapeutic properties in many diseases. For example, omeprazole, which contains benzimidazole and pyridine, is the best selling anti-ulcer drug nowadays (Carlsson *et al.*, 2002). The aforementioned compounds show versatile pharmacological activities, such as antibacterial, antifungal, antihelmintic, anti-allergic, antineoplastic, local analgesic, antihistaminic, vasodilative, hypotensive and spasmolytic activities (Easmon *et al.*, 2001; Güneş & Coşar, 1992; Küçükbay *et al.*, 2004). We have also synthesized and investigated the crystal structures of some benzimidazole derivatives (Akkurt *et al.*, 2004, 2005; Türktekin *et al.*, 2004; Karaca *et al.*, 2005). The object of the present study was to elucidate the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles (Table 1) are comparable with those of similar structures previously reported (Öztürk Yıldırım *et al.*, 2005, Akkurt *et al.*, 2004; Karaca *et al.*, 2005). The benzimidazole ring system is essentially planar, with a maximum deviation of 0.023 (2) Å for atom N1. The two phenyl rings, C9–C14 and C17–C22, make dihedral angles of 83.03 (8) and 52.99 (9)°, respectively, with the benzimidazole ring system.

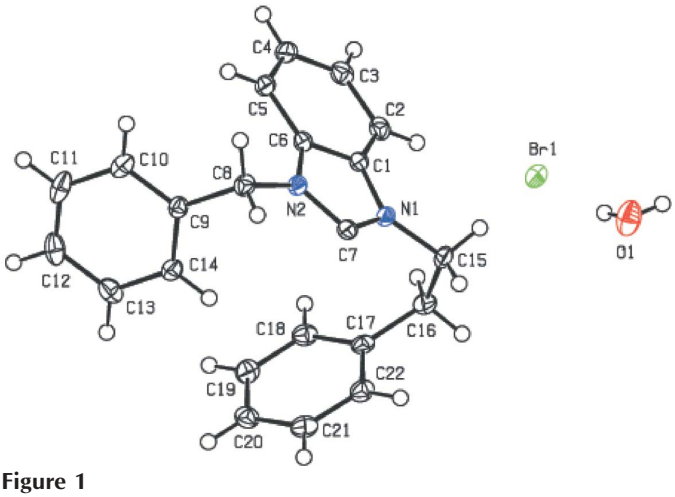


Figure 1
View of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

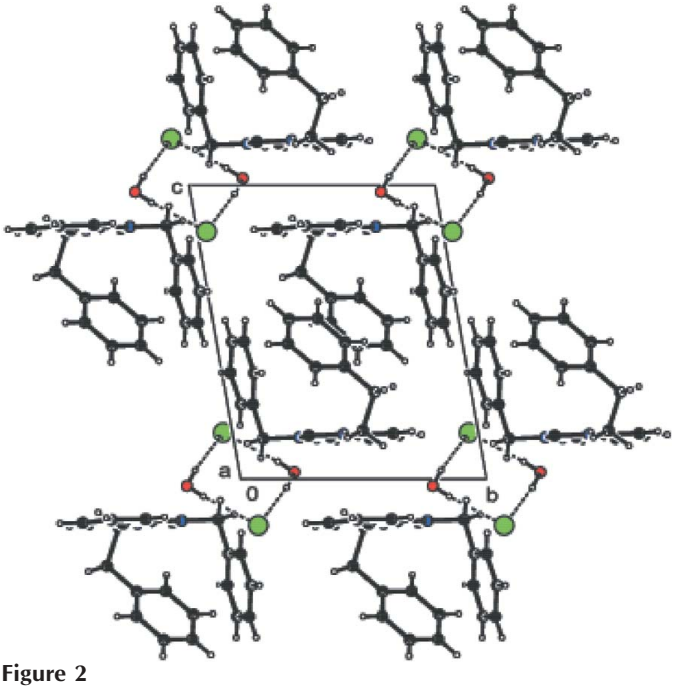


Figure 2
A view of the crystal packing along the *a* axis. Dashed lines indicate O—H···Br hydrogen bonds.

The dihedral angle between these phenyl rings is 70.6 (1)°. The crystal packing (Fig. 2) is stabilized by intermolecular C—H···Br and O—H···Br hydrogen bonds (Table 2).

Experimental

1-Benzylbenzimidazole (2.0 g, 9.62 mmol) and 2-bromoethylbenzene (1.3 ml, 9.62 mmol) in dimethylformamide (DMF, 3 ml) were heated for 3 h. All the volatiles were then removed under vacuum. The title compound was crystallized from EtOH–Et_2O (3:1 (*v*/*v*) (yield: 3.28 g, 83%; m.p. 435–436 K). ^{1}H NMR (DMSO-d_6): δ 3.29 (*t*, NCH_2CH_2Ph, 2H), 4.84 (*t*, $N—CH_2CH_2Ph$, 2H), 5.77 (*s*, CH_2Ph, 2H), 7.22–8.13 (*m*, Ar—H, 14H), 9.99 (*s*, benzimidazole-C^2—H, 1H). ^{13}C NMR (DMSO-d_6): δ 34.77, 48.50, 50.14, 114.32, 127.12, 127.17, 128.51, 129.06, 129.26, 129.41, 131.06, 131.60, 134.42, 137.27, 142.79. Analysis calculated for $C_{22}H_{23}BrN_2O$: C 64.23, H 5.59, N 6.81%; found: C 63.88, H 5.69, N 6.38%.

Crystal data

$C_{22}H_{20}N_2^+\cdot Br^-\cdot H_2O$
M_r = 410.32
Triclinic, $P\overline{1}$
a = 9.2334 (9) Å
b = 9.3684 (10) Å
c = 11.3028 (12) Å
α = 99.895 (8)°
β = 90.607 (8)°
γ = 95.637 (8)°
V = 958.14 (17) Å^3
Z = 2
D_x = 1.422 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10373 reflections
θ = 2.2–26.8°
μ = 2.16 mm^{-1}
T = 100 K
Prism, colourless
0.66 × 0.47 × 0.26 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.330, T_{max} = 0.604
10373 measured reflections
4023 independent reflections
3811 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 26.7°
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.09
4023 reflections
244 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2 + 0.4181P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.45 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.393 (3)	N2—C7	1.334 (3)
N1—C15	1.471 (3)	N2—C8	1.473 (3)
N1—C7	1.331 (3)	N2—C6	1.389 (3)
C1—N1—C7	108.76 (17)	N1—C1—C2	131.49 (18)
C7—N1—C15	124.55 (17)	N2—C6—C5	131.7 (2)
C1—N1—C15	126.54 (17)	N2—C6—C1	106.60 (16)
C6—N2—C8	126.43 (16)	N1—C7—N2	109.83 (17)
C7—N2—C8	124.91 (17)	N2—C8—C9	111.57 (16)
C6—N2—C7	108.63 (17)	N1—C15—C16	111.07 (16)
N1—C1—C6	106.16 (17)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*W*···Br1	0.84 (4)	2.54 (4)	3.373 (2)	170 (4)
O1—H2*W*···Br1^{i}	0.76 (5)	2.61 (5)	3.356 (2)	168 (5)
C2—H2···Br1	0.93	2.82	3.7431 (19)	175
C15—H15*A*···O1^{ii}	0.97	2.58	3.458 (3)	151

Symmetry codes: (i) $-x, -y, -z+2$; (ii) $-x, -y+1, -z+2$.

The water molecule H atoms were found in difference Fourier maps and refined freely. The other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.97 Å, and with U_{iso} = 1.2U_{eq}(parent atom). The highest residual peak and the deepest hole are located 0.89 and 0.90 Å, respectively, from atom Br1.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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