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Bis[2-(1*H*-benzimidazol-1-yl)ethyl] ether monohydrate

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In the approximately mirror-symmetric molecule of the title compound, $C_{18}H_{18}N_4O{\cdot}H_2O$, each benzimidazole group is essentially planar and the dihedral angle between them is 75.10 (5)°. O—H···N and C—H···O hydrogen bonds generate a centrosymmetric $R_4^4(10)$ cluster of two organic and two water molecules.

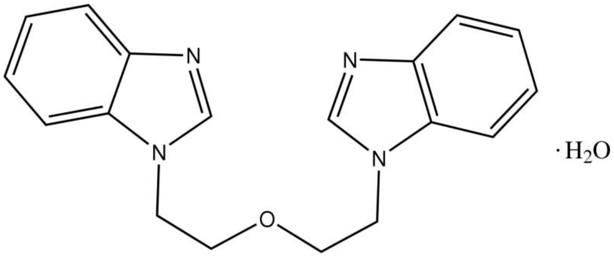
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.101
Data-to-parameter ratio = 14.8

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

Comment

In our ongoing studies of benzimidazole derivatives, the title compound, (I), was obtained from the dehydration reaction of 1*H*-benzimidazole and diglycol.



(I)

In the approximately mirror-symmetric molecule, each benzimidazole group is planar (Fig. 1), with dihedral angles of 0.13 (8) and 1.64 (8)°, respectively, between the benzene ring and its fused imidazole ring. The mean planes of these two benzimidazole systems make a dihedral angle of 75.10 (5)° with each other. All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987), and the bond lengths in the benzimidazole groups show a character intermediate between single and double bonds.

In the crystal structure, the water molecules play an important role as hydrogen-bond acceptors and donors. O—H···N and C—H···O hydrogen bonds (Table 2) link the molecules into centrosymmetric $R_4^4(10)$ clusters of two organic and two water molecules (Fig. 2).

Experimental

Diglycol (24 ml, 0.25 mol) was added dropwise to a solution of 4-methylbenzenesulfonyl chloride (100 g, 0.5 mol) in pyridine (170 ml) with stirring in an ice-water bath. After the addition was complete, the mixture was stirred at 273 K for 2 h, and then poured into cold water (600 ml) containing concentrated hydrochloric acid (170 ml). The volatiles were removed *in vacuo* to give a white solid. The solid (4.1 g, 0.01 mol) and benzimidazole (2.6 g, 0.02 mol) were refluxed in THF (45 ml) for 5 h and the solution was filtered. Single crystals suitable for X-ray diffraction study were obtained by slow evaporation of the filtrate.

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Crystal data

$C_{18}H_{18}N_4O{\cdot}H_2O$
$M_r = 324.38$
Orthorhombic, *Pbca*
$a = 18.230$ (3) Å
$b = 9.4065$ (16) Å
$c = 19.578$ (3) Å
$V = 3357.2$ (10) Å^3
$Z = 8$
$D_x = 1.284$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
$0.46 \times 0.34 \times 0.10$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.961$, $T_{\max} = 0.991$
17849 measured reflections
3319 independent reflections
2536 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 26.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.101$
$S = 1.05$
3319 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.4543P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···N4	0.90 (2)	2.10 (2)	2.962 (2)	161 (2)
O1W—H2W1···N2	0.90 (3)	2.15 (3)	3.021 (2)	165 (3)
C12—H12A···O1$W^{\rm i}$	0.93	2.44	3.352 (2)	168

Symmetry code: (i) $-x, -y + 1, -z + 1$.

After their location in a difference Fourier map, all C-bound H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å), and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The H atoms of the water molecule were located in a difference Fourier and refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

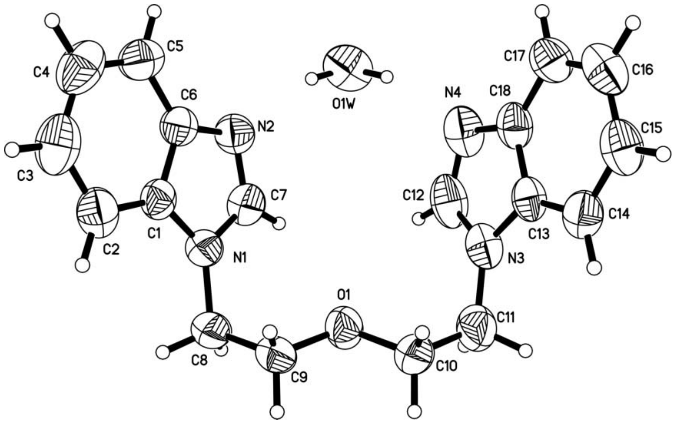

Figure 1
The molecular structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

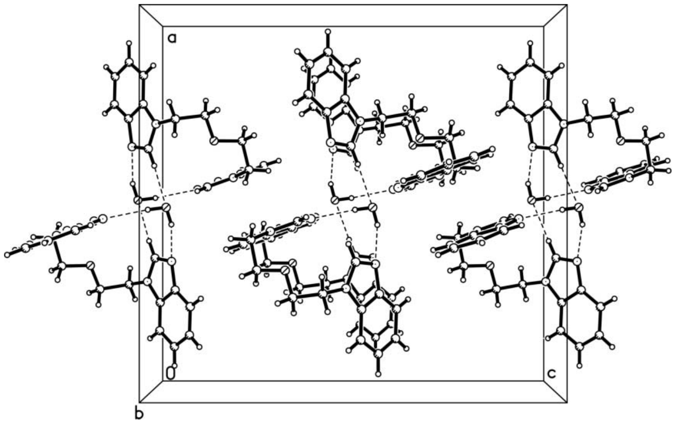

Figure 2
A partial packing diagram, showing the O—H···N and C—H···O hydrogen-bonded (dashed lines) clusters of (I).

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