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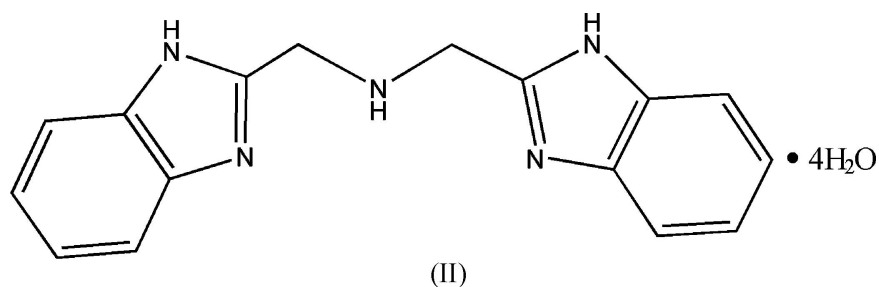
Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.008$ Å
 R factor = 0.068
 wR factor = 0.160
Data-to-parameter ratio = 8.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Bis(benzimidazol-2-ylmethyl)amine tetrahydrate

In the title compound, $\text{C}_{16}\text{H}_{15}\text{N}_5 \cdot 4\text{H}_2\text{O}$, the two independent
molecules of the asymmetric unit are linked into a three-
dimensional structure by a combination of classical hydrogen
bonds, $\text{C}-\text{H} \cdots \pi$ and aromatic $\pi-\pi$ interactions.Received 31 July 2006
Accepted 22 August 2006

Comment

We have recently reported the centrosymmetric structure of
(benzimidazol-3-ium-2-ylmethyl)(benzimidazol-2-ylmethyl)-
aminium sulfate, (I) (Meng *et al.*, 2005). In an attempt to
further study the influence of the solvent on the crystal
structure of bis(benzimidazol-2-yl-methyl)amine (IDB), we
report here the structure of the title compound, (II), crystal-
lized from an aqueous solution under hydrothermal condi-
tions.

In contrast to the related structures (I) and bis(benzimidazol-2-ylmethyl)amine, (III) (Tarazon Navarro & McKee, 2003), in which the dihedral angles between the benzimidazole

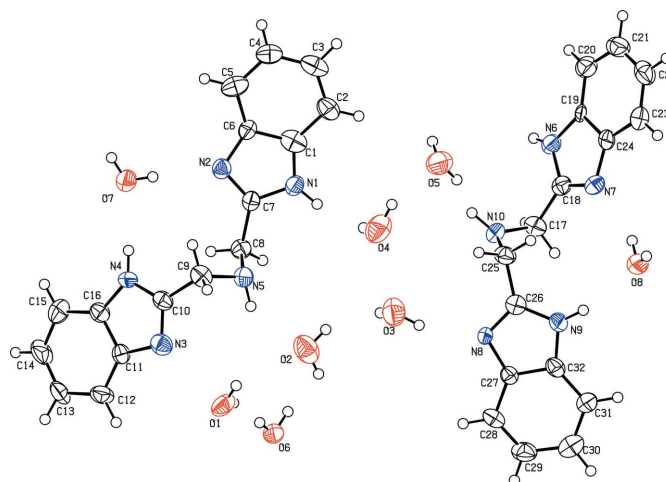


Figure 1
The asymmetric unit of (II), showing atom-labelling scheme and 50% probability displacement ellipsoids.

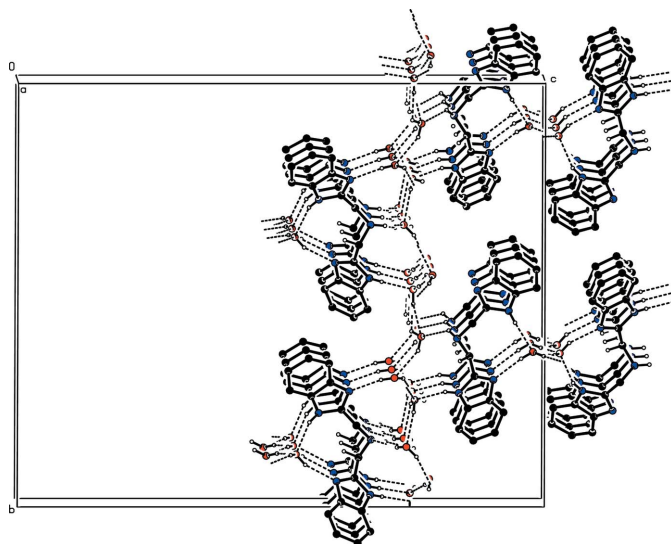


Figure 2

Plot of the packing of (II), showing O—H...O and N—H...O hydrogen bonds as dashed lines. H atoms not involved in the hydrogen-bonding scheme have been omitted for clarity.

groups are less than 5.0° , in the two independent molecules comprising the asymmetric unit of (II) (Fig. 1), the comparable dihedral angles are $36.2(1)$ and $39.8(1)^\circ$. Apart from this, the bond lengths and angles present no unexpected values between the structures.

The supramolecular structures formed by (I) and (II) are both three-dimensional, but they are different not only in their detailed construction but also in the types of direction-specific intermolecular interactions in their crystal structures. In (I), there are intramolecular N—H...O and N—H...N hydrogen bonds, as well as aromatic π - π interactions (Meng *et al.*, 2005). In contrast, the molecules in (II) are linked into a three-dimensional framework structure (Fig. 2) by a combination of N—H...O, O—H...O and C—H... π hydrogen bonds (as detailed in Table 1) and aromatic π - π interactions. The N1/C1/C6/N2/C7 and (C1—C6)ⁱ rings are almost parallel, with an interplanar spacing of approximately 3.28 \AA [symmetry code: (i) $-1 + x, y, z$]; the ring-centroid separation is $3.631(3) \text{ \AA}$.

Experimental

Bis(benzimidazol-2-yl-methyl)amine (IDB) was prepared according to the method described by Adams *et al.* (1990). IDB (0.27 g, 1 mmol) and water (10 ml) were sealed in a 25 ml stainless steel reactor with a Teflon liner. The reaction solution was heated at 393 K for 24 h. After slow cooling to room temperature, pale-yellow crystals were collected by filtration.

Crystal data

$C_{16}H_{15}N_5 \cdot 4H_2O$
 $M_r = 349.39$
 Orthorhombic, *Pbc*₂
 $a = 4.7111(6) \text{ \AA}$
 $b = 24.857(3) \text{ \AA}$
 $c = 30.823(4) \text{ \AA}$
 $V = 3609.5(8) \text{ \AA}^3$

$Z = 8$
 $D_x = 1.286 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 292(2) \text{ K}$
 Block, yellow
 $0.40 \times 0.20 \times 0.06 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2001)
 $T_{\min} = 0.963, T_{\max} = 0.994$

25072 measured reflections
 3608 independent reflections
 3171 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.160$
 $S = 1.17$
 3608 reflections
 451 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 1.7967P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.005$
 $\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

Cg1 is the centroid of the N1/C1/C6/N2/C7 ring and Cg2 is the centroid of the N6/C18/N7/C24/C19 ring.

D—H...A	D—H	H...A	D...A	D—H...A
O1—H1B...O6	0.82	2.10	2.789 (7)	142
O2—H2A...O6	0.83	2.49	2.795 (7)	103
O2—H2B...O3	0.83	2.18	2.895 (7)	145
O3—H3B...N8	0.83	2.00	2.782 (7)	157
O4—H4A...O5	0.83	2.16	2.788 (8)	133
O4—H4B...N1	0.82	2.24	2.823 (7)	128
O5—H5B...N10	0.83	2.04	2.853 (6)	169
O6—H6A...O2	0.82	2.01	2.795 (7)	159
O6—H6B...O1	0.82	1.97	2.789 (7)	176
O7—H7B...N2	0.82	2.01	2.828 (6)	173
O8—H8C...N7	0.82	2.09	2.858 (6)	155
N1—H1...O4	0.86	1.98	2.823 (7)	166
N4—H4C...O7	0.86	2.09	2.939 (6)	171
N5—H5A...O2	0.93	2.57	3.387 (7)	148
N6—H6...O6 ⁱ	0.86	2.02	2.875 (6)	175
N9—H9...O8	0.86	2.12	2.913 (6)	153
N10—H10...O5	0.84	2.40	2.853 (6)	114
O1—H1A...O6 ⁱⁱ	0.83	2.01	2.823 (6)	169
O3—H3A...O4 ⁱⁱⁱ	0.82	2.09	2.807 (7)	145
O5—H5C...O1 ^{iv}	0.83	2.11	2.877 (7)	155
O7—H7A...O8 ^v	0.83	2.09	2.903 (6)	168
O8—H8D...O7 ^{vi}	0.82	2.10	2.886 (6)	160
C8—H8B...Cg1 ⁱⁱⁱ	0.97	2.85	3.545 (1)	129
C17—H17A...Cg2 ⁱⁱⁱ	0.97	2.95	3.612 (1)	127

Symmetry codes: (i) $-x, y + \frac{1}{2}, z$; (ii) $x + 1, y, z$; (iii) $x - 1, y, z$; (iv) $-x + 1, y + \frac{1}{2}, z$; (v) $x + 1, -y + \frac{3}{2}, z + \frac{1}{2}$; (vi) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

The C-bound H atoms were included in the riding-model approximation, with C—H = 0.93 – 0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The remaining H atoms were located in difference maps and their positions were fixed at their indicated separations, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ or $1.5U_{\text{eq}}(\text{O})$. In the absence of significant anomalous scattering effects, 3457 Friedel pairs were averaged in the final refinement.

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

This work was supported by the Key Fundamental Project (No. 2002CCA00500) and the National Natural Science Foundation of China (Nos. 29971012 and 29972014).

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