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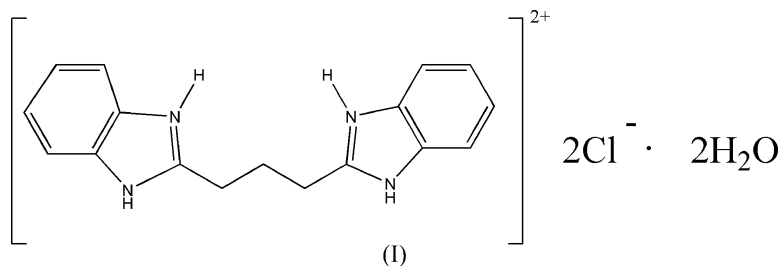
Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(C-C) = 0.004$ Å
 R factor = 0.053
 wR factor = 0.134
Data-to-parameter ratio = 17.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2,2'-(Propane-1,3-diyl)bis(benzimidazolium)
dichloride dihydrateIn the title compound, $C_{17}H_{18}N_4^{2+} \cdot 2Cl^- \cdot 2H_2O$, anions, cations and water molecules are linked into a two-dimensional framework by a combination of intermolecular $N-H \cdots O$, $N-H \cdots Cl$ and $O-H \cdots Cl$ hydrogen bonds.

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Comment

Interest in bis(2-benzimidazolyl)alkanes is widespread, due to their wide-ranging antiviral activity (Roderick, *et al.*, 1972; Salunke *et al.*, 1994). We report here the crystal structure of such a compound, (I). The asymmetric unit of (I) is shown in Fig. 1. It contains one H_2dbz [dbz = 1,3-bis(2-benzimidazolyl)propane] cation, two chloride anions and two solvent water molecules. In (I), the two imine N atoms of the dbz cation are protonated, unlike in a previously reported structure (Sun *et al.*, 2004). All the bond lengths and angles in the organic cation are normal (Allen *et al.*, 1987).In the crystal structure, anions, cations and water molecules are linked into a two-dimensional layer structure parallel to the *ac* plane by a combination of intermolecular $N-H \cdots O$, $N-H \cdots Cl$, $N-H \cdots Cl$ and $O-H \cdots Cl$ hydrogen bonds (Fig. 2 and Table 1). There are also significant $\pi-\pi$ stacking interactions involving four different rings; $Cg1$, $Cg2$, $Cg3$ and $Cg4$ are the centroids of the ring atoms $N1/C12/C17/N2/C11$, $N3/C1/C6/N4/C7$, $C1-C6$, and $C12-C17$, respectively. The relevant centroid-centroid and perpendicular distances defining these interactions are 3.6231 (13) and 3.451 Å for $Cg1 \cdots Cg2^i$ [symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$], 3.5990 (13) and 3.450 Å for $Cg1 \cdots Cg3^i$, and 3.8079 (15) and 3.506 Å for $Cg1 \cdots Cg4^{ii}$ [symmetry code: (ii) $x, \frac{1}{2} - y, -\frac{1}{2} + z$].

Experimental

1,3-Bis(2-benzimidazolyl)propane (dbz) was prepared according to a literature method (van Albada *et al.*, 1995; Wang & Joullié, 1957). Dbz (0.27 g, 1 mmol) was then added to a mixture of CH_3OH (30 ml) and H_2O (5 ml). The solution was adjusted to $pH = 1$ (using concentrated HCl) and then stirred for 30 min at room temperature. The pale-yellow solution was allowed to stand at room temperature and

red crystals suitable for X-ray diffraction were obtained over a period of about one week.

Crystal data

$C_{17}H_{18}N_4^{2+} \cdot 2Cl^- \cdot 2H_2O$
 $M_r = 385.29$
 Monoclinic, $P2_1/c$
 $a = 9.6420$ (8) Å
 $b = 13.6336$ (11) Å
 $c = 16.9921$ (10) Å
 $\beta = 123.729$ (3)°
 $V = 1857.7$ (2) Å³

$Z = 4$
 $D_x = 1.378$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.37$ mm⁻¹
 $T = 298$ (2) K
 Block, red
 $0.35 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART CCD diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2001)
 $T_{min} = 0.882$, $T_{max} = 0.930$

13103 measured reflections
 4242 independent reflections
 3203 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.033$
 $\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.134$
 $S = 1.05$
 4242 reflections
 250 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.3667P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.30$ e Å⁻³
 $\Delta\rho_{min} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1A \cdots Cl1^i$	0.851 (12)	2.295 (13)	3.0971 (18)	157 (2)
$N2-H2A \cdots O2^{ii}$	0.86 (3)	1.885 (12)	2.726 (3)	167 (2)
$N3-H3A \cdots Cl1$	0.86 (3)	2.308 (13)	3.1349 (19)	160 (2)
$N4-H4A \cdots O1$	0.86 (3)	1.86 (3)	2.703 (2)	164 (3)
$O1-H1C \cdots Cl1^i$	0.82 (3)	2.29 (3)	3.1055 (18)	176 (3)
$O1-H1B \cdots Cl2$	0.82 (3)	2.305 (11)	3.1253 (19)	174 (3)
$O2-H2B \cdots Cl1^{iii}$	0.81 (3)	2.34 (3)	3.142 (2)	170 (4)
$O2-H2C \cdots Cl2$	0.82 (4)	2.35 (4)	3.159 (2)	172 (3)

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

H atoms bonded to O and N atoms were located in difference maps and then included in the refinement with bond-length restraints of $O-H = 0.82$ (1) Å and $N-H = 0.86$ (1) Å, with $U_{iso}(H) = 1.5U_{eq}(N,O)$. H atoms bonded to C atoms were placed in calculated positions and included in the riding-model approximation, with $C-H = 0.93-0.97$ Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL.

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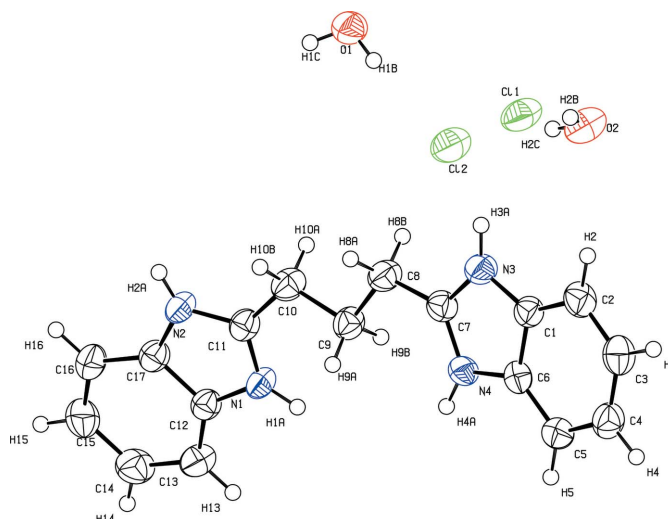


Figure 1

The asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level.

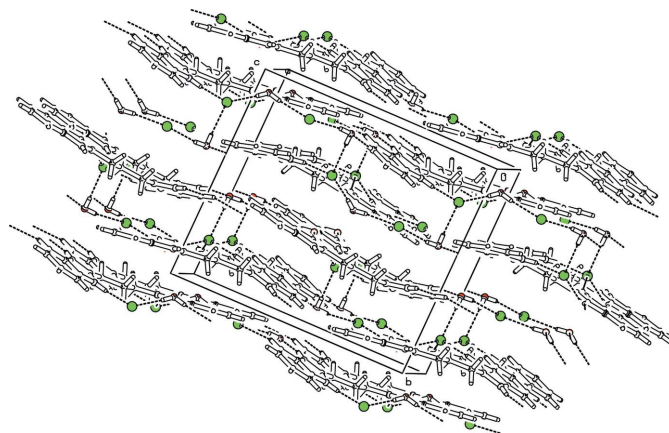


Figure 2

Part of the crystal structure of (I), showing the hydrogen bonds as dashed lines.

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