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(Chloromethyl)triethylammonium chloride monohydrate

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The title compound, $C_7H_{17}ClN^+\cdot Cl^-\cdot H_2O$, is composed of discrete (chloromethyl)triethylammonium cations, Cl^- anions and water molecules, which are held together by O—H···Cl hydrogen bonds.

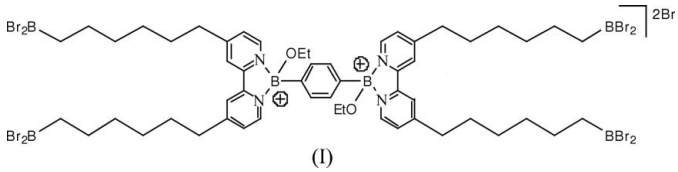
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.112
Data-to-parameter ratio = 27.6

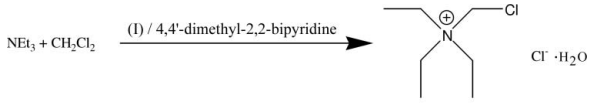
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Treatment of a solution of the diboronium, (I) (Haberecht, 2006), and 4,4′-dimethyl-2,2′-bipyridine in CH_2Cl_2 with NEt_3 led to the formation of the title compound, (II), $(Et_3NCH_2Cl)^+(Cl)^-\cdot H_2O$.



(I)



(II)

Compound (II) consists of discrete (chloromethyl)triethylammonium cations, Cl^- anions and water molecules. Geometric parameters adopt normal values (Cambridge Structural Database, Version 5.27, updated May 2006; *MOGUL* Version 1.1; Allen, 2002). Two water molecules and two Cl^- anions form a hydrogen-bonded eight-membered centrosymmetric ring (Fig. 2). In addition to these classical hydrogen bonds, there are also intramolecular C—H···Cl contacts, as well as intermolecular C—H···O, O—H···Cl and C—H···Cl contacts (Table 1).

Experimental

To a solution of diboronium dibromide, (I) (1 mmol), and 4,4′-dimethyl-2,2′-bipyridine (0.7 g, 4 mmol) in CH_2Cl_2 (40 ml), NEt_3 (1.5 ml) was added. $(Et_3NCH_2Cl)^+(Cl)^-\cdot H_2O$ was obtained as a side-product. X-ray quality crystals of the title compound were grown from a solution in CH_2Cl_2 at ambient temperature.

Crystal data

$C_7H_{17}ClN^+\cdot Cl^-\cdot H_2O$
M_r = 204.13
Monoclinic, $P2_1/n$
a = 11.1642 (8) Å
b = 7.9798 (4) Å
c = 12.3239 (9) Å
β = 106.087 (6)°
V = 1054.92 (12) Å^3
Z = 4
D_x = 1.285 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 100 (2) K
Block, colourless
0.50 × 0.40 × 0.30 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.764, T_{max} = 0.848
26921 measured reflections
2977 independent reflections
2664 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 29.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.112
S = 1.06
2977 reflections
108 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2 + 0.5992P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1D···Cl1	0.83 (1)	2.49 (1)	3.3051 (13)	170 (3)
O1—H1C···Cl1^{i}	0.83 (1)	2.34 (1)	3.1660 (13)	172 (3)
C7—H7A···O1	0.99	2.36	3.3131 (19)	161
C7—H7B···O1^{ii}	0.99	2.57	3.429 (2)	145
C1—H1A···Cl1^{iii}	0.99	2.75	3.6809 (15)	156
C1—H1B···Cl1^{iv}	0.99	2.76	3.7471 (15)	176
C3—H3A···Cl7	0.99	2.72	3.1677 (15)	108
C5—H5B···Cl7	0.99	2.75	3.0704 (18)	100

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

H atoms bonded to C atoms were located in a difference map but were subsequently refined with fixed individual isotropic displacement parameters [U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(C_{methyl})] using a riding model, with C—H = 0.98 and 0.99 Å for methyl and methylene groups, respectively. The water H atoms were refined with a distance restraint of O—H = 0.84 (1) Å.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

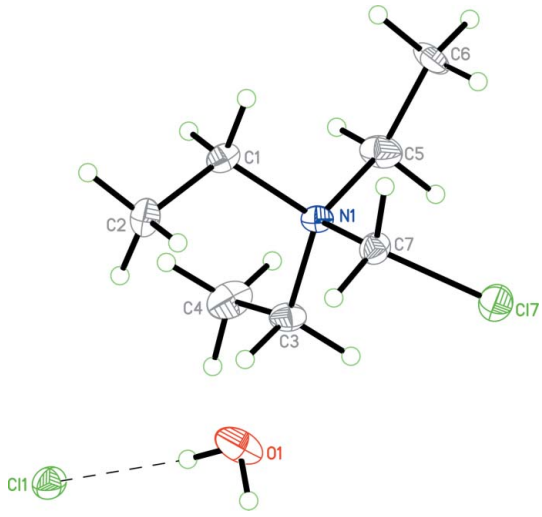


Figure 1
A perspective view of the asymmetric unit of (II), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

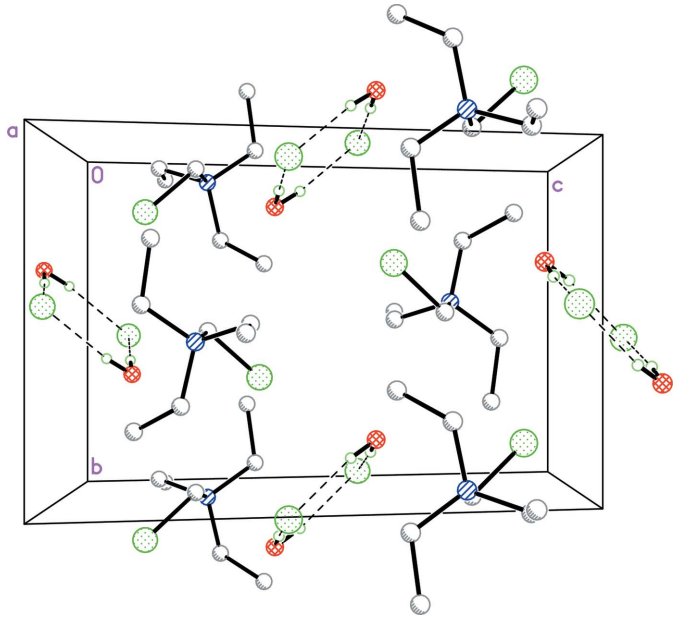


Figure 2
A packing diagram for (II), viewed along the *a* axis. H atoms bonded to C atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds.

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