(2-Hydroxyethyl)hydrazinium(2+) dichloride

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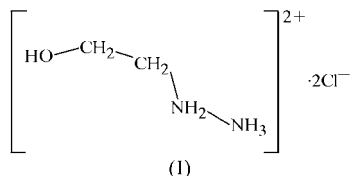The crystal structure of the title compound, $C_2H_{10}N_2O^{2+}\cdot 2Cl^-$, is built up from one 2-hydroxyethylhydrazinium(2+) cation and two Cl^- anions. The molecular structure is stabilized by $O-H\cdots Cl$ and $N-H\cdots Cl$ hydrogen bonds. The crystal structure is stabilized by one $N-H\cdots O$ and three $N-H\cdots Cl$ interactions, and the three-dimensional network of hydrogen bonds stabilizes the crystal packing. All five hydrazinium H atoms are involved in hydrogen bonds to Cl^- anions. The $Cl\cdots H$ contact distances range from 2.122 (15) to 2.809 (14) Å.

Comment

Hydrogen bonding plays a key role in molecular recognition and the engineering of organic solids (Desiraju, 1989; Melendez & Hamilton, 1998). The design of highly specific solid-state compounds is of considerable significance in organic chemistry, due to the important applications of these compounds in the development of new optical, magnetic and electronic systems (Lehn, 1992).


(I)

The structure of the title compound, (I), is presented in Fig. 1, and selected bond distances and angles are given in Table 1. The asymmetric unit contains one protonated 2-hydroxyethylhydrazinium(2+) cation and two Cl^- counter-anions. Atoms N1 and N2 exhibit approximately ideal tetrahedral geometry, with average angles of 109.45 (13) and 109.48 (13)°, respectively.

Hydrogen bonds are abundant in this structure, as might be expected from the structural formula and the liability of amino

groups to act as donors. In fact, five different $N-H\cdots Cl$ bonds are found, with $H\cdots Cl$ distances ranging from 2.122 (15) to 2.809 (14) Å. The shortest, *viz.* $N2-H42\cdots Cl2$ [2.122 (15) Å], has a nearly linear contact angle [171.1 (13)°]. According to Balmer *et al.* (2001), this bond is the strongest among those found for $N-H\cdots Cl$ contacts. Table 2 gives details of the hydrogen-bond geometry of (I). The H atoms on N1 and N2, with the exception of H31, have only one hydrogen bond, while atom H31 forms a three-centre inter-action with two Cl atoms. Our investigation shows that the 2-hydroxyethylhydrazinium cation is linked to the two Cl^- anions through $O1-H1\cdots Cl1$ [$O1\cdots Cl1 = 3.0874$ (7) Å] and $N1-H31\cdots Cl1$ [$N1\cdots Cl1 = 3.4104$ (8) Å] hydrogen bonds, resulting in the formation of cyclic seven-membered hydrogen-bonded rings, and an $N2-H41\cdots Cl2$ [$N2\cdots Cl2 = 3.0701$ (8) Å] hydrogen bond (Fig. 1).

The 2-hydroxyethylhydrazinium(2+) dichloride units are arranged in such a way as to form a two-dimensional network *via* $O-H\cdots Cl$ and $N-H\cdots Cl$ interactions, which develop parallel to the *bc* plane. There is also another $N-H\cdots Cl$ interaction, which connects two symmetry-related planar networks (Fig. 2). The $N1-H31\cdots O1$ interaction builds an approximately zigzag chain, which develops parallel to the *c* axis (Fig. 3). Importantly, the $N1-H32\cdots Cl1$ and $N2-$
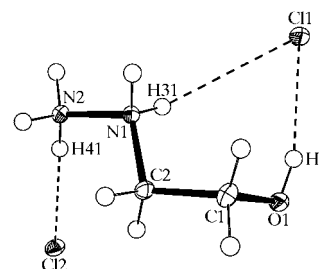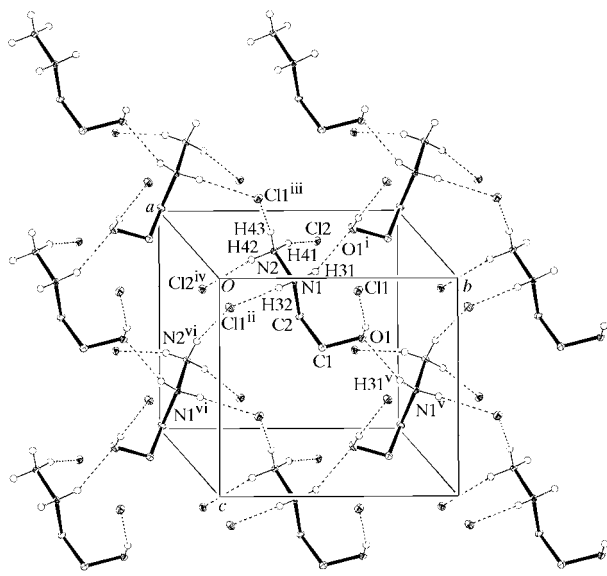

Figure 1
A view of the ionic components of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.
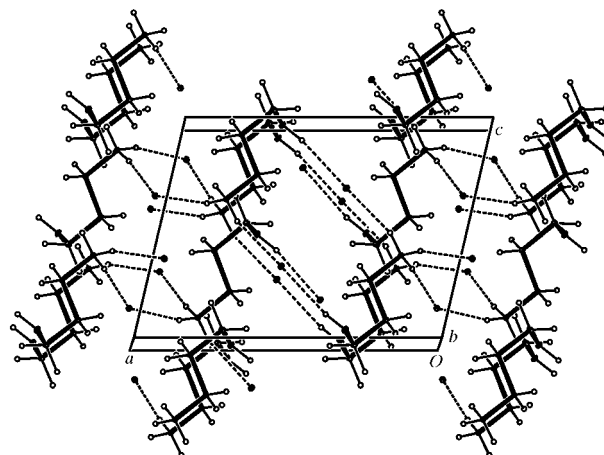
Figure 2
A packing diagram for (I), with hydrogen bonds indicated by dashed lines.

organic compounds
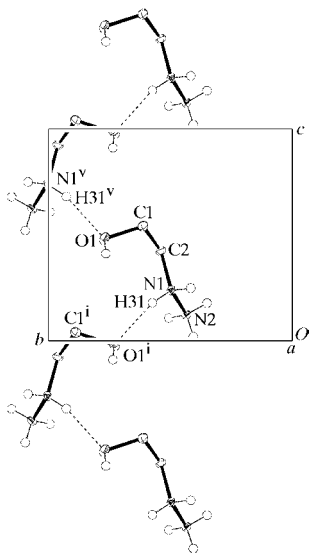
Figure 3
The zigzag chain parallel to the *c* axis built up by N—H···O interactions. Cl atoms have been omitted for clarity. [Symmetry codes: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (v) $x, \frac{3}{2} - y, \frac{1}{2} + z$.]

Figure 4
The two-dimensional network, including the rings built up by N—H···Cl and N—H···O interactions. [Symmetry codes: (i) $x, \frac{3}{2} - y, z - \frac{1}{2}$; (ii) $1 - x, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $1 - x, 1 - y, -z$; (iv) $2 - x, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $x, \frac{3}{2} - y, \frac{1}{2} + z$; (vi) $x, \frac{1}{2} - y, \frac{1}{2} + z$.]

H43···Cl1 interactions link symmetry-related zigzag-like chains to build up a two-dimensional network as a layer, which includes $R_6^6(20)$ rings (Bernstein *et al.*, 1995) and develops parallel to the *bc* plane (Fig. 4).

Experimental

HCl (aqueous, 37% *w/w*, 0.93 ml, 30 mmol) was added dropwise to 2-hydroxyethylhydrazine (1.01 ml, 15 mmol) in ether (20 ml) and the resulting solution was stirred for 15 min at 293 K. Colourless single crystals of (I) were obtained by slow evaporation of the solvent and these crystals were dried in air (m.p. 406–408 K).

Crystal data

$C_2H_{10}N_2O^{2+} \cdot 2Cl^-$	$D_x = 1.571$ Mg m^{-3}
$M_r = 149.02$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 11 440
$a = 10.2367$ (9) Å	reflections
$b = 8.4158$ (6) Å	$\theta = 2.8–29.4°$
$c = 7.5111$ (7) Å	$\mu = 0.93$ mm^{-1}
$\beta = 103.208$ (7)°	$T = 150$ (2) K
$V = 629.96$ (9) Å^3	Block, colourless
$Z = 4$	$0.54 \times 0.50 \times 0.43$ mm

Data collection

Stoe IPDS-II diffractometer	1625 reflections with $I > 2\sigma(I)$
Rotation method scans	$R_{int} = 0.077$
Absorption correction: integration	$\theta_{max} = 29.1°$
(*X-RED32*; Stoe & Cie, 2002)	$h = -13 \rightarrow 13$
$T_{min} = 0.680$, $T_{max} = 0.735$	$k = -11 \rightarrow 11$
11 440 measured reflections	$l = -10 \rightarrow 10$
1678 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0248P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.019$	$+ 0.1595P]$
$wR(F^2) = 0.050$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{max} = 0.001$
1678 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
104 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.429 (2)	N1—N2	1.449 (2)
C2—N1	1.502 (2)		
O1—C1—C2	111.20 (7)	N2—N1—C2	110.86 (6)
N1—C2—C1	110.94 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Cl1	0.83 (2)	2.28 (2)	3.0874 (7)	164 (2)
N1—H31···O1^i	0.86 (2)	1.99 (1)	2.7257 (10)	144 (1)
N1—H31···Cl1	0.86 (2)	2.81 (1)	3.4104 (8)	129 (1)
N1—H32···Cl1^{ii}	0.94 (2)	2.19 (2)	3.0832 (8)	161 (1)
N2—H43···Cl1^{iii}	0.87 (1)	2.25 (2)	3.0864 (8)	162 (1)
N2—H41···Cl2	0.88 (2)	2.21 (2)	3.0701 (8)	164 (1)
N2—H42···Cl2^{iv}	0.90 (2)	2.12 (2)	3.0098 (8)	171 (1)

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

All H atoms were located in a difference map and were refined isotropically, with N—H = 0.86 (2)–0.94 (2) Å, O—H = 0.83 (2) Å and C—H = 0.94 (2)–0.98 (2) Å, and with $U_{iso}(H)$ values in the range 0.015 (3)–0.030 (4) Å^2.

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, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997), *CAMERON* (Watkin *et al.*, 1993) and *PLUTON* (Spek, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DN1076). Services for accessing these data are described at the back of the journal.

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