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trans-1-Hydroxycyclopentan-2-aminium chloride

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Key indicators

Single-crystal X-ray study
T = 103 K
Mean σ(C–C) = 0.001 Å
R factor = 0.031
wR factor = 0.079
Data-to-parameter ratio = 46.4

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

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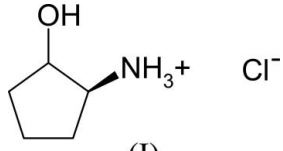
The crystal structure of the title compound, $C_5H_{12}NO^+\cdot Cl^-$, is stabilized by ionic, hydrogen-bonding and hydrophobic interactions. The cyclopentane ring of the *trans*-1-hydroxycyclopentan-2-aminium cation has a twist conformation, with both substituent groups in equatorial positions.

Comment

trans-2-Aminocyclopentanol, of which the hydrochloride structure, (I), is reported (Fig. 1), is used in the synthesis of Amaryllidaceae alkaloids (Overman *et al.*, 1983; Overman & Sugai, 1985). In the November 2006 release of the Cambridge Structural Database (Allen, 2002; Version number 5.28), there are 96 structures which contain a cyclopentane ring that does not participate in multi-ring cyclic systems, and which have three or more unsubstituted C atoms. Among them, only 19 have amino or hydroxyl groups as substituents. For these compounds, the C—O bond lengths range from 1.409 to 1.472 Å [with an average value of 1.429 (5) Å] and the C—N bond lengths range from 1.479 to 1.540 Å [with an average value of 1.509 (9) Å]. The corresponding values for (I) are close to the averages, being 1.422 (1) Å for C1—O1 and 1.489 (1) Å for C2—N1.



(I)

In the crystal structure of the title compound, *trans*-1-hydroxycyclopentan-2-aminium cations form dimers through

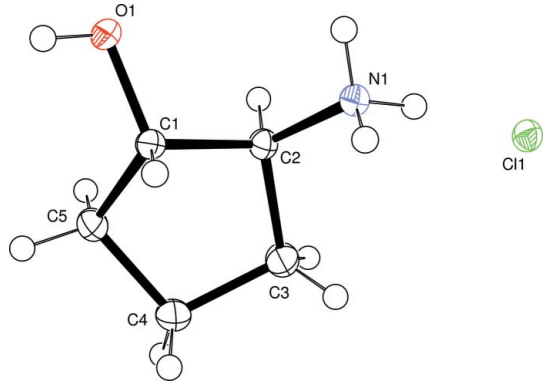


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius.

hydrogen bonds (Table 1 and Fig. 2). The cations forming dimers are related by an inversion center ($-x+1$, $-y$, $-z+1$). Four dimers surround a pair of Cl^- ions, being 3.925 (1) Å apart and related by the inversion center ($-x+1$, $-y+1$, $-z+1$). Each Cl^- ion is an acceptor for four hydrogen bonds. Atom H2*N* is involved in bifurcated hydrogen bonds. The crystal packing is stabilized not only by ionic and hydrogen-bonding interactions, but also by hydrophobic interactions between cyclopentane rings. The cyclopentane rings of (I) have a twist conformation (Cremer & Pople, 1975), with the hydroxyl and the amino groups in equatorial positions.

Experimental

The title compound was purchased from Aldrich and crystallized from ethanol by slow evaporation at 293 K.

Crystal data

$C_5H_{12}NO^+\cdot Cl^-$
M_r = 137.61
Monoclinic, $P2_1/c$
a = 10.130 (1) Å
b = 8.736 (1) Å
c = 7.657 (1) Å
β = 98.68 (1)°
V = 669.86 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 103 (2) K
0.45 × 0.2 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (Otwinowski *et al.*, 2003)
T_{min} = 0.89, T_{max} = 0.96
40913 measured reflections
5611 independent reflections
4628 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
S = 0.90
5611 reflections
121 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···Cl1^{i}	0.87 (1)	2.32 (1)	3.191 (1)	176 (1)
N1—H2*N*···O1^{ii}	0.88 (1)	2.35 (1)	2.922 (1)	123 (1)
N1—H2*N*···Cl1^{iii}	0.88 (1)	2.64 (1)	3.317 (1)	135 (1)
N1—H3*N*···Cl1	0.89 (1)	2.29 (1)	3.162 (1)	165 (1)
O1—H1*O*···Cl1^{iv}	0.81 (1)	2.36 (1)	3.162 (1)	167 (1)

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

H atoms were located in a difference map and all their parameters were refined.

Data collection: *HKL-2000* (Otwinowski & Minor, 1997); cell refinement: *HKL-2000*; data reduction: *HKL-2000*; program(s) used to solve structure: *HKL-3000SM* (Minor *et al.*, 2006) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *HKL-3000SM* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *HKL-3000SM*, *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3* (Farrugia, 1997) and Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: *HKL-3000SM*.

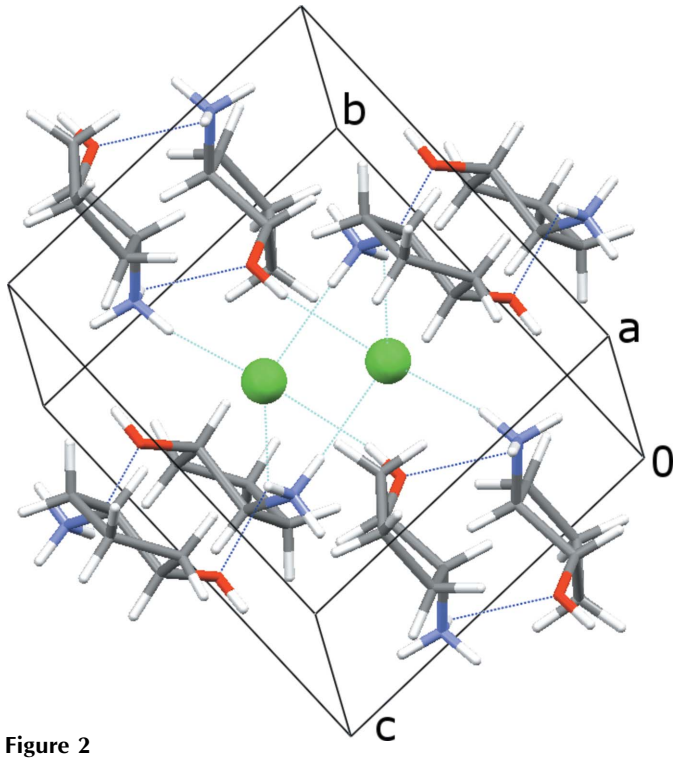


Figure 2
The packing of (I). The chloride ions are shown as green spheres. The hydrogen bonds with Cl atoms as acceptors are colored light blue. The hydrogen bonds within the dimers are colored navy blue.

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