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## Structure Reports

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**(*tert*-Butyl)(2-hydroxyethyl)ammonium chloride****Cintya Valerio-Cárdenas,\* Simón Hernández-Ortega and David Morales-Morales**Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Coyoacán, México, DF 04510, Mexico  
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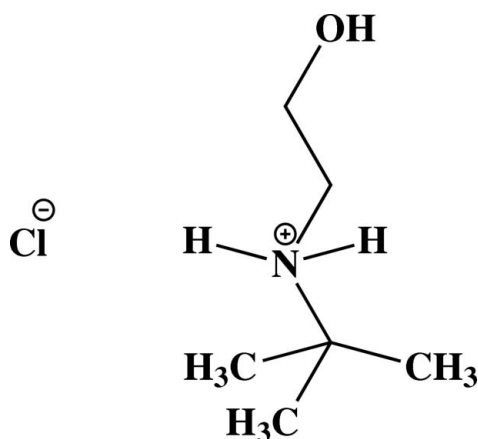
Received 18 February 2014; accepted 2 June 2014

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.046;  $wR$  factor = 0.124; data-to-parameter ratio = 17.7.

In the cation of the title molecular salt,  $\text{C}_6\text{H}_{16}\text{NO}^+\cdot\text{Cl}^-$ , the  $\text{N}-\text{C}-\text{C}-\text{O}$  torsion angle is  $176.5$  (2)°. In the crystal, the cations and chloride ions are linked by  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, generating a two-dimensional network parallel to (100).

**Related literature**

For the chiral pool synthesis of naturally occurring molecules, see: Coppola & Schuster (1987); Bergmeier & Stanchina (1999). For pharmacologic synthesis, see: Gante (1994); Tok & Rando (1998).

**Experimental***Crystal data*

$\text{C}_6\text{H}_{16}\text{NO}^+\cdot\text{Cl}^-$   
 $M_r = 153.65$   
 Monoclinic,  $P2_1/c$   
 $a = 8.5204$  (3) Å  
 $b = 7.8742$  (3) Å  
 $c = 14.1844$  (5) Å  
 $\beta = 105.804$  (1)°

$V = 915.68$  (6) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.35$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.40 \times 0.10 \times 0.03$  mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer  
 5487 measured reflections  
 1668 independent reflections  
 1071 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.058$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.124$   
 $S = 1.00$   
 1668 reflections  
 94 parameters  
 3 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{Cl1}^{\text{i}}$	0.86 (1)	2.29 (1)	3.140 (2)	167 (3)
$\text{N3}-\text{H3A}\cdots\text{Cl1}$	0.90 (1)	2.27 (1)	3.144 (2)	166 (2)
$\text{N3}-\text{H3B}\cdots\text{Cl1}^{\text{ii}}$	0.89 (1)	2.30 (1)	3.190 (2)	175 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: GW2144).

**References**

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## supporting information

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**(*tert*-Butyl)(2-hydroxyethyl)ammonium chloride****Cintya Valerio-Cárdenas, Simón Hernández-Ortega and David Morales-Morales****S1. Comment**

Amino alcohols are some of the most versatile starting materials both at the laboratory and at the industrial scale and have been widely used for a large number of applications. Among which stands the chiral pool synthesis of naturally occurring molecules (Coppola *et al.* 1987; Bergmeier *et al.* 1999). These compounds have also displayed important biological activities and are of interest for the development of synthetic methods in the pharmaceutical industry (Gante, 1994; Tok *et al.* 1998). Based on the above, we report here the crystal structure of *N*-((2-hydroxyethyl)tertbutyl)ammonium chloride and discuss its geometry and intermolecular interactions.

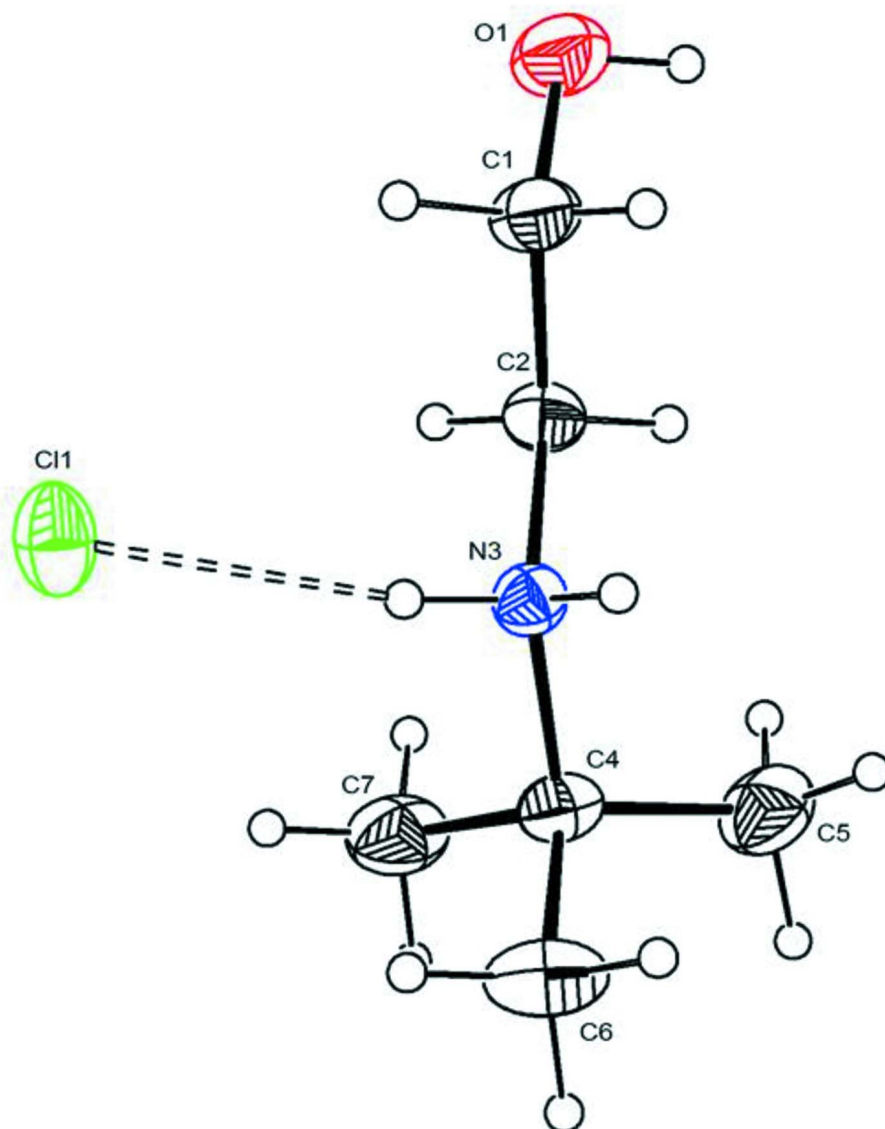
The molecular structure of the title compound [(HOC<sub>2</sub>H<sub>4</sub>)((CH<sub>3</sub>)<sub>3</sub>C)NH<sub>2</sub>]<sup>+</sup>Cl<sup>-</sup> (Fig. 1), consists of an ionic species, exhibiting the nitrogen atom in a tetrahedral geometry. The dihedral angle between the tertbutyl and the 2-hydroxyethyl moieties is almost plane (173.34 (2)°) as a result of the reduced steric effects. In the asymmetric unit the Cl atom is linked by a N3—H3A⋯Cl1 interaction (2.266 (11) Å). In the crystal the Cl atom is acting as tri-acceptor H-bonding, such that, the anion and cation species are linked through O1—H1⋯Cl1 with distances of 2.294 (13) Å, leading to stairs aligned along the *ac* plane (symmetry code *x*, -*y* + 3/2, *z* + 1/2). These stairs are expanded by a third intermolecular interaction N3—H3B⋯Cl1 (2.304 (10) Å) along the *b* axis with symmetry code -*x* + 1, *y* - 1/2, -*z* + 3/2 (see Table 1, Fig. 2).

**S2. Experimental**

The title compound was isolated from the reaction of [S<sub>2</sub>CN(*t*Bu)(EtOH)] and [NiCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>] in a 1:1 molar ratio in ethanol. Colourless crystals suitable for single-crystal X-ray diffraction analysis were obtained from a solvent system ether/CH<sub>2</sub>Cl<sub>2</sub>.

**S3. Refinement**

The atoms H1, H3A and H3B were located from a difference Fourier map and N3—H3A, N3—H3B and O1—H1 distances are restrained to 0.90 and 0.85 Å respectively. H atoms were included in calculated position (C—H = 0.97 Å for methylene H, and C—H = 0.96 Å for methyl H), and refined using a riding model with *U*<sub>iso</sub>(H) = 1.2 *U*<sub>eq</sub> of the carrier atoms. 3 badly fitting reflections were omitted from the final refinement.



**Figure 1**

The molecular structure of the title compound showing the atom labelling and displacement ellipsoids at the 40% of probability.

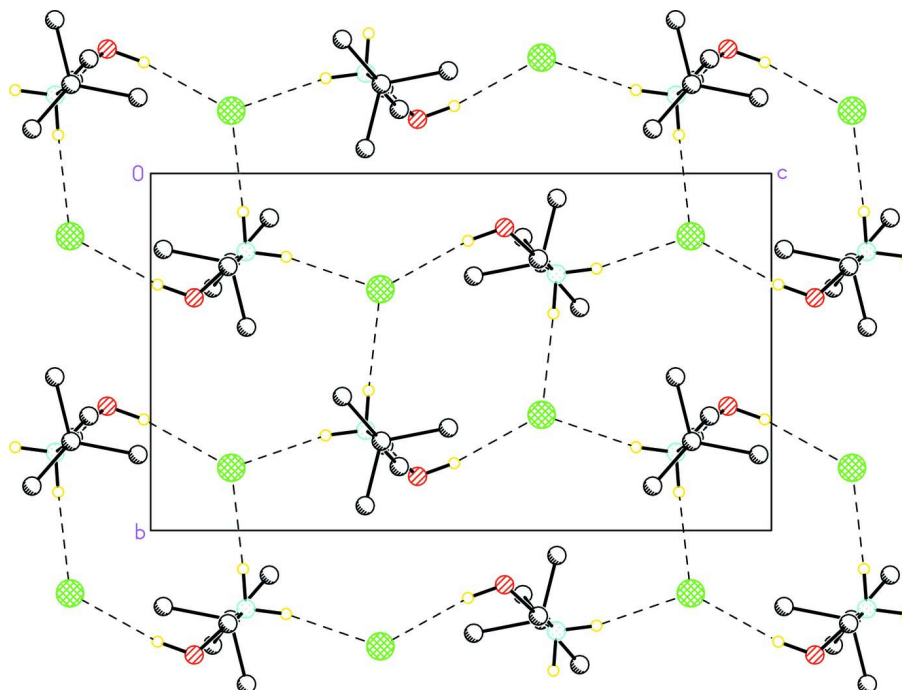


Figure 2

A view in projection on the direction of the chain. The O—H...Cl and N—H...Cl interactions are shown as dashed lines.

### (*tert*-Butyl)(2-hydroxyethyl)ammonium chloride

#### Crystal data

$C_6H_{16}NO^+Cl^-$

$M_r = 153.65$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 8.5204\ (3)\ \text{\AA}$

$b = 7.8742\ (3)\ \text{\AA}$

$c = 14.1844\ (5)\ \text{\AA}$

$\beta = 105.804\ (1)^\circ$

$V = 915.68\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 336$

$D_x = 1.115\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2475 reflections

$\theta = 2.5\text{--}25.3^\circ$

$\mu = 0.35\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Prism, colourless

$0.40 \times 0.10 \times 0.03\ \text{mm}$

#### Data collection

Bruker APEXII CCD area-detector  
diffractometer

Detector resolution:  $0.83\ \text{pixels mm}^{-1}$

$\omega$  scans

5487 measured reflections

1668 independent reflections

1071 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.058$

$\theta_{\text{max}} = 25.3^\circ$ ,  $\theta_{\text{min}} = 2.5^\circ$

$h = -5 \rightarrow 10$

$k = -8 \rightarrow 9$

$l = -17 \rightarrow 16$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.124$

$S = 1.00$

1668 reflections

94 parameters

3 restraints

Hydrogen site location: inferred from  
neighbouring sites

H atoms treated by a mixture of independent  
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$$

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.44289 (9)	0.82425 (9)	0.62991 (4)	0.0579 (3)
O1	0.2643 (2)	0.8483 (3)	0.92991 (15)	0.0690 (6)
H1	0.303 (4)	0.811 (4)	0.9889 (11)	0.083*
C1	0.3512 (3)	0.7606 (4)	0.87548 (19)	0.0531 (7)
H1A	0.3003	0.7781	0.8062	0.064*
H1B	0.3488	0.6400	0.8889	0.064*
C2	0.5253 (3)	0.8207 (3)	0.90041 (18)	0.0436 (6)
H2A	0.5280	0.9397	0.8832	0.052*
H2B	0.5742	0.8098	0.9704	0.052*
N3	0.6212 (2)	0.7191 (3)	0.84643 (15)	0.0383 (5)
H3A	0.579 (3)	0.734 (3)	0.7818 (8)	0.046*
H3B	0.607 (3)	0.6079 (13)	0.8511 (17)	0.046*
C4	0.8038 (3)	0.7496 (3)	0.87151 (19)	0.0454 (7)
C5	0.8775 (3)	0.7126 (4)	0.9796 (2)	0.0686 (9)
H5A	0.8423	0.6028	0.9950	0.082*
H5B	0.8427	0.7976	1.0181	0.082*
H5C	0.9944	0.7142	0.9941	0.082*
C6	0.8687 (3)	0.6245 (4)	0.8087 (2)	0.0728 (9)
H6A	0.8452	0.5105	0.8247	0.087*
H6B	0.9845	0.6386	0.8214	0.087*
H6C	0.8172	0.6459	0.7407	0.087*
C7	0.8344 (3)	0.9303 (4)	0.8456 (2)	0.0678 (9)
H7A	0.9497	0.9489	0.8584	0.081*
H7B	0.7906	1.0071	0.8844	0.081*
H7C	0.7825	0.9498	0.7774	0.081*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cl1	0.0865 (6)	0.0441 (4)	0.0413 (4)	0.0031 (3)	0.0142 (4)	-0.0011 (3)
O1	0.0533 (13)	0.0912 (16)	0.0646 (13)	0.0179 (11)	0.0194 (11)	0.0001 (13)
C1	0.0387 (17)	0.0772 (19)	0.0429 (15)	0.0068 (14)	0.0103 (12)	-0.0066 (15)
C2	0.0407 (16)	0.0462 (15)	0.0467 (14)	0.0013 (11)	0.0166 (12)	-0.0050 (13)
N3	0.0377 (13)	0.0364 (11)	0.0406 (11)	0.0007 (9)	0.0101 (10)	-0.0003 (11)
C4	0.0342 (15)	0.0438 (14)	0.0584 (17)	0.0013 (11)	0.0130 (13)	-0.0028 (14)
C5	0.0472 (19)	0.084 (2)	0.0657 (19)	0.0039 (15)	-0.0004 (15)	0.0017 (18)

C6	0.0513 (19)	0.079 (2)	0.095 (2)	0.0051 (16)	0.0311 (17)	-0.020 (2)
C7	0.0463 (18)	0.0607 (19)	0.099 (2)	-0.0077 (14)	0.0232 (17)	0.0038 (19)

*Geometric parameters (Å, °)*

O1—C1	1.390 (3)	C4—C5	1.519 (4)
O1—H1	0.862 (10)	C4—C6	1.529 (4)
C1—C2	1.504 (4)	C5—H5A	0.9600
C1—H1A	0.9700	C5—H5B	0.9600
C1—H1B	0.9700	C5—H5C	0.9600
C2—N3	1.495 (3)	C6—H6A	0.9600
C2—H2A	0.9700	C6—H6B	0.9600
C2—H2B	0.9700	C6—H6C	0.9600
N3—C4	1.518 (3)	C7—H7A	0.9600
N3—H3A	0.896 (9)	C7—H7B	0.9600
N3—H3B	0.888 (10)	C7—H7C	0.9600
C4—C7	1.510 (4)		
C1—O1—H1	104 (2)	C7—C4—C6	110.5 (2)
O1—C1—C2	110.7 (2)	N3—C4—C6	105.8 (2)
O1—C1—H1A	109.5	C5—C4—C6	110.4 (2)
C2—C1—H1A	109.5	C4—C5—H5A	109.5
O1—C1—H1B	109.5	C4—C5—H5B	109.5
C2—C1—H1B	109.5	H5A—C5—H5B	109.5
H1A—C1—H1B	108.1	C4—C5—H5C	109.5
N3—C2—C1	110.6 (2)	H5A—C5—H5C	109.5
N3—C2—H2A	109.5	H5B—C5—H5C	109.5
C1—C2—H2A	109.5	C4—C6—H6A	109.5
N3—C2—H2B	109.5	C4—C6—H6B	109.5
C1—C2—H2B	109.5	H6A—C6—H6B	109.5
H2A—C2—H2B	108.1	C4—C6—H6C	109.5
C2—N3—C4	117.61 (19)	H6A—C6—H6C	109.5
C2—N3—H3A	109.4 (16)	H6B—C6—H6C	109.5
C4—N3—H3A	108.7 (16)	C4—C7—H7A	109.5
C2—N3—H3B	112.9 (15)	C4—C7—H7B	109.5
C4—N3—H3B	106.6 (15)	H7A—C7—H7B	109.5
H3A—N3—H3B	100 (2)	C4—C7—H7C	109.5
C7—C4—N3	109.1 (2)	H7A—C7—H7C	109.5
C7—C4—C5	112.0 (2)	H7B—C7—H7C	109.5
N3—C4—C5	108.8 (2)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H1 $\cdots$ C11 <sup>i</sup>	0.86 (1)	2.29 (1)	3.140 (2)	167 (3)

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N3—H3A···Cl1	0.90 (1)	2.27 (1)	3.144 (2)	166 (2)
N3—H3B···Cl1 <sup>ii</sup>	0.89 (1)	2.30 (1)	3.190 (2)	175 (2)

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Symmetry codes: (i)  $x, -y+3/2, z+1/2$ ; (ii)  $-x+1, y-1/2, -z+3/2$ .