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(2-Hydroxyethyl)diisopropylammonium chloride and its derivatives

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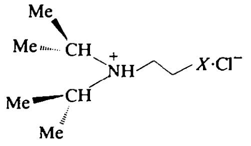
Abstract

The crystal structure of the title compound, $C_8H_{20}NO^+\cdot Cl^-$, (I), and the structures of its derivatives, (2-chloroethyl)diisopropylammonium chloride, $C_8H_{19}ClN^+\cdot Cl^-$, (II), and diisopropyl(2-mercaptoethyl)ammonium chloride, $C_8H_{20}NS^+\cdot Cl^-$, (III), are described. The conformations of the isopropyl groups in (II) (*gauche–gauche*) are different from those in (I) and (III) (both *gauche–trans*). The structures are stabilized by hydrogen bonds of the type Y—H···Cl (Y = N, O, S) and C—H···X (X = Cl, S).

Comment

Crystallographic evidence for the existence of C—H···X (X = O, N, S, Cl) hydrogen bonds was postulated in the pioneering work of Taylor & Kennard (1982). The importance of this type of hydrogen bonding is now well established in crystal engineering and in the supramolecular architectures of organic species, as well as in biomolecular structures and transition metal complexes (Desiraju, 1989, 1996; Jeffrey, 1997; Braga & Grepioni, 1997). Such weak interactions not only play a part in crystal packing, but also have an important role in determining the crystal conformations of flexible molecules (Desiraju, 1989). Recently, the existence of C—H···Cl hydrogen bonding has been described in the crystal structure of triisopropylammonium chloride and it is regarded as being responsible for the conformations of the isopropyl groups on the N atom (Bock *et al.*, 1994).

As part of an on-going study to investigate the electronic and steric effects on the coordination chemistry of *N*-alkylated aminoethanols and the corresponding thiols with Co, Ni and Cu, we prepared (2-hydroxyethyl)diisopropylammonium chloride, (I), (2-chloroethyl)diisopropylammonium chloride, (II), and diisopropyl(2-mercaptoethyl)ammonium chloride, (III). The relationship between the structure and reactivity of these molecules when bulky and rigid groups are incorporated in the main skeleton of the ligands is of interest.



(I) $X = OH$
(II) $X = Cl$
(III) $X = SH$

The molecular structure of (I) is shown in Fig. 1. The O atom is almost *trans* with respect to the N atom and the corresponding N1—C2—C1—O1 torsion angle is 171.9 (2)°. The isopropyl groups on the N atom are arranged in such a way that the H6—C6—N1—H1 and H3—C3—N1—H1 torsion angles are −67.7 and −176.8°, respectively. Thus, H6 is *gauche* and H3 is *trans* (eclipsed) with respect to the ammonium H1 atom. The crystal packing and hydrogen-bonding

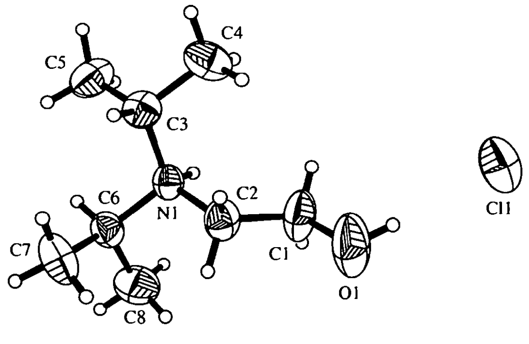


Fig. 1. The molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as spheres of an arbitrary radius.

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scheme are shown in Fig. 2. There are two medium-strength hydrogen bonds (Gilli, 1995) of the O—H···Cl and N—H···Cl types, with donor–acceptor distances of 3.063 (3) and 3.129 (2) Å, respectively. However, there are also weak C—H···Cl hydrogen bonds with atoms C6 and C8 as donors.

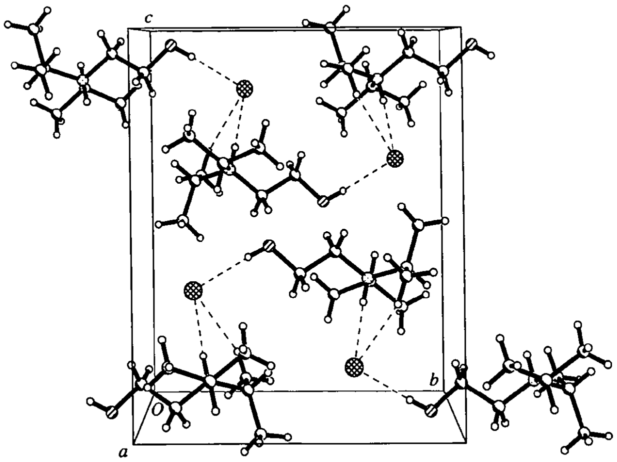

Fig. 2. The crystal packing in a projection along the *a* axis and the hydrogen-bonding scheme for (I).

The molecular structure of (II) is shown in Fig. 3. It crystallizes in space group $P2_1/n$, the same as (I). The N1—C2—C1—Cl1 torsion angle is −173.37 (12)° and the torsion angles H3—C3—N1—H1 and H6—C6—N1—H1 are −84.9 and −62.4°, respectively. Thus, both H6 and H3 are almost *gauche* with respect to H1 on the N atom. The crystal structure is stabilized by a network of hydrogen bonds (Fig. 4). This network consists of a medium-strength N—H···Cl hydrogen bond, with a donor–acceptor distance of 3.125 (2) Å. There are several C—H···Cl hydrogen bonds between the Cl2 anion and atoms C1, C4, C7 and C6. The covalently bonded chlorine, Cl1, also takes part in a C—H···Cl hydrogen bond with atom C4. Thus, both isopropyl groups are involved in C—H···Cl hydrogen bonding which stabilizes *gauche* conformations for these groups.

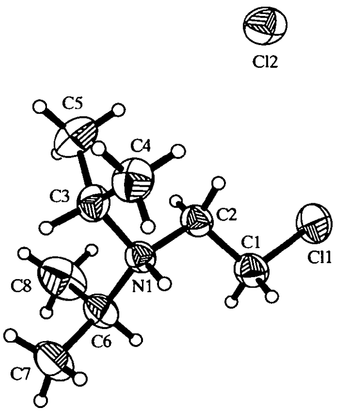

Fig. 3. The molecular structure of (II). Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as spheres of an arbitrary radius.

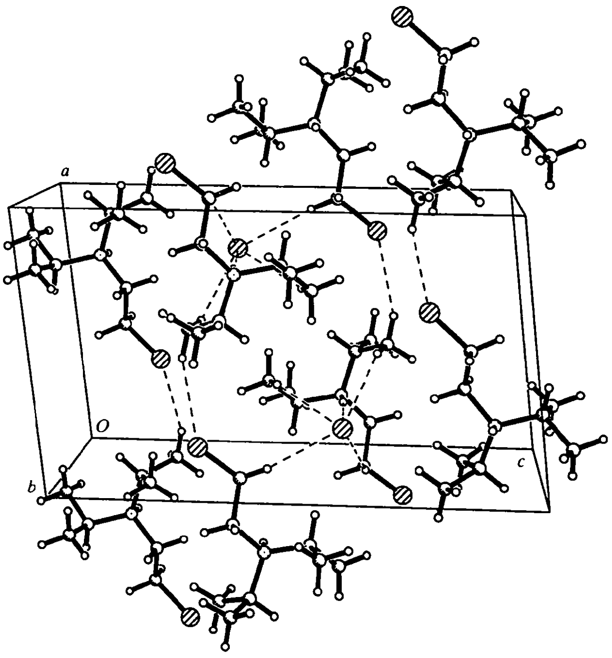

Fig. 4. The crystal packing in a projection along the *b* axis and the hydrogen-bonding scheme for (II).

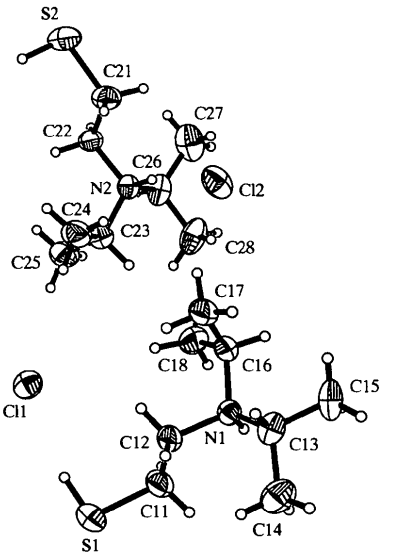

Fig. 5. The molecular structure of (III), showing the two independent molecules in the asymmetric unit. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as spheres of an arbitrary radius.

The molecular structure of (III) is shown in Fig. 5. It crystallizes in the orthorhombic system with two molecules in the asymmetric unit, which are related by an additional approximate twofold screw axis parallel to **a** at 0.74/**b** and 0.26/**c**. The torsion angles N1—C12—C11—S1 and N2—C22—C21—S2 are 177.0 (2) and 175.7 (2)°, respectively. The torsion angles H16—C16—N1—H1, H13—C13—N1—H1, H23—C23—N2—H2 and H26—C26—N2—H2 are −61.0, −174.9, −61.1 and −172.5°, respectively. Thus, the crystal contains two molecules in the asymmetric unit with the same conformation (*gauche–trans*) for the isopropyl groups on the N atoms. The crystal packing and hydrogen-bonding scheme are shown in Fig. 6. The packing consists of N—H···Cl and S—H···Cl hydrogen bonds for both molecules. The Cl2 anion is involved in two C—H···Cl hydrogen bonds with atoms C13 and C24, while there is only one of the same type for the Cl1 anion, with atom C26. The covalently bonded atom S2 also participates in a C—H···S hydrogen bond, with atom C11.

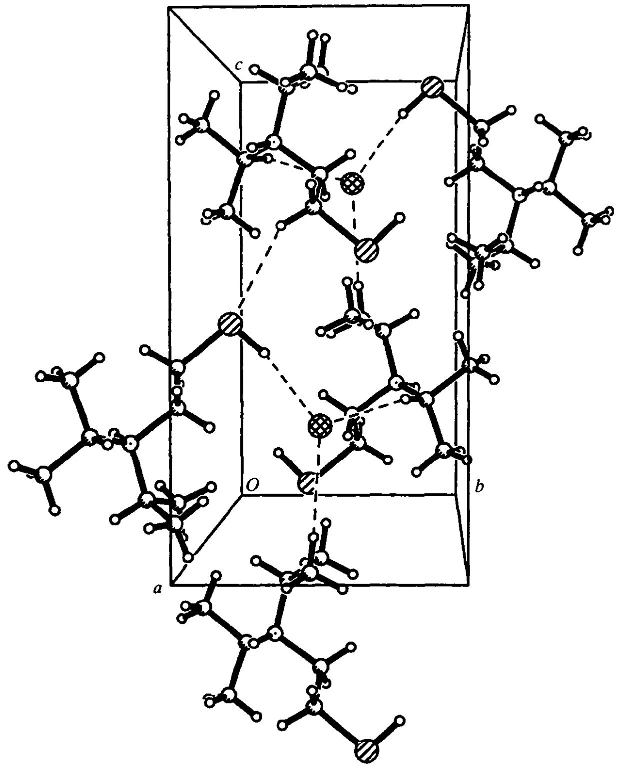

Fig. 6. The crystal packing in a projection along the *a* axis and the hydrogen-bonding scheme for (III).

The N—H···Cl hydrogen bonds in the structures presented here, with *D*—H···*A* angles in the range 166.3–173.4°, are more directional than the C—H···*X* hydrogen bonds. All but one of the N···Cl distances [3.129 (2), 3.125 (2), 3.128 (2) and 3.155 (2) Å] are significantly shorter than those in both triisopropylammonium chloride [3.150 (2) Å; Bock *et al.*, 1994] and diisopropylammonium chloride [3.163 (3) and 3.180 (3) Å; Prince *et al.*, 1990]. The C—H···Cl hydrogen bonds contribute to the crystal packing forces and, moreover, determine the conformation of the isopropyl groups in these structures. Although bulky, these isopropyl groups are flexible enough to provide space for the N atom to act as an electron donor. This has been also shown in the structures of the copper complexes of diisopropylaminoethanol and 1-diisopropylamino-2-propanol ligands, in which diisopropylamine groups are coordinated to the metal ion (Mikuriya *et al.*, 1994).

Experimental

Compound (I) was prepared by the slow addition of an aqueous solution of HCl (20%) to an ethanolic solution (20%) of commercially available diisopropylaminoethanol (Merck). The solvents were removed by azeotropic distillation with toluene. Crystals of (I) were obtained by slow evaporation of a solution in acetone when allowed to stand over silica gel in a desiccator. Compound (II) was prepared by chlorination of diisopropylaminoethanol with $SOCl_2$ according to the method described by Vogel (1989). Crystals of (II) were obtained by recrystallization from a toluene–ethanol (5:1) solution. Compound (III) was synthesized by the reaction of (II) with thiourea according to the method described by Cossar *et al.* (1962). After treatment with HCl [the same procedure as for (I)], crystals of (III) were obtained from benzene–acetone (3:1) solution by slow evaporation. All crystals were stable enough for data collection under normal conditions.

Compound (I)

Crystal data

$C_8H_{20}NO^+ \cdot Cl^-$
$M_r = 181.70$
Monoclinic
$P2_1/n$
$a = 7.2665\ (3)$ Å
$b = 10.9212\ (4)$ Å
$c = 13.2862\ (4)$ Å
$\beta = 96.477\ (1)°$
$V = 1047.65\ (7)$ Å^3
$Z = 4$
$D_x = 1.152$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 3036 reflections
$\theta = 1$–$25°$
$\mu = 0.319$ mm^{-1}
$T = 297\ (2)$ K
Parallelepiped
0.35 × 0.20 × 0.15 mm
Colourless

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.897$, $T_{max} = 0.954$
6870 measured reflections
1765 independent reflections

1221 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.18°$
$h = -8 \rightarrow 7$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.124$
$S = 1.031$
1765 reflections
126 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 0.474P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.339$ e Å^{-3}
$\Delta\rho_{\min} = -0.203$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997*a*)
Extinction coefficient: 0.030 (4)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °) for (I)*

N1—C2	1.508 (3)	N1—C3	1.523 (3)
N1—C6	1.520 (3)	O1—C1	1.400 (3)
C2—N1—C6	112.4 (2)	C2—N1—H1	106.1
C2—N1—C3	111.9 (2)	C6—N1—H1	106.1
C6—N1—C3	113.6 (2)	C3—N1—H1	106.1
H3—C3—N1—H1	−176.8	N1—C2—C1—O1	171.9 (2)
H6—C6—N1—H1	−67.7		

Table 2. *Hydrogen-bonding geometry (Å, °) for (I)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1^{i}	0.91	2.22	3.129 (2)	173.4
O1—H1O···Cl1	0.82	2.24	3.063 (3)	176.1
C6—H6···Cl1^{ii}	0.98	2.93	3.707 (3)	136.9
C8—H8*B*···Cl1^{i}	0.96	2.91	3.698 (3)	140.3

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

Compound (II)

Crystal data

$C_8H_{19}ClN^+{\cdot}Cl^-$
$M_r = 200.14$
Monoclinic
$P2_1/n$
$a = 8.9772$ (2) Å
$b = 8.0690$ (1) Å
$c = 15.3032$ (2) Å
$\beta = 95.937$ (1)°
$V = 1102.57$ (3) Å^3
$Z = 4$
$D_x = 1.206$ Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 5070 reflections
$\theta = 1$–25°
$\mu = 0.537$ mm^{-1}
$T = 297$ (2) K
Rectangular prism
0.5 × 0.3 × 0.1 mm
Colourless

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.775$, $T_{\max} = 0.948$
8239 measured reflections
1854 independent reflections
1499 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\max} = 25.18°$
$h = -10 \rightarrow 10$
$k = -9 \rightarrow 9$
$l = -17 \rightarrow 17$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.080$
$S = 1.062$
1854 reflections
124 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 0.3199P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.208$ e Å^{-3}
$\Delta\rho_{\min} = -0.148$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997*a*)
Extinction coefficient: 0.0203 (19)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 3. *Selected geometric parameters (Å, °) for (II)*

Cl1—C1	1.7765 (18)	N1—C3	1.530 (2)
N1—C2	1.501 (2)	N1—C6	1.532 (2)
C2—N1—C3	112.12 (13)	C2—N1—H1	104.7
C2—N1—C6	113.17 (13)	C3—N1—H1	104.7
C3—N1—C6	116.03 (14)	C6—N1—H1	104.7
H1—N1—C3—H3	−84.9	N1—C2—C1—Cl1	−173.4 (1)
H1—N1—C6—H6	−62.4		

Table 4. *Hydrogen-bonding geometry (Å, °) for (II)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···Cl2^{i}	0.97	2.72	3.662 (2)	163.6
C1—H1*B*···Cl2^{ii}	0.97	2.76	3.560 (2)	140.5
C4—H4*A*···Cl2^{ii}	0.96	2.87	3.641 (2)	138.0
C4—H4*B*···Cl1^{iii}	0.96	2.89	3.777 (2)	155.0
C7—H7*A*···Cl2^{ii}	0.96	2.90	3.692 (2)	140.1
C6—H6···Cl2^{i}	0.98	2.92	3.857 (2)	160.4
N1—H1···Cl2^{ii}	0.91	2.22	3.125 (2)	171.6

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

Compound (III)

Crystal data

$C_8H_{20}NS^+{\cdot}Cl^-$
$M_r = 197.76$
Orthorhombic
$Pca2_1$
$a = 25.0910$ (6) Å
$b = 6.7447$ (2) Å
$c = 13.3049$ (2) Å
$V = 2251.60$ (9) Å^3
$Z = 8$
$D_x = 1.167$ Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 5563 reflections
$\theta = 1$–25°
$\mu = 0.474$ mm^{-1}
$T = 297$ (2) K
Polyhedron
0.7 × 0.6 × 0.5 mm
Colourless

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.733$, $T_{\max} = 0.798$
8760 measured reflections
3374 independent reflections
3009 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 25.20°$
$h = -28 \rightarrow 25$
$k = -5 \rightarrow 8$
$l = -15 \rightarrow 11$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.079$
$S = 1.090$
$(\Delta/\sigma)_{\max} = 0.008$
$\Delta\rho_{\max} = 0.192$ e Å^{-3}
$\Delta\rho_{\min} = -0.163$ e Å^{-3}
Extinction correction: none

3374 reflections
253 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.4855P]$
where $P = (F_o^2 + 2F_c^2)/3$

Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 5. *Selected geometric parameters (Å, °) for (III)*

S2—C21	1.807 (3)	N1—C16	1.529 (3)
S1—C11	1.808 (3)	N2—C22	1.526 (3)
N1—C12	1.515 (3)	N2—C23	1.525 (4)
N1—C13	1.524 (3)	N2—C26	1.530 (3)
C21—S2—H2*S*	96.2 (16)	C16—N1—H1	106.2
C11—S1—H1*S*	96.3 (16)	C22—N2—C23	112.2 (2)
C12—N1—C13	112.4 (2)	C22—N2—C26	111.0 (2)
C12—N1—C16	112.0 (2)	C23—N2—C26	115.1 (2)
C13—N1—C16	113.3 (2)	C22—N2—H2	105.9
C12—N1—H1	106.2	C23—N2—H2	105.9
C13—N1—H1	106.2	C26—N2—H2	105.9
H13—C13—N1—H1	−174.9	H23—C23—N2—H2	−61.1
H16—C16—N1—H1	−61.0	H26—C26—N2—H2	−172.5
N1—C12—C11—S1	177.0 (2)	N2—C22—C21—S2	175.7 (2)

Table 6. *Hydrogen-bonding geometry (Å, °) for (III)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1^{i}	0.91	2.26	3.155 (2)	166.3
C11—H11*A*···S2^{ii}	0.97	2.89	3.670 (3)	138.4
C13—H13···Cl2^{iii}	0.98	2.84	3.707 (3)	148.0
C24—H24*B*···Cl2	0.96	2.93	3.703 (4)	137.8
C26—H26···Cl1^{iv}	0.98	2.95	3.873 (3)	157.8
S1—H1*S*···Cl1	1.23 (2)	2.59 (2)	3.799 (1)	169 (2)
N2—H2···Cl2	0.91	2.24	3.128 (2)	166.4
S2—H2*S*···Cl2^{v}	1.24 (2)	2.47 (2)	3.694 (1)	169 (2)

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

A full sphere [(I) and (II)] or hemisphere [(III)] of reciprocal space was scanned by 0.3° steps in ω with a crystal-to-detector distance of 6.22 cm. The non-H atoms were refined anisotropically. H(—S) atoms were refined isotropically with a restrained S—H distance, whereas other H atoms were treated isotropically using an appropriate riding model.

For all compounds, data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT* and *SADABS* (Sheldrick, 1996); program(s) used to solve structures: *SHELXS*97 (Sheldrick, 1997*b*); program(s) used to refine structures: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*c*).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1104). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1999). C**55**, 1167-1170

(1*S*,2*R*)-1-Amino-2-methoxycyclohexane-1-carboxamide hydrochloride 0.25-hydrate

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Abstract

The title compound, (1-carboxamido-2-methoxycyclohexyl)ammonium chloride 0.25-hydrate, $C_8H_{17}N_2O_2^+\cdot Cl^-\cdot 0.25H_2O$, (I), was obtained in the course of our research efforts towards 2,4-propano analogues of the naturally occurring α-amino acid L_s-threonine. In order to elucidate the absolute stereochemistry of (I), the absolute configuration was determined by exploiting anomalous dispersion effects. The crystal structure contains four independent molecules within the asymmetric unit, which are linked by a network of hydrogen bonds and include the Cl^- ions. The absolute configuration of all four molecules is the same; however, differences in the conformation of some groups are present.

Comment

It has been shown that the asymmetric Strecker synthesis is a valuable tool for the preparation of 2-substituted