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The crystal structure of 3-chloropropylammonium chloride, $C_3H_9Cl_2N$

<https://doi.org/10.1515/ncrs-2020-0527>

Received October 8, 2020; accepted November 8, 2020;

published online November 23, 2020

Abstract

$C_3H_9Cl_2N$, monoclinic, $I2/a$ (no. 15), $a = 8.7694(5)$ Å, $b = 9.6963(6)$ Å, $c = 14.8577(9)$ Å, $\beta = 98.266(3)^\circ$, $V = 1250.24(13)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0193$, $wR_{ref}(F^2) = 0.0511$, $T = 200$ K.

CCDC no: 2042546

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The compound was obtained commercially (Fluka). Crystals suitable for the diffraction study were taken directly from the provided product.

Experimental details

Carbon-bound H atoms were placed in calculated positions (C–H 0.99 Å) and were included in the refinement

Table 1: Data collection and handling.

Crystal:	Colourless platelet
Size:	$0.42 \times 0.41 \times 0.39$ mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.91 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	28.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	5906, 1560, 0.011
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1483
$N(param)_{refined}$:	67
Programs:	Bruker [1, 2], SHELX [3], WinGX/ORTEP [4], Mercury [5], PLATON [6]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Cl1	0.61530 (3)	0.52982 (3)	0.12230 (2)	0.03503 (9)
N1	0.40081 (10)	0.17699 (9)	0.16933 (6)	0.02508 (17)
H711	0.2992 (19)	0.1596 (15)	0.1652 (10)	0.041 (4)*
H712	0.4264 (17)	0.2321 (16)	0.2143 (10)	0.040 (4)*
H713	0.4478 (17)	0.0911 (16)	0.1809 (10)	0.040 (4)*
C1	0.43768 (11)	0.23458 (11)	0.08204 (7)	0.0273 (2)
H1A	0.386245	0.325109	0.070845	0.033*
H1B	0.396437	0.172162	0.031636	0.033*
C2	0.60956 (12)	0.25245 (12)	0.08250 (7)	0.0297(2)
H2A	0.660164	0.162244	0.096840	0.036*
H2B	0.627344	0.278402	0.020406	0.036*
C3	0.68722 (11)	0.35840 (11)	0.14845 (8)	0.0290 (2)
H3A	0.799623	0.356712	0.146663	0.035*
H3B	0.670062	0.333828	0.210888	0.035*
Cl2	0.04089 (3)	0.12061 (2)	0.15846 (2)	0.02772 (8)

in the riding model approximation, with $U(H)$ set to $1.2U_{eq}(C)$.

All three nitrogen-bound H atoms were located on a difference Fourier map and refined freely.

Comment

The effect of size and steric pretense of large ions on chemical and spectroscopic properties of compounds have

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been a focus of research for many decades and have been reported to influence the glass transition temperature in ionomers [7], surfactant modifying properties [8], the charge transfer in radical ions [9] and polymer-modified electrodes [10], as well as the structural and vibrational spectroscopic behaviour of DNA building blocks [11]. Furthermore, the benefit of choosing the adequate size of counterions to crystallize ionic compounds has been confirmed and reviewed on many occasions [12]. In continuation of our interest in metrical features of large cations [13–19] the structure of the title compound has been determined.

In the title compound, the C–Cl as well as the C–N bond lengths of 1.8003(11) and 1.4896(13) Å, respectively, are in good agreement with other primary ammonium salts and compounds featuring chloromethylene moieties whose metrical parameters have been deposited with the Cambridge Structural Database [20].

In the crystal, classical hydrogen bonds of the N–H...Cl type are observed with all of the pnictogen-bound hydrogen atoms acting as donors. In terms of graph-set analysis [21, 22], the descriptor for these hydrogen bonds is *DDD* at the unary level. In total, the entities of the crystal structure are connected to double layers perpendicular to the crystallographic *c* axis.

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: National Research Foundation.

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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