Redetermination of the crystal structure of ethylenediammonium chloride, $C_2H_{10}Cl_2N_2$

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Table 1. Parameters used for the X-ray data collection

Crystal:	colorless needle, size 0.15 x 0.15 x 0.35 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	9.39 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	64°
$N(hkl)_{\text{unique}}$:	1058
Criterion for I_0 :	$I_0 > 2 \sigma(I_0)$
$N(\text{param})_{\text{refined}}$:	34
Program:	SHELXTL

Source of material: The title compound was obtained by reaction of ethylenediamine with HCl in DMF/H₂O (5:1) solvent.

The crystal structure of ethylenediammonium chloride first described by T. Ashida and S. Hirokawa (see ref. 1) was redetermined by single crystal X-ray diffraction. The asymmetric unit contains 0.5 formula units. There are two formula units in the monoclinic unit cell. All three hydrogen atoms of the ammonium groups form hydrogen bonds (in the figure indicated by broken lines) to chloride ions. The N–Cl distance is 3.183 Å, the H–Cl distances are 2.296 Å, 2.267 Å and 2.321 Å.

$C_2H_{10}Cl_2N_2$, monoclinic, $P12_1/c1$ (No. 14), $a = 4.426(1)$ Å, $b = 6.888(1)$ Å, $c = 9.958(1)$ Å, $\beta = 91.32(2)^\circ$, $V = 303.5$ Å³, $Z = 2$, $R(F) = 0.024$, $R_w(F) = 0.073$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1A)	4e	0.2520(2)	−0.4813(1)	0.9085(1)	0.033(4)
H(1B)	4e	0.2678(2)	−0.3804(1)	1.0500(1)	0.037(4)
H(1C)	4e	0.4150(2)	−0.1686(1)	0.88831(9)	0.054(5)
H(1D)	4e	0.6561(2)	−0.2974(1)	0.84726(9)	0.049(5)
H(1E)	4e	0.6721(2)	−0.2046(1)	0.97829(9)	0.055(5)

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Cl(1)	4e	0.09266(6)	0.08003(4)	0.82959(2)	0.0348(2)	0.0295(2)	0.0267(2)	0.00051(8)	−0.0010(1)	0.00150(8)
C(1)	4e	0.3877(2)	−0.4244(1)	0.9755(1)	0.0221(4)	0.0252(4)	0.0292(5)	0.0034(3)	−0.0013(3)	0.0015(3)
N(1)	4e	0.5489(2)	−0.2570(1)	0.91642(9)	0.0335(4)	0.0237(4)	0.0285(4)	0.0029(3)	0.0000(3)	0.0013(3)

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References

1. Ashida, T.; Hirokawa, H.: The Crystal Structure of Ethylenediammonium Chloride. Bull. Chem. Soc. Jpn. **36** (1963) 704–707.
2. Sheldrick, G. M.: Program Package SHELXTL. Release 5. Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1994.