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Acta Cryst. (1988). C**44**, 1152–1153

Structure of 1,7-Heptanediamine Dihydrochloride

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(*Received* 14 *January* 1988; *accepted* 25 *January* 1988)

Abstract. 1,7-Heptanediyldiammonium dichloride, $C_7H_{20}N_2^{2+}.2Cl^-$, $M_r = 203{\cdot}16$, monoclinic, $P2_1/c$, $a = 4{\cdot}648\,(2)$, $b = 16{\cdot}079\,(6)$, $c = 15{\cdot}027\,(4)$ Å, $\beta = 95{\cdot}52\,(3)°$, $V = 1117{\cdot}8$ Å^3, $Z = 4$, $D_m = 1{\cdot}20$, $D_x = 1{\cdot}207$ Mg m^{-3}, $\lambda(\text{Cu } K\bar{\alpha}) = 1{\cdot}54178$ Å, $\mu = 4{\cdot}94$ mm^{-1}, $F(000) = 440$, $T = 173$ K, final $R = 0{\cdot}031$ for 1562 unique observed reflections. The compound is isomorphous with the corresponding dibromide. The $[NH_3C_7H_{14}NH_3]^{2+}$ cation has an all-*trans* conformation. The NH_3^+ groups form N—H···Cl hydrogen bonds with the Cl^- ions with N—Cl distances ranging from 3·123 (2) to 3·339 (2) Å.

Experimental. Compound prepared by the same method as 1,3-diaminopropane dihydrochloride (Brisson & Brisse, 1982). Crystals grown from ethanol, 0·10 (010–0$\bar{1}$0) × 0·33 (001–00$\bar{1}$) × 0·46 (100–$\bar{1}$00) mm, density by flotation in chlorobenzene/bromobenzene. Enraf–Nonius CAD-4 diffractometer, cell dimensions and Laue symmetry from 25 centered reflections ($25 \leq \theta \leq 30°$) checked with oscillation photographs, data-collection procedure described elsewhere (Bélanger-Gariépy & Beauchamp, 1980), Cu $K\bar{\alpha}$ graphite-monochromatized radiation, $2\theta_{\max} = 120°$, $0 \leq h \leq 5$, $0 \leq k \leq 18$, $-17 \leq l \leq 17$; orientation checked every 100 measurements, intensity of seven standards checked every hour, max. fluctuation 3·1%, 1656 independent reflections measured, 1562 with $I > 3{\cdot}0\sigma(I)$. Data corrected for Lp and absorption, transmission range 0·23–0·60. Cl located from Patterson map, other atoms from ΔF map; structure refined on F by full-matrix least squares. H refined isotropically, other atoms anisotropically. Final $R = 0{\cdot}031$, $wR = 0{\cdot}043$ (weights based on counting statistics), $S = 1{\cdot}97$, mean shift/$\sigma = 0{\cdot}04$, max. $= 0{\cdot}10$. Residual electron density on final ΔF map: $-0{\cdot}23$ and $0{\cdot}21$ e Å^{-3}. Scattering factors for Cl, N and C from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965). Anomalous-dispersion f' and f'' terms for Cl from Cromer & Liberman (1970). Programs used listed elsewhere (Authier-Martin & Beauchamp, 1977). Final positional and isotropic thermal parameters are listed in Table 1,† and selected bond distances and angles in Table 2.

Related literature. 1,7-Heptanediamine dihydrochloride is isomorphous with the corresponding di-

Table 1. *Refined coordinates* (× 10^4, Cl × 10^5, H × 10^3), U_{eq} (Å^2 × 10^3) *for* C, N, Cl and U_{iso} (Å^2 × 10^3) *for* H

$$U_{\rm eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Cl(1)	11262 (8)	60510 (2)	45077 (3)	27
Cl(2)	5720 (8)	27511 (3)	128849 (3)	31
N(1)	6373 (3)	5766 (1)	6010 (1)	27
N(7)	5216 (3)	2316 (1)	11550 (1)	29
C(1)	4608 (3)	5421 (1)	6696 (1)	27
C(2)	6455 (3)	5030 (1)	7470 (1)	27
C(3)	4618 (3)	4665 (1)	8157 (1)	28
C(4)	6325 (4)	4168 (1)	8886 (1)	28
C(5)	4415 (4)	3813 (1)	9558 (1)	27
C(6)	5990 (3)	3251 (1)	10260 (1)	26
C(7)	3878 (4)	2902 (1)	10867 (1)	29
H(N1)1	736 (4)	540 (1)	582 (1)	35 (5)
H(N1)2	753 (4)	620 (1)	622 (1)	32 (5)
H(N1)3	502 (5)	597 (1)	551 (1)	48 (6)
H(N7)1	583 (4)	193 (1)	1131 (1)	35 (5)
H(N7)2	679 (4)	257 (1)	1191 (1)	42 (5)
H(N7)3	402 (4)	217 (1)	1194 (1)	42 (6)
H(11)	355 (4)	588 (1)	686 (1)	31 (5)
H(12)	333 (4)	503 (1)	641 (1)	33 (5)
H(21)	762 (4)	462 (1)	724 (1)	28 (5)
H(22)	784 (4)	546 (1)	774 (1)	33 (5)
H(31)	351 (4)	512 (1)	843 (1)	41 (5)
H(32)	316 (4)	433 (1)	785 (1)	37 (5)
H(41)	730 (4)	374 (1)	865 (1)	42 (6)
H(42)	787 (4)	453 (1)	920 (1)	32 (5)
H(51)	359 (4)	425 (1)	988 (1)	32 (5)
H(52)	294 (4)	348 (1)	921 (1)	33 (5)
H(61)	684 (4)	282 (1)	996 (1)	32 (5)
H(62)	754 (4)	354 (1)	1061 (1)	27 (5)
H(71)	313 (4)	337 (1)	1121 (1)	30 (5)
H(72)	232 (4)	260 (1)	1054 (1)	41 (5)

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† Lists of observed and calculated structure-factor amplitudes, anisotropic thermal parameters, distances and angles involving H atoms, and data on the geometry of the hydrogen bonds have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44727 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/88/061152-02$03.00

Table 2. *Distances* (Å), *angles* (°), *hydrogen-bond lengths* (Å) *and torsion angles* (°)

N(1)–C(1)	1·485 (2)	N(1)–C(1)–C(2)	112·2 (1)
C(1)–C(2)	1·514 (2)	C(1)–C(2)–C(3)	111·6 (1)
C(2)–C(3)	1·519 (2)	C(2)–C(3)–C(4)	113·9 (1)
C(3)–C(4)	1·517 (2)	C(3)–C(4)–C(5)	112·3 (1)
C(4)–C(5)	1·519 (2)	C(4)–C(5)–C(6)	114·3 (1)
C(5)–C(6)	1·522 (2)	C(5)–C(6)–C(7)	110·0 (1)
C(6)–C(7)	1·511 (2)	C(6)–C(7)–N(7)	113·6 (1)
C(7)–N(7)	1·485 (2)		
N(1)···Cl(1)	3·193 (2)	N(1)–C(1)–C(2)–C(3)	−178·9 (1)
N(1)···Cl(1^{i})	3·339 (2)	C(1)–C(2)–C(3)–C(4)	172·5 (1)
N(1)···Cl(1^{ii})	3·266 (2)	C(2)–C(3)–C(4)–C(5)	−179·9 (1)
N(1)···Cl(2^{iii})	3·163 (2)	C(3)–C(4)–C(5)–C(6)	175·3 (1)
N(7)···Cl(2)	3·163 (2)	C(4)–C(5)–C(6)–C(7)	−177·5 (1)
N(7)···Cl(2^{iv})	3·174 (2)	C(5)–C(6)–C(7)–N(7)	177·5 (1)
N(7)···Cl(2^{i})	3·123 (2)		

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

hydrobromide (Brisson & Brisse, 1984), and in both compounds the $C_7H_{20}N_2^{2+}$ cations present a similar curvature (Fig. 1). Unit-cell packing is the same as Fig. 2 in the publication on the dihydrobromide. The cation has an all-*trans* zigzag conformation (Table 2). Although there is an exception (Holmes, Day, Harland, Sau & Holmes, 1984), the all-*trans* structure is the most common for long-chain aliphatic α,ω-diamines and diammonium ions (Borkakoti, Lindley, Moss & Palmer, 1978; McNeil, Scheidt & Thomas, 1981; Oouchi, Takenaka & Sasada, 1986; Binnie & Robertson, 1950; Brown, 1966).

We are grateful to M. Simard for collecting the X-ray data and B. Lagarde for his participation in the structure determination.

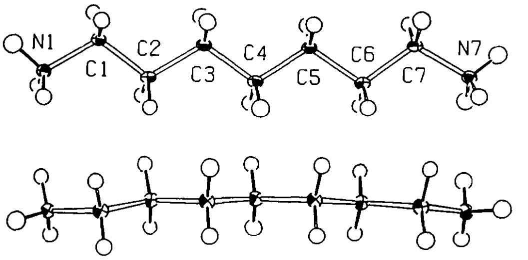

Fig. 1. Two views 90° apart of the 1,7-heptanediyldiammonium cation. The ellipsoids correspond to 50% probability.

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Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1988). C**44**, 1153–1154

Crystallographic databases. Edited by F. H. Allen, G. Bergerhoff and R. Sievers. Pp. 221. Chester, England: International Union of Crystallography, 1987. Price US$ 20.00. (Paper.)

This book is a collection of articles dealing with methods of crystallographic database compilation and searching, and deals specifically with those crystallographic databases already in existence. It is a useful reference if one wishes to do large-scale analysis of published crystallographic data, or if one needs to provide easy access to crystallographic data as part of a service. The book would also be useful to non-crystallographers as an introduction to the various crystallographic databases that are available.

The articles are divided into four sections, with the first consisting of an overview of crystal structure analysis for the non-specialist, and an introduction to printed crystallographic archives and reference works. The second section is the most interesting to structural scientists as it contains descriptions of the major crystal structure databases. This section contains information on the inclusion criteria, abstraction methods, error checking and availability of the Cambridge Structural Database (CSD), the Inorganic Crystal Structure Database (ICSD), the NRCC metals