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Unit Cells of Choline Halides and Structure of Choline Chloride*

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Three choline halides have been studied by single-crystal X-ray diffraction methods at room temperature. Choline chloride is orthorhombic, space group $P2_12_12_1$,

$$a = 11{\cdot}21 \pm 0{\cdot}02,\ b = 11{\cdot}59 \pm 0{\cdot}02,\ c = 5{\cdot}87 \pm 0{\cdot}02 \text{ Å},\ Z = 4\,.$$

Atomic coordinates have been determined by least-squares refinement of three-dimensional data. Bond distances in Å are: N–C (methyl), 1·53, 1·52, 1·50; N–C (side chain), 1·60; C–C, 1·56; C–O, 1·39 (each ±0·03 Å). Choline bromide is orthorhombic, probable space group $Pna2_1$ or $Pnam$,

$$a = 19{\cdot}55 \pm 0{\cdot}04,\ b = 7{\cdot}35 \pm 0{\cdot}03,\ c = 5{\cdot}69 \pm 0{\cdot}02 \text{ Å},\ Z = 4\,.$$

Choline iodide is monoclinic, probable space group $P2_1$,

$$a = 5{\cdot}88 \pm 0{\cdot}02,\ b = 8{\cdot}20 \pm 0{\cdot}02,\ c = 9{\cdot}10 \pm 0{\cdot}02 \text{ Å},\ \beta = 91 \pm 1^\circ,\ Z = 2\,.$$

Introduction

At room temperature choline chloride is remarkably sensitive to decomposition into trimethylamine and acetaldehyde by ionizing radiations because of a chain reaction which occurs extensively only in the solid state (Tolbert *et al.*, 1953; Lemmon *et al.*, 1955, 1958). We have determined the structure of this crystal and have made preliminary studies of choline bromide and choline iodide, which are more stable, to aid in the interpretation of this phenomenon. Collin (1957) discovered that at elevated temperature choline chloride changes to a disordered cubic phase, which is also more stable than the room-temperature phase with respect to radiation damage (Serlin, 1957).

Unit-cell data

Crystals of the three salts were kindly given us by Dr Richard E. Lemmon. Weissenberg and precision patterns, calibrated with quartz, $a = 4{\cdot}913$ Å, yielded the following cell dimensions:

Choline chloride, $[(CH_3)_3NCH_2CH_2OH]^+Cl^-$, orthorhombic

$$a = 11{\cdot}21 \pm 0{\cdot}02,\ b = 11{\cdot}59 \pm 0{\cdot}02,\ c = 5{\cdot}87 \pm 0{\cdot}02 \text{ Å}.$$

Space group $P2_12_12_1$ (by determination of the structure).

$Z = 4$ molecules/cell; $d_x = 1{\cdot}216$ g.cm.$^{-3}$, $d_m = 1{\cdot}205 \pm 0{\cdot}02$ g.cm.$^{-3}$.‡

Choline bromide, $[(CH_3)_3NCH_2CH_2OH]^+Br^-$, orthorhombic

$$a = 19{\cdot}55 \pm 0{\cdot}04,\ b = 7{\cdot}35 \pm 0{\cdot}03,\ c = 5{\cdot}69 \pm 0{\cdot}02 \text{ Å}.$$

Probable space group $Pna2_1$ or $Pnam$.
$Z = 4$ molecules/cell: $d_x = 1{\cdot}495$ g.cm.$^{-3}$.

Choline iodide, $[(CH_3)_3NCH_2CH_2OH]^+I^-$, monoclinic.

$$a = 5{\cdot}88 \pm 0{\cdot}02,\ b = 8{\cdot}20 \pm 0{\cdot}02,\ c = 9{\cdot}10 \pm 0{\cdot}02 \text{ Å};\ \beta = 91 \pm 1^\circ.$$

Probable space group $P2_1$.
$Z = 2$ molecules/cell; $d_x = 1{\cdot}749$ g.cm.$^{-3}$.

Crystal structure of choline chloride

Crystals of choline chloride after recrystallization from dimethyl formamide were colorless, transparent needles with the long dimension in the *c* direction. Their hygroscopic nature made it necessary to mount them in glass capillaries. After about 40 hr. of exposure to nickel-filtered copper X-rays under normal diffraction conditions they became opaque and slightly yellow and yielded very diffuse diffraction spots. This instability limited the available diffraction data to reflections with $\sin^2\theta \le 0{\cdot}60$. The atomic positions are derived from intensity data from a set of multiple-film Weissenberg photographs for $l = 0$ to 4 with rotation about the *c* axis. The calculations are based

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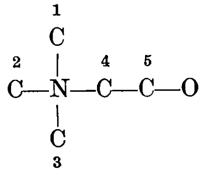
‡ R. E. Lemmon, private communication, 1956.

on a total of 357 independent reflections including 72 too weak to be observed.

The systematic absences correspond to space group $P2_12_12_1$, and a satisfactory structure was found with that symmetry. Each atom of the molecule is crystallographically independent and occurs in the four-fold general set of positions:

$$x, y, z;\ \tfrac{1}{2}-x, \bar{y}, \tfrac{1}{2}+z;\ \tfrac{1}{2}+x, \tfrac{1}{2}-y, \bar{z};\ \bar{x}, \tfrac{1}{2}+y, \tfrac{1}{2}-z\,.$$

In describing the structure, the carbon atoms are designated as follows:



$$\begin{array}{c} \overset{1}{C} \\ {}^{2}C-\overset{|}{\underset{|}{N}}-\overset{4}{C}-\overset{5}{C}-O \\ \underset{3}{C} \end{array}$$

The x, y coordinates of chloride ion were located by the Patterson projection $P(x, y)$. An electron-density projection with signs based on the chloride ion showed the molecule without resolution of any atoms. Consideration of bond lengths led to a trial structure which on refinement in this projection by Fourier and least-squares methods gave x, y coordinates for N and the methyl carbons which agree within 0·1 Å with the final structure. At this point C_4, C_5 and O were not resolved. Consideration of the Harker sections $P(x, \frac{1}{2}, z)$ and $P(\frac{1}{2}, y, z)$ with bond length considerations gave a complete structure which was refined by least squares using the IBM-650 computer and the three-dimensional data. The method of weighting and the treatment of unobserved reflections have been described by Hardgrove & Templeton (1959). The resulting structure is reported elsewhere (Senko, 1957). Subsequently it was discovered that by an arithmetic error the standard deviations had been overestimated. To obtain the accuracy indicated by the new standard deviations the refinement was continued for 8 additional cycles to give the slightly different structure reported here. In the last cycles the treatment of unobserved reflections was changed so that $F_o - F_c$ was taken as $F_{\text{min.}} - F_c$ rather than $-F_c$, when $F_c > F_{\text{min.}}$, to diminish erratic shifts which the earlier method produced. The final 'unreliability factors' (as designated by Senko & Templeton, 1958) were:

$$R_1 = 0{\cdot}109;\ R_2 = 0{\cdot}127;\ R_3 = 0{\cdot}148$$

for 285 observed reflections. The final atomic coordinates, their standard deviations, and the isotropic temperature factors are listed in Table 1. No allowance has been made for systematic errors due to omission of hydrogen atoms from the calculations nor for effects of the radiation damage to the crystals. The temperature factors are considered to be upper limits because effects of the radiation damage tend to make them larger than the true values for the intact crystal.

Table 1. *Final atomic parameters and isotropic temperature factors*

	x	y	z	B (Å^2)
Cl	−0·2203 ± 0·0003	0·2287 ± 0·0003	0·1627 ± 0·0007	5
O	0·1247 ± 0·0010	0·1091 ± 0·0009	0·114 ± 0·002	6
N	−0·0059 ± 0·0008	−0·0024 ± 0·0009	0·558 ± 0·002	4
C_1	−0·0545 ± 0·0014	−0·0560 ± 0·0012	0·337 ± 0·003	5
C_2	−0·1011 ± 0·0017	0·0678 ± 0·0014	0·679 ± 0·004	7
C_3	0·0320 ± 0·0013	−0·0983 ± 0·0012	0·714 ± 0·003	5
C_4	0·1199 ± 0·0017	0·0587 ± 0·0015	0·519 ± 0·004	7
C_5	0·1122 ± 0·0016	0·1538 ± 0·0015	0·332 ± 0·004	7

Observed and calculated structure factors are listed in Table 3.

Discussion of the structure

The bond distances in the choline molecule are listed in Table 2. The N–C_4 bond, which is broken in the radiation-induced decomposition, is observed longer than an ordinary single bond. All the other bonds have normal lengths. The configuration of the molecule with respect to rotation about the C_4–C_5 bond is approximately *gauche*, with an angle of 84° between the planes of N, C_4, C_5 and C_4, C_5, O. This angle would be 60° for an ideal *gauche* configuration. Takeuchi & Pepinsky (1956) reported a *gauche* configuration in choline reineckate.

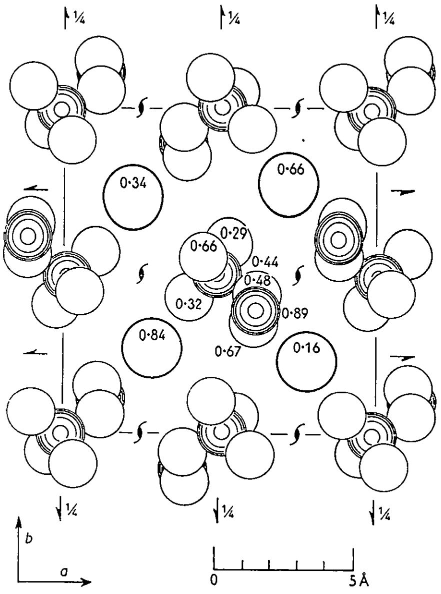


Fig. 1. Crystal structure of choline chloride, projected along c. The larger circles represent chlorine atoms. Nitrogen and oxygen atoms are shaded. The numbers on or near atoms are their z coordinates. Hydrogen atoms are not shown.

The packing of the molecules, shown in Fig. 1, is dominated by ionic forces. Each nitrogen has three chloride neighbors nested between the methyl substituents at distances of 4·08, 4·22, and 4·28 Å (each ±0·02 Å). A total of six chloride ions can be considered as neighbors of some part of the choline molecule, but the configuration of these ions is not that

Table 2. *Bond distances in choline chloride*, in Å, *each* ±0·03 Å

N–C_1	1·53	N–C_4	1·60
N–C_2	1·52	C_4–C_5	1·56
N–C_3	1·50	C_5–O	1·39

of any symmetrical polyhedron. Each chloride ion has three nitrogen neighbors and is also close to an oxygen atom. The C₅–O–Cl angle of 109° suggests hydrogen bonding between oxygen and chloride, although the O–Cl distance of 3·03 ± 0·02 Å is more like the non-bonded distance 3·05 Å in hydroxylammonium chloride (Jerslev, 1948) than the distance 2·99 Å in the same crystal which presumably is hydrogen-bonded. Other O–H · · · Cl bonds are reported with lengths 2·91 and 2·99 Å in tropolone hydrochloride (Sasada, Osaki & Nitta, 1954) and 2·95 Å in hydronium chloride (Yoon & Carpenter, 1959). In choline chloride the hydrogen bonding, if any, must be considered relatively weak.

It is noteworthy that the oxygen atoms are not hydrogen bonded to each other in chains, as is common for alcohols. The absence of such chains must be attributed to dominance by the ionic forces which

Table 3. *Observed and calculated structure factors for choline chloride*

Each structure factor has been multiplied by 2·5

An asterisk after an observed structure factor denotes that it is the observational limit for an unobserved reflection

h	k	ℓ	$\|F_o\|$	$\|F_c\|$
0	2	0	55	34
0	4	0	30	47
0	6	0	72	81
0	8	0	30	27
1	1	0	32	33
1	2	0	65	66
1	3	0	7*	1
1	4	0	20	18
1	5	0	77	82
1	6	0	11*	4
1	7	0	54	59
1	8	0	14*	5
1	9	0	30	29
1	10	0	15*	4
1	11	0	28	27
2	0	0	57	29
2	1	0	28	27
2	2	0	206	225
2	3	0	95	103
2	4	0	80	64
2	5	0	42	39
2	6	0	46	48
2	7	0	13*	12
2	8	0	14*	15
2	9	0	15*	3
3	1	0	33	41
3	2	0	132	137
3	3	0	96	96
3	4	0	39	30
3	5	0	14	14
3	6	0	17	19
3	7	0	21	21
3	8	0	25	29
3	9	0	37	42
4	0	0	18	16
4	1	0	67	72
4	2	0	66	56
4	3	0	61	61
4	4	0	105	114
4	5	0	34	42
4	6	0	13*	2
4	7	0	14*	4
4	8	0	32	30
4	9	0	28	15
5	1	0	51	57
5	2	0	62	63
5	3	0	11	10
5	4	0	64	59
5	5	0	22	19
5	6	0	40	36
5	7	0	30	23
5	8	0	22	22
6	0	0	35	32
6	1	0	90	101
6	2	0	43	41
6	3	0	20	22
6	4	0	13*	2
6	5	0	28	17
6	6	0	28	30
6	7	0	40	39
7	1	0	16	18
7	2	0	13	8
7	3	0	13*	3
7	4	0	34	35
7	5	0	14*	1
7	6	0	25	27
7	7	0	20	15
7	8	0	23	23
8	0	0	35	44
8	1	0	42	40
8	2	0	15	12
8	3	0	40	41
8	4	0	15*	2
8	5	0	40	37
8	6	0	15*	5
9	1	0	15*	15
9	2	0	31	38
9	3	0	15*	9
9	4	0	15*	1
9	5	0	15*	14
9	6	0	28	21
10	0	0	23	19
10	1	0	25	23
10	2	0	15*	2
10	3	0	32	29
0	2	1	85	91
0	3	1	47	45
0	4	1	86	85
0	5	1	23	23
0	6	1	15*	11
0	7	1	37	42
0	8	1	44	47
1	1	1	114	127
1	2	1	50	55
1	3	I	149	166
1	4	1	26	26
1	5	1	60	65
1	6	1	44	46
1	7	1	25	24
1	8	1	18*	9
2	1	1	67	72
2	2	1	38	35
2	3	1	64	68
2	4	1	39	44
2	5	1	39	39
2	6	1	54	59
2	7	1	24	29
2	8	1	26	24
3	0	1	102	113
3	1	1	150	161
3	2	1	43	46
3	3	1	14	17
3	4	1	24	23
3	5	1	54	54
3	6	1	20	16
3	7	1	23	28
3	8	1	40	41
4	0	1	45	51
4	1	1	44	46
4	2	1	14	15
4	3	1	40	31
4	4	1	38	32
4	5	1	46	53
4	6	1	47	43
4	7	1	18*	16
4	8	1	27	28
5	0	1	29	19
5	1	1	43	41
5	2	1	61	54
5	3	1	56	56
5	4	1	52	54
5	5	1	17*	6
5	6	1	43	34
5	7	1	36	36
6	0	1	34	26
6	1	1	51	58
6	2	1	44	41
6	3	1	36	38
6	4	1	34	30
6	5	1	18*	8
6	6	1	23	23
6	7	1	33	30
7	0	1	48	50
7	1	1	19	14
7	2	1	39	32
7	3	1	18*	13
7	4	1	53	46
7	5	1	38	35
8	0	1	29	29
8	1	1	19*	14
8	2	1	23	25
8	3	1	19*	10
8	4	1	22	21
8	5	1	34	30
9	0	1	31	28
9	1	1	20*	12
9	2	1	43	41
0	2	2	62	72
0	3	2	16	14
0	4	2	18*	12
0	5	2	21*	14
0	6	2	42	42
0	7	2	32	35
0	8	2	29*	1
0	9	2	54	53
1	1	2	41	48
1	2	2	88	103
1	3	2	42	33
1	4	2	80	82
1	5	2	45	39
1	6	2	23	21
1	7	2	27	32
1	8	2	29*	14
2	0	2	25	32
2	1	2	27	31
2	2	2	33	30
2	3	2	41	49
2	4	2	65	64
2	5	2	43	41
2	6	2	38	36

Table 3 (*cont.*)

h	k	ℓ	$\|F_o\|$	$\|F_c\|$
2	7	2	49	44
2	8	2	28	20
3	0	2	81	92
3	1	2	54	60
3	2	2	45	51
3	3	2	32	34
3	4	2	30	35
3	5	2	31	31
3	6	2	44	46
3	7	2	28	29
3	8	2	27	21
4	0	2	29	24
4	1	2	16	19
4	2	2	35	33
4	3	2	40	32
4	4	2	35	39
4	5	2	53	58
4	6	2	41	38
4	7	2	29*	3
4	8	2	29	19
5	0	2	28	34
5	1	2	32	39
5	2	2	38	37
5	3	2	69	70
5	4	2	21	20
5	5	2	27*	22
5	6	2	29	23
6	0	2	27	31
6	1	2	28	28
6	2	2	28	33
6	3	2	30	31
6	4	2	26	20
6	5	2	29*	2
6	6	2	27	18
7	0	2	27*	21
7	1	2	45	43
7	2	2	28*	12
7	3	2	34	36
7	4	2	30*	9
7	5	2	32	32
8	0	2	30*	16
8	1	2	30	29
9	1	2	31	30
0	2	3	13	11
0	3	3	22	30
0	4	3	17*	3
0	5	3	57	63
0	6	3	22*	5
0	7	3	34	32
0	8	3	26*	2
1	1	3	13	12
1	2	3	17	17
1	3	3	18	14
1	4	3	63	65
1	5	3	18	21
1	6	3	43	41
1	7	3	24*	8
1	8	3	27	21
2	0	3	12	12
2	1	3	40	61
2	2	3	59	60
2	3	3	71	71
2	4	3	18*	18
2	5	3	36	33
2	6	3	23*	13
2	7	3	25*	20
3	0	3	25	26
3	1	3	15*	17
3	2	3	30	30
3	3	3	18*	16
3	4	3	21	14
3	5	3	22*	6
3	6	3	28	26
3	7	3	29	29
3	8	3	40	35
4	0	3	47	52
4	1	3	41	50
4	2	3	24	33
4	3	3	29	36
4	4	3	28	35
4	5	3	23*	20
4	6	3	40	29
5	0	3	20*	18
5	1	3	20*	19
5	2	3	20	24
5	3	3	22*	16
5	4	3	23*	5
5	5	3	32	31
5	6	3	31	25
6	0	3	46	54
6	1	3	18	15
6	2	3	31	28
6	3	3	22	21
6	4	3	28	24
6	5	3	26*	15
6	6	3	30	29
7	0	3	25*	7
7	1	3	25*	14
7	2	3	25*	8
7	3	3	26	23
7	4	3	28	25
8	0	3	26*	26
8	1	3	26*	9
8	2	3	37	36
0	2	4	25	31
0	3	4	23	26
0	4	4	8*	9
0	5	4	9*	2
0	6	4	17	15
0	7	4	33	33
0	8	4	11*	10
0	9	4	16	15
1	1	4	4*	3
1	2	4	38	40
1	3	4	7	7
1	4	4	25	24
1	5	4	27	26
1	6	4	25	23
1	7	4	23	20
1	8	4	14	12
1	9	4	10*	6
2	0	4	25	30
2	1	4	21	20
2	2	4	32	40
2	3	4	20	20
2	4	4	15	18
2	5	4	39	38
2	6	4	16	16
2	7	4	11	10
2	8	4	11*	11
2	9	4	16	16
3	0	4	23	25
3	1	4	17	17
3	2	4	31	28
3	3	4	28	26
3	4	4	29	30
3	5	4	17	15
3	6	4	16	16
3	7	4	12	13
3	8	4	12	11
3	9	4	15	14
4	0	4	8*	2
4	1	4	19	21
4	2	4	18	19
4	3	4	32	31
4	4	4	34	34
4	5	4	11	12
4	6	4	10*	10
4	7	4	14	17
5	0	4	9*	2
5	1	4	27	29
5	2	4	25	27
5	3	4	25	26
5	4	4	16	17
5	5	4	12	9
5	6	4	20	15
5	7	4	12	10
6	0	4	13	14
6	1	4	21	21
6	2	4	10*	7
6	3	4	16	19
6	4	4	10*	9
6	5	4	14	13
6	6	4	12	14
6	7	4	12	10
7	0	4	24	27
7	1	4	24	27
7	2	4	11*	4
7	3	4	16	13
7	4	4	12	9
7	5	4	18	18
7	6	4	11	12
8	0	4	11*	2
8	1	4	15	17
9	0	4	10*	7
9	1	4	11	13

disperse the bulky molecules. For example, it may be that no chain structure is consistent with sufficient dispersal. It can also be shown that hydrogen bonds do not exist between oxygen atoms in choline bromide or choline iodide, if the space groups suggested above are correct. In these space groups, with the stated cell contents, all oxygen atoms must be equivalent. An examination of the coordinates of equivalent sets of the proper multiplicities reveals in each case that no two atoms can be closer than half the shortest cell dimension, because of the translation components of the symmetry elements. The shortest possible distance is 2·84 Å, in the bromide. This distance is long for an O–H · · · O bond and corresponds to all the oxygen atoms being on a straight line. Any deviation sufficient to achieve a reasonable bond angle leads to a distance which is much too long to be considered a hydrogen bond.

The radiation sensitivity remains to be explained. We offer no explanation based on the long C–N bond because that distance may be a spurious effect of the radiation damage of our crystal and because we know of no accurate measurement of this bond in the more stable phases. We hope that the present work will at least rule out some of the speculations which otherwise might be proposed as explanations of this effect.

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Structures of 1:3:5-Trichlorobenzene at 20 °C. and −183 °C., and of 1:3:5-Tribromobenzene at 20 °C.

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$C_6H_3Cl_3$, $C_6H_3Br_3$ are isomorphous, $P2_12_12_1$ with $Z = 4$. The structure is of a layer type, the molecules being planar and inclined at about ±27° to (001). The mean thermal expansion coefficients for $C_6H_3Cl_3$ from −183 °C. to 20 °C. are 58, 46, 109×10^{-6} along *a*, *b*, *c* respectively. The lack of exact triangular symmetry of the molecule is shown both in the lengths of intermolecular bonds and in the anisotropy of the atomic Debye factors. The structure is compared with those of other symmetrically-substituted ring compounds.

Introduction

This work was undertaken for the following reasons:

(1) Derivation of structures at different temperatures is essential for knowledge of the way in which various physical phenomena are related—for example, atomic and molecular vibrations and thermal expansion coefficients.

(2) A study of isomorphous compounds is useful not only for the actual process of structure analysis, but also for giving information about the degree of reliability of determination of light-atom parameters in the presence of heavier atoms.

(3) 1:3:5-triphenylbenzene is a polar structure of a layer type (Farag, 1954). It was interesting to see whether other symmetrically-substituted derivatives $C_6H_3R_3$ would crystallize similarly.

(4) A comparison of the structures of $C_6H_3Cl_3$, of cyanuric trichloride $C_3N_3Cl_3$ and of B-trichloroborazole $B_3N_3H_3Cl_3$, and of their molecular diamagnetic susceptibilities (which can only be deduced from the crystal susceptibilities when the structures are known) would give valuable information concerning the π-electron orbital areas for these three compounds and perhaps throw some light on packing forces.

Experimental details

The X-ray examination was carried out by L. M. Pant, who also deduced the preliminary structures. H. J. Milledge prepared Pegasus computer programmes and refined the structures.

$C_6H_3Cl_3$ and $C_6H_3Br_3$ are isomorphous and there is no discontinuous structure transition between room and liquid-nitrogen temperatures.

The only systematic absences are $\{h00\}$ for h odd, $\{0k0\}$ for k odd, $\{00l\}$ for l odd. The space group $P2_12_12_1$ was confirmed by Patterson and Fourier projections. Unit-cell dimensions are as follows:

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