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Crystal Structure and Absolute Configuration of the Hydrochloride and Hydrobromide of D(—)-Isoleucine

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The hydrochloride and hydrobromide of D(−)-isoleucine crystallize with one molecule water in the orthorhombic space group $P2_12_12_1$. The cell edges of the hydrochloride are: $a = 6{\cdot}13$, $b = 25{\cdot}01$, $c = 6{\cdot}79$ Å, and those of the hydrobromide are: $a = 6{\cdot}21$, $b = 24{\cdot}4$, $c = 7{\cdot}00$ Å. There are four molecules in the unit cell. The two compounds appear not to be isomorphous. The crystal structure of both has been determined mainly by the use of the heavy-atom techniques. The 'inorganic part' of the structure is nearly identical in the two compounds, but the carbon chain has a different orientation. The molecules are arranged in double layers parallel to the *ac* plane, with their aliphatic chains protruding and their carboxyl and amino groups linked by hydrogen bonds to the halogen ions and the water molecules; between the layers only van der Waals forces act. In the molecule the methyl group and the amino group are in *cis* position with respect to each other. By exciting the bromine with U $L\alpha_1$ radiation the absolute configuration of D-isoleucine has been checked; the result is in agreement with the convention of Fischer and confirms expectation.

Introduction

Up till now the crystal structures of some fifteen amino acids have been determined. The present paper describes the crystal structure of the hydrochloride and the hydrobromide of isoleucine, one of the essential constituents of proteins, occurring, for example, in casein from cow's milk. The molecule contains two asymmetric carbon atoms; consequently there are four stereo-isomers: D- and L-isoleucine and D- and L-allo-isoleucine (Greenstein, Levintow, Baker & White, 1951). Chemically it is unknown which configuration corresponds to isoleucine. A Fourier synthesis will immediately reveal the relation between the two centres of asymmetry. The hydrobromide was chosen because of the possibility of checking the *absolute* configuration of the molecule (Bijvoet, Peerdeman & van Bommel, 1951).

Experimental

Crystals of D-isoleucine hydrochloride and hydrobromide were obtained by adding concentrated hydrochloric acid or hydrobromic acid to a suspension in acetone of pure D(−)-isoleucine from Hoffmann–La Roche and Co. and allowing the solution to evaporate slowly over soda lime *in vacuo*. The crystals of the hydrochloride are thin laths elongated along [100]. Always {010} is prominently developed and {001}, {100} and {101} are the terminal faces. Easy cleavage along (010) occurs. The crystals of the hydrobromide grow in the shape of flat squares with {010} as basal plane and {101} and sometimes also {100} as terminal faces. The crystals cleave easily along (010) and less prominently along (100). On exposure to air they lose slowly their crystal water; they were therefore sealed in thin capillaries of 'Sibor' glass before X-ray examination. Chemical analysis indicated the presence of one molecule water per molecule isoleucine.

The cell dimensions have been determined from rotation photographs with Cu $K\alpha$ radiation; the density was measured by flotation in a toluene–chloroform mixture. The results for the hydrochloride are:

$$a=6{\cdot}13,\ b=25{\cdot}01,\ c=6{\cdot}79\ \text{Å}\pm0{\cdot}3\%,\ U=104(1)\text{Å}^3,$$
$$D_m=1{\cdot}19\ \text{g.cm.}^{-3},\ Z=4,\ D_X=1{\cdot}18(4)\ \text{g.cm.}^{-3}.$$

For the hydrobromide the corresponding data are determined somewhat less accurately as:

$$a = 6{\cdot}21,\ b = 24{\cdot}4,\ c = 7{\cdot}00\ \text{Å}\pm0{\cdot}6\%,$$
$$U = 106(2)\ \text{Å}^3,\ Z = 4,\ D_X = 1{\cdot}44\ \text{g.cm.}^{-3}.$$

On Weissenberg photographs systematic absences in the $h00$, $0k0$ and $00l$ reflexions indicated for both compounds that the space group is $P2_12_12_1$.

Intensity data for the $hk0$ and $0kl$ reflexions were recorded with Cu $K\alpha$ radiation on zero-level Weissenberg films about the c and a axes by the multiple-film technique and were measured by visual comparison with an intensity scale. Absorption was minimized, but not corrected for, by cutting very small parallelopipida of almost uniform cross-section from the crystals. Corrections for Lorentz and polarization factors were applied and the observed structure amplitudes were brought to an absolute scale afterwards by scaling against the calculated values. The scattering curves for Br^-, Cl^-, O, N and C as given in *Internationale Tabellen* were corrected by a temperature factor, obtained from the ratio $|F_o|/|F_c|$ against $\sin^2\theta$.

The Fourier summations were made partially with Beevers–Lipson strips at intervals of 6° along the a

and c axes and of 3° along the b axis and partially with IBM punched cards.

For the determination of the absolute configuration a crystal of the hydrobromide was carefully ground on a watchmaker's lathe into a cylindrical rod about the c axis. A first-level Weissenberg photograph was recorded with U $L\alpha_1$ rays, which were monochromatized with a curved quartz crystal. As the X-ray tube could operate at only 100 W., an exposure time of 400 hr. was necessary.

Structure determination of the hydrochloride

Since the a and c axes are comparatively short and the b axis is rather long, only projections on (100) and (001) are used in the investigation.

The a-axis projection

A Patterson projection along the a axis was constructed for the hydrochloride and the hydrobromide. Since the space group $P2_12_12_1$ contains only fourfold general positions halogen–halogen vector peaks will occur at $(2y, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}-2z)$ and $(\frac{1}{2}-2y, 2z)$. The Patterson projections showed three heavy peaks corresponding to these vector sets and gave for the chlorine ion the co-ordinates: $y = 61°$, $z = 26°$ and for the bromine ion: $y = 58°$, $z = 26°$. These values, the cell dimensions and the approximately identical appearance of the two Patterson projections seemed to indicate the isomorphism of the hydrochloride and the hydrobromide.

The isomorphous replacement method was therefore applied to fix the phases of the majority of the reflexions. On the Fourier projection of the hydrochloride, obtained with these phases, several models could be matched. Structure factors were calculated for these models and the decrease of the value of the reliability index $R = \Sigma(|F_o - F_c|)/\Sigma|F_o|$ after one adjustment of the co-ordinates from a Fourier projection was used as a test for the correctness of the model.

After some successive Fourier refinements of the model selected the [100] projection of Fig. 1 was obtained with $R = 0{\cdot}23$. Further refinement of the co-ordinates was carried out with a least-squares method, minimizing $\sum\limits_{kl}(F_o - F_c)^2$. After one refinement the reliability index had decreased very little. A $(F_o - F_c)$ synthesis was constructed (Cochran, 1951) and revealed that the methyl group must be displaced. With this new model the least-squares method rapidly diminished the value of R down to 0·18. This model was confirmed afterwards by the [001] projection.

A temperature factor with $B = 2{\cdot}80$ Å^2 was applied for all atoms, obtained from the ratio $|F_o|/|F_c|$ against $\sin^2\theta$. The $(F_o - F_c)$ synthesis indicated an asymmetric temperature factor for the chlorine ion and larger temperature factors for C_4, C_5 and C_6 (for the numbering of the atoms see Fig. 4(b)). To the chlorine ion a temperature factor $\exp[-(B+\beta\cos^2\varphi) \times (\sin\theta/\lambda)^2]$ was attributed, where φ denotes the angle between the direction of maximum vibration and the normal of the reflecting net plane (Helmholtz, 1936). For the chlorine ion was chosen $B = 2{\cdot}80$ Å^2 and $\beta = 1{\cdot}00$ Å^2, for the C_4 atom $B = 4{\cdot}40$ Å^2 and for the C_5 and C_6 atoms $B = 6{\cdot}00$ Å^2. With these values the agreement between calculated and observed structure factors had notably improved and the final value of R is 0·147.

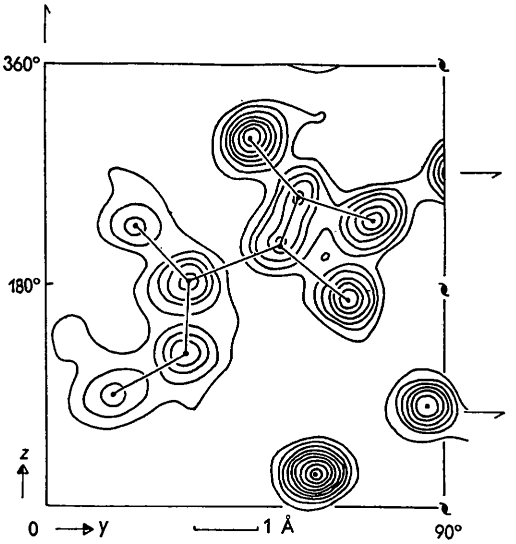

Fig. 1. Electron density of isoleucine-HCl.1H$_2$O, projected on (100). Wrong model with $R = 0{\cdot}23$.

The final projection of the electron density along the a axis is shown in Fig. 2(a) and the arrangement of the molecules in the a-axis projection is drawn in Fig. 5(a).

The c-axis projection

The x parameter of the halogen ion was derived from Patterson projections along the c axis in the same way as described above for the y and z parameters. The results are: $x_{Cl} = 57°$ and $x_{Br} = 66°$. The y parameters were in full agreement with those found in the a-axis projection.

A Fourier projection of the hydrochloride, constructed with the phases obtained by the isomorphous-replacement method, had many spurious peaks. It was not possible to fit a model that gave a reasonable agreement between calculated and observed structure factors. Then, for the hydrochloride and the hydrobromide, Fourier projections were made with their strongest reflexions only, using the phases of the halogen contribution. These two Fouriers had a quite different appearance. Consequently the tentative conclusion was drawn that the hydrochloride and the hydrobromide are not isomorphous.

With the Patterson projection of the hydrochloride a vector-convergence map (Beevers & Robertson, 1950) was constructed. Combining the results of this map,

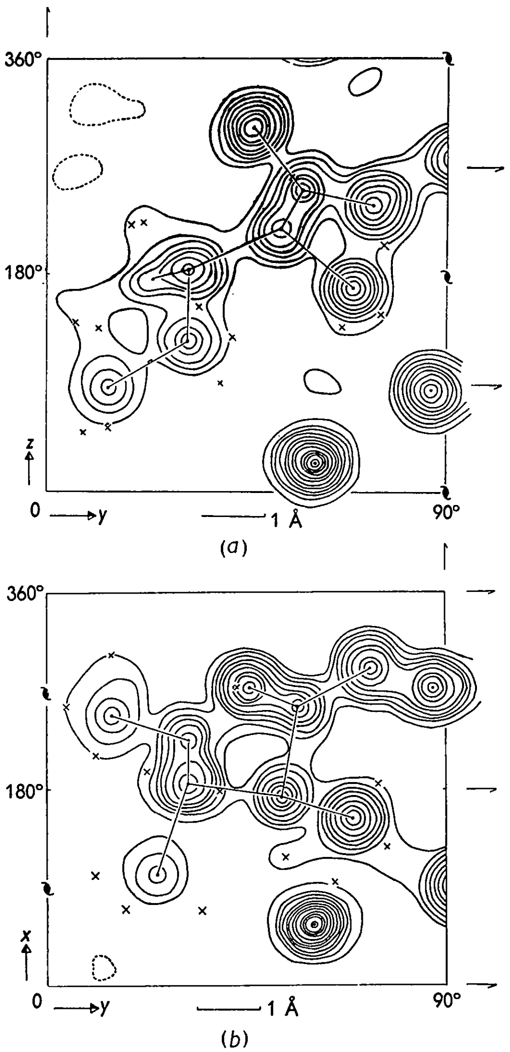

Fig. 2. Electron density of isoleucine-HCl. $1H_2O$, projected (*a*) on (100), (*b*) on (001). Contours are drawn at intervals of 1 e.Å^{-2} (for the chlorine 2 e.Å^{-2}); the zero level is broken and the first full line is drawn at 2 e.Å^{-2}.

the Fourier projection constructed with the phases of the chlorine, spatial considerations and the *a*-axis projection already determined at that moment, it was possible to find a model which gave reasonable agreement between calculated and observed structure factors. The refinement of the coordinates was carried out with successive Fourier syntheses and later with the least-squares method, as for the *a*-axis projection. The same temperature factors as applied in the *a*-axis projection were indicated by the (F_o-F_c) synthesis. Inclusion of these temperature factors gave a further reduction of the reliability index and the final value of R is 0·143.*

The projection of the electron density along the *c* axis is shown in Fig. 2(*b*) and the arrangement of the molecules in this projection can be seen in Fig. 5(*b*). The shape of the molecule in the hydrochloride is drawn in Fig. 4(*b*); Fig. 4(*a*) gives the ordinary structure formula.

The final atomic coordinates, relative to the origin in *Internationale Tabellen*, are listed in Table 1†.

Table 1. *Atomic coordinates of the hydrochloride*

	$-x$	y	z
C_1	0·708	0·158	0·692
C_2	0·487	0·148	0·600
C_3	0·503	0·090	0·522
C_4	0·628	0·090	0·328
C_5	0·694	0·038	0·231
C_6	0·276	0·065	0·489
O_1	0·758	0·129	0·839
O_2	0·799	0·203	0·660
N	0·417	0·190	0·467
Cl	0·153	0·168	0·072
H_2O	0·756	0·243	0·226

An attempt was made to locate the hydrogen atoms. However, the (F_o-F_c) syntheses of both axes, though indicating maxima at some of the expected positions, gave no conclusive evidence for the location of all the H atoms. The positions expected from spatial considerations, except for the H atoms belonging to the water molecule and to the carboxyl group, are indicated by crosses in the Fig. 2. The calculation of the structure factors for these positions indeed indicated that appreciable influence on the intensities is to be expected for only a very few reflexions.

Structure determination of the hydrobromide

The phases of the greater part of the reflexions of the hydrobromide could be fixed from the phases of the contributions of the bromine ion. Fourier syntheses along the *a* and *c* axes were constructed with these phases and showed quite clearly the layout of the molecule. Refinement of the coordinates was done by successive Fourier syntheses. Owing to the very strong scattering of the bromine ion no further refinement with least-squares methods was judged to be worthwhile.

The final value of R amounts to 0·145 for the $0kl$ reflexions and 0·141 for the $hk0$ reflexions. The same asymmetric temperature factor as in the case of the chlorine has been applied for the bromine in the structure-factor calculations.

The projection of the electron density along the *a* and *c* axes is shown in Fig. 3. In both projections the electron density of the C_5 atom is a little too low. The same must be remarked with respect to the C_5 and the C_6 atom in the projections of the hydrochloride. The explanation for this fact is that chiefly weak reflexions with high value of sin θ happened to contribute to the electron density of these atoms and

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* The list of observed and calculated structure factors F_{hk0} and F_{0kl} will be published in the thesis of J. Trommel, Utrecht 1954.

† The minus sign is explained in the paragraph on the absolute configuration.

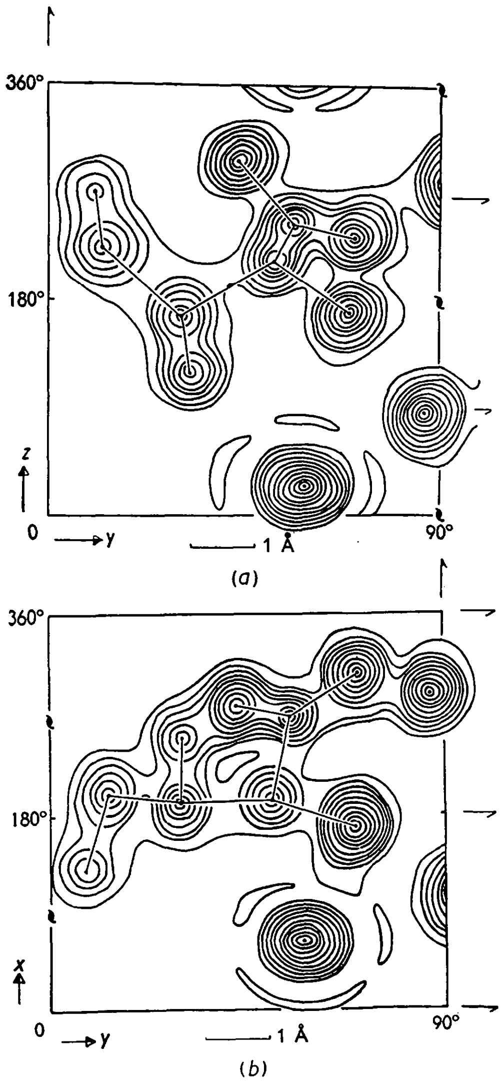

Fig. 3. Electron density of isoleucine-HBr.1H$_2$O, projected (a) on (100), (b) on (001). Contours drawn approximately at intervals of 1 e.Å^{-2} (for the bromine at 10 e.Å^{-2}); the first full line is at about 2 e.Å^{-2}.

the unobserved reflexions were not included in the calculation of the Fourier syntheses.

The arrangement of the molecules in the *a*- and *c*-axis projections is drawn in Fig. 6. The final atomic coordinates are listed in Table 2. Fig. 4(*c*) shows the shape of the molecule in the crystal of the hydrobromide.

Table 2. *Atomic coordinates of the hydrobromide.*

	$-x$	y	z
C_1	0·733	0·156	0·678
C_2	0·528	0·144	0·575
C_3	0·517	0·087^5	0·478
C_4	0·542	0·039	0·622
C_5	0·350	0·033	0·761
C_6	0·692	0·092	0·325
O_1	0·761	0·122	0·825
O_2	0·856	0·194	0·650
N	0·467	0·192	0·467
Br	0·186	0·161	0·072
H_2O	0·794	0·242	0·242

Accidentally it was found that crystals of the hydrochloride obtained by crystallization from a 96% alcoholic solution are isomorphous with the hydrobromide, as shown by structure-factor calculations. These crystals are unstable, however, and recrystallize into the (stable) modification obtained from the solution in acetone.

Determination of the absolute configuration

The principle on which it is possible to distinguish with X-rays between optical antipodes, was outlined by Bijvoet (1949). In using Zr $K\alpha$ rays, which excite the rubidium atom, Peerdeman, van Bommel & Bijvoet (1951) determined the absolute configuration of sodium rubidium tartrate and found it to be in agreement with the chemical convention of Fischer. With this determination all compounds which can be related chemically to tartaric acid are determined with respect to their optical behaviour.

Nevertheless, it was thought worthwhile to check the absolute configuration of isoleucine. The absorption edge of the *K* electrons of bromine is 0·918 kX. X-rays with a wave length a little shorter than this value will excite the *K* electrons, and it was found that for U $L\alpha_1$ radiation with $\lambda = 0{\cdot}9087$ kX., $\Delta f' = -4{\cdot}48$ and the imaginary part of the anomalous scattering $\Delta f'' = +3{\cdot}39$ (James, 1948).

Intensities were calculated for the model which corresponds to the D-configuration of Fischer. Using a positive coordinate system, one of the coordinates of Tables 1 and 2 must have a minus sign in order to correspond with the D-antipode. In Table 3 experimental and calculated relations between I_{hkl} and $I_{h\bar{k}l}$ are compared, the latter being equal to $I_{\bar{h}k\bar{l}}$ by symmetry. The visual estimations of the last column have been made by a few people independently. It is seen that the configuration is in agreement with the chemical convention.

Table 3. *Determination of the absolute configuration*

	Calculated		Observed
hkl	I_{hkl}	$I_{h\bar{k}l}$	I_{hkl} $I_{h\bar{k}l}$
111	395	449	<
121	474	428	>
131	164	185	<
141	281	314	<
151	590	620	<
161	15	20	Not observed
171	151	129	>
181	265	222	>
191	72	58	>
1,10,1	289	239	>
211	386	373	>
221	108	79	>
231	85	69	?
241	21	29	<

Discussion of results

Table 4. *Interatomic distances*

Intramolecular

	Hydrochloride	Hydrobromide
C_1–O_1	1·27 Å	1·33 Å
C_1–O_2	1·27	1·22
C_2–N	1·43	1·45
C_1–C_2	1·51	1·51
C_2–C_3	1·55	1·54
C_3–C_4	1·53	1·56
C_4–C_5	1·52	1·54
C_3–C_6	1·54	1·53

Intermolecular

	Hydrochloride	Hydrobromide
(Cl, Br)–N	3·18 Å	3·35 Å
(Cl, Br)–O_1	3·05	3·29
(Cl, Br)–H_2O	3·07	3·30
	3·24	3·35
N–H_2O	2·85	2·82
	2·96	2·84
N–O_2'	2·90	2·98
C_5–C_5'	3·95	4·05
C_5–C_3'	3·96	—
C_5–C_6'	4·03	4·20

The interatomic distances are given in Table 4 and the bond angles can be read from Fig. 4(*b*) and (*c*). The errors in the bond lengths are estimated to be of the order of 0·05 Å and in the angles of the order of 10°. Within these limits of error, all distances agree with those found in other similar compounds.

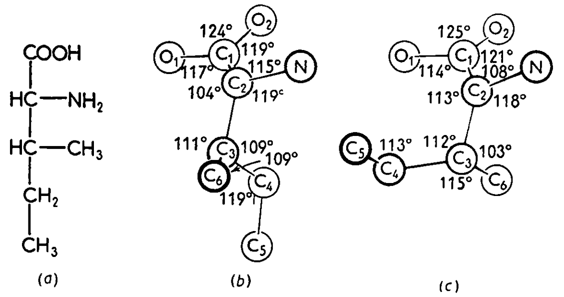

Fig. 4. Structure formulae of D-isoleucine, according (*a*) to chemical custom, (*b*) to the model in the hydrochloride and (*c*) to the model in the hydrobromide.

The shape of the molecule, seen as projected along the *a* axis, is drawn in Fig. 4(*b*) as in the hydrochloride and in Fig. 4(*c*) as in the hydrobromide. The ordinary chemical formula is given in Fig. 4(*a*). Contrary to expectation, the carbon chain C_1–C_5 is not flat. However, closer examination shows that a plane chain would give rise to an improbable short distance between O_1 and the methyl group C_6. In the crystal of the hydrochloride the carbon atoms C_1, C_2, C_3 and C_6 are approximately in a plane, and so are the carbon atoms C_2, C_3, C_4 and C_5. In the crystal of the hydrobromide only C_6, C_3, C_4 and C_5 are in one plane.

Within the limits of error the group $NC_2C_1O_1O_2$ is planar. In the hydrochloride the same value is found for the distances C_1–O_1 and C_1–O_2. In view of the inaccuracy of the bond lengths, no conclusions about the structure of the carboxyl group can be drawn from these distances. From the intermolecular distances, hydrogen bonds are possible between O_1 and Cl and between O_2' and N; the angle C_2–N–O_2', however, amounts to 160°, so it is concluded that the latter distance corresponds only to a short approach without a hydrogen bond (see Fig. 7). Consequently the O_1 atom must be the hydroxyl group. This is in agreement with the distances found in the crystal of the hydrobromide.

The amino group and the methyl group are in the *cis* position with respect to each other. So D-isoleucine is D-α-amino-D-β-methylvaleric acid and consequently D-allo-isoleucine is D-α-amino-L-β-methylvaleric acid.

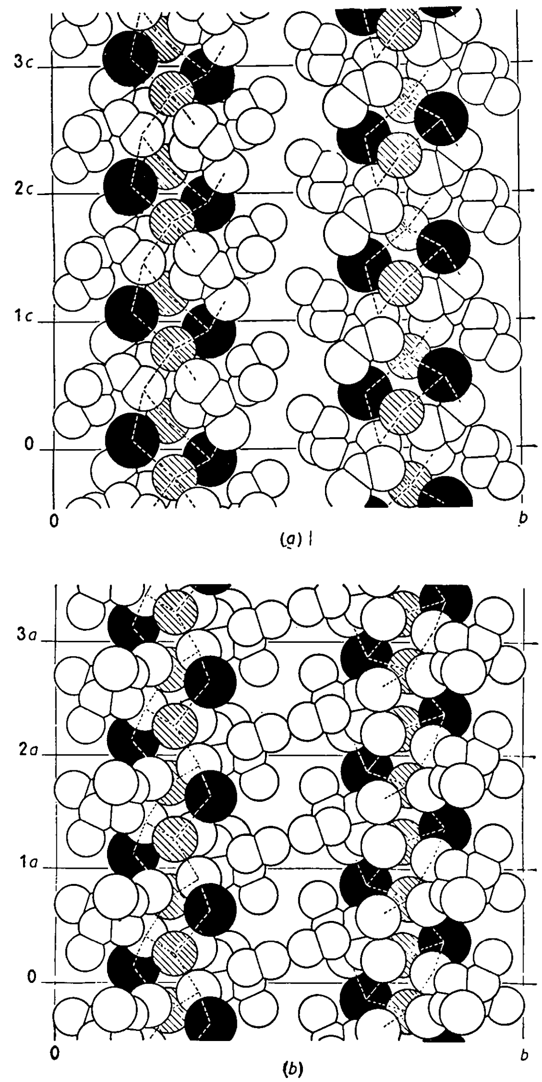

Fig. 5. Structure of D-isoleucine-HCl.1H_2O projected (*a*) on (100), (*b*) on (001). The chlorine ions are black and the water molecules are shaded. The dashed lines represent hydrogen bonds.

The molecular arrangement of the hydrochloride viewed along the *a* and *c* axes is shown in Fig. 5, and the arrangement of the hydrobromide in Fig. 6. The 'inorganic part' of the structure is nearly the same in both compounds. A network of hydrogen bonds in the *a* and *c* direction, indicated by dashed lines in the Fig. 5, exists between the halogen ions, the water molecules and the amino group and carboxyl group of the isoleucine molecule.

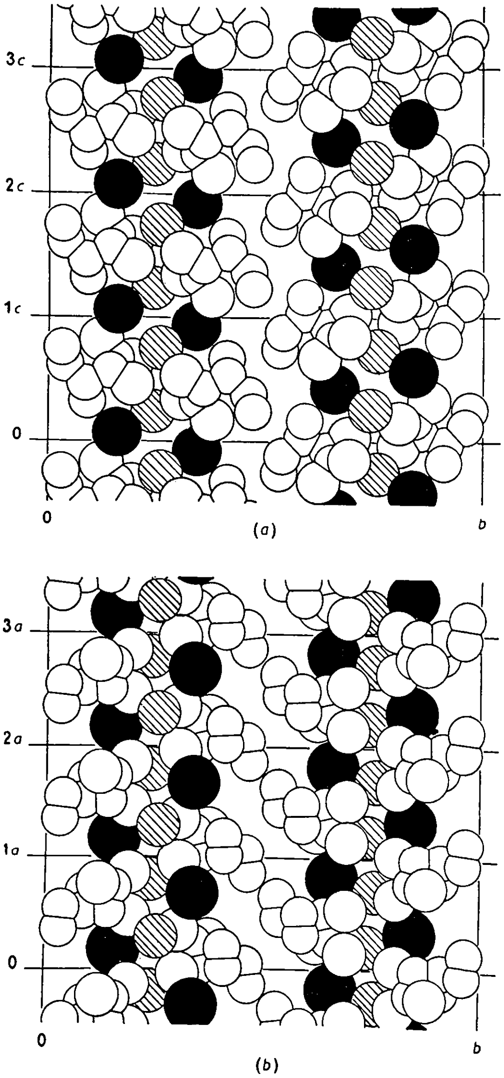

Fig. 6. Structure of D-isoleucine-HBr.$1H_2O$ projected (*a*) on (100), (*b*) on (001). The bromine ions are black and the water molecules are shaded. Hydrogen bonds are not indicated, but are the same as in Fig. 5.

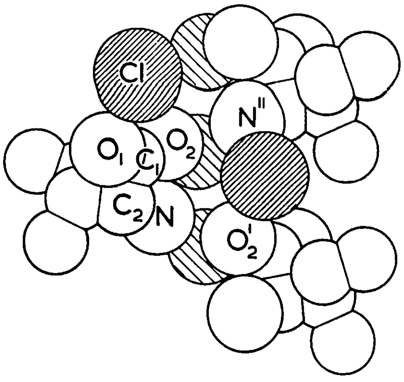

Fig. 7.

The amino group forms three hydrogen bonds directed along the apices of a tetrahedron, two with water molecules and one with the halogen ion. The water molecule is surrounded nearly tetrahedrally by two halogen ions and two amino groups at distances corresponding with hydrogen bonds (Table 4). The halogen ion is linked by four hydrogen bonds directed along the edges of a flat pyramid to two water molecules, the O_1 atom and the amino group. In this way firmly packed layers are formed parallel to (010) from which the carbon tails of the molecules protrude.

In the *b* direction only van der Waals forces between carbon atoms keep these layers together. This is in full accordance with the observed easy cleavage along (010). From the Figs. 5(*b*) and 6(*b*) it is clear that only the hydrobromide has some tendency to cleave along (100), as is found experimentally. The distances between carbon atoms of neighbouring molecules amount to 4·0 Å, as expected from the van der Waals radius of 2·0 Å of a methyl group (Pauling, 1940).

In spite of the small difference in radius of Cl^- and Br^- the hydrochloride and the hydrobromide are not isomorphous. In organic compounds the inorganic part of the structure, if present, evidently determines the general layout of the structure and the remaining organic part somehow fits as best it can. When branched carbon chains are present they seem to have a tendency to form plane zigzag chains of four carbon atoms.

It may be noted that the molecule of methionine (Mathieson, 1952) also crystallizes in two modifications, differing only in the orientation of the end of the carbon chain.

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A Theoretical Possibility of Correcting the Collimation Error in Small-Angle X-ray Scattering

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A general solution for correcting the collimation error in small-angle X-ray scattering is considered. The experimentally obtained intensity function can be expressed analytically as the convolution of the correct intensity function and the intensity distribution on the trace of the primary beam in the film. The correction of the experimental scattering curve is possible by using the convolution theorem for multiple Fourier transforms.

The effect of imperfect collimation of the primary beam on the angular intensity distribution of scattered radiation at small angles is called collimation error (Yudowitch, 1949*a*). Several authors have studied the possibility of correcting the experimentally obtained scattering curve (Jellinek & Fankuchen, 1945; Guinier & Fournet, 1947; DuMond, 1947; Shull & Roess, 1947; Franklin, 1950; Kratky, Porod & Kahovec, 1951). It was shown that the correction is possible only assuming that certain properties are attributed to the energy distribution in the primary beam, or to the shape of the beam-defining apertures, or to the shape of the scattering function. Yudowitch (1949*a*, *b*, 1952) investigated the geometrical conditions of the collimating system under which the collimation error may be reduced to its minimum.

Hosemann (1951) gave a general formula expressing the relationship between the experimental scattering function I and the correct function I_0; the latter would be obtainable if an incident parallel beam of infinitely small cross section were available. This formula does not imply any assumption of the energy distribution in the primary beam and of the shapes of the collimation apertures or of the shapes of scattering curves. The aim of this paper is to show that the correcting of experimental scattering function I is possible also in such a general case, using the convolution theorem for multiple Fourier transforms. The method to be described is analogous to the method of correcting the experimentally obtained line widths and shapes in Debye–Scherrer diagrams, proposed by Shull (1946) and applied by Stokes (1948). The difference between these two methods lies in the fact that the functions to be considered in the collimation-error problem are two-variable functions, while line-shape correcting could be regarded as a one-dimensional problem.

Let us deduce Hosemann's formula for the case of registering the small-angle scattering on a photographic film. The rectangle in Fig. 1 represents the trace of the primary beam on the film. We want to get the intensity of the scattered rays reaching the point $P(x, 0)$ on the film equator. A part of the energy of primary X-rays falling on the surface element $d\xi d\eta$ around the point M is scattered in the specimen towards the point P. The scattering angle of these rays is directly proportional to the distance MP. Thus the intensity of these scattered rays is proportional to $I_0(MP)$, or to $I_0(x-\xi, \eta)$. If we denote the intensity distribution function on the trace of the primary beam by $G(\xi, \eta)$, the contribution of the examined part of the incident beam to the intensity at point P is

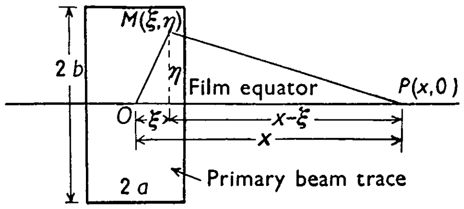

Fig. 1. See text for explanation.

$$dI = G(\xi, \eta)I_0(x-\xi, \eta)d\xi d\eta \, .$$

We obtain the whole intensity of radiation scattered