contraction of 2% is largely in a direction normal to the shearing movement:

Parameter of γ: $a = 3{\cdot}585$ Å;
whence $\frac{1}{2}a_\gamma\sqrt{2} = 2{\cdot}535$ Å, $\frac{2}{3}a_\gamma\sqrt{3} = 4{\cdot}140$ Å.
Parameters of ε: $a = 2{\cdot}528$ Å, $c = 4{\cdot}080$ Å.

The mechanism is of the type which produces a 'Widmanstätten' pattern of strain bands; and the contraction associated with the transformation limits the growth of ε around each nucleus. A photomicrograph (Fig. 2) confirms both the strain pattern and the absence of massive precipitate, although individual phases cannot be distinguished.

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Some implications of a theorem due to Shannon.

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Shannon (1949), in the field of communication theory, has given the following theorem: If a function $d(x)$ is known to vanish outside the points $x = \pm a/2$, then its Fourier transform $F(X)$ is completely specified by the values which it assumes at the points $X = 0, \pm 1/a, \pm 2/a, \ldots$. In fact, the continuous $F(X)$ may be filled in merely by laying down the function $\sin \pi aX/\pi aX$ at each of the above points, with weight equal to the value of $F(X)$ at that point, and adding.

Now the electron-density function $d(x)$ describing a single unit cell of a crystal vanishes outside the points $x = \pm a/2$, where a is the length of the cell. The reciprocal-lattice points are at $X = 0, \pm 1/a, \pm 2/a, \ldots$, and hence the experimentally observable values of $F(X)$ would suffice, by the theorem, to determine $F(X)$ everywhere, if the phases were known. (In principle, the necessary points extend indefinitely in reciprocal space, but by using, say, Gaussian atoms both $d(x)$ and $F(X)$ can be effectively confined to the unit cell and the observable region, respectively.)

For centrosymmetrical structures, to be able to fill in the $|F|^2$ function would suffice to yield the structure, for sign changes could occur only at the points where $|F|^2$ vanishes. The structure corresponding to the $|F|^2$ function is the Patterson of a single unit cell. This has twice the width of the unit cell, and hence to fill in the $|F|^2$ function would require knowledge of $|F|^2$ at the half-integral, as well as the integral h's. This is equivalent to a statement made by Gay (1951).

I think the conclusions which may be stated at this point are:

1. Direct structure determination, for centrosymmetric structures, could be accomplished as well by finding the sizes of the $|F|^2$ at half-integral h as by the usual procedure of finding the signs of the F's at integral h.

2. In work like that of Boyes-Watson, Davidson & Perutz (1947) on haemoglobin, where $|F|^2$ was observed at non-integral h, it would suffice to have only the values at half-integral h.

The extension to three dimensions is obvious.

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Unit-cell dimensions and space groups of synthetic peptides. I. Glycyl-L-tyrosine, glycyl-L-tyrosine hydrochloride, glycyl-DL-serine and glycyl-DL-leucine.

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The data presented here form part of an extended survey of crystalline peptides recently begun by the Wool Industries Research Association. The objects of the investigation are first to obtain some knowledge of the factors influencing the crystallization of these materials; secondly, from their unit-cell dimensions to obtain information regarding the types of molecular arrangements present, and thirdly to select materials suitable for a more detailed X-ray examination.

Source of peptides.

Glycyl-L-tyrosine was obtained from Roche Products, Welwyn Garden City, England, and the monohydrochloride was prepared from it by treatment with excess of 2N.HCl, followed by evaporation at room temperature. (Found 12·1% Cl; calculated 12·9%.)

Glycyl-DL-leucine and glycyl-DL-serine were synthesized by the chloracetyl chloride method first described by

Table 1. *Crystallographic data*

Peptide	Crystal system	Space group	Unit-cell dimensions	Density (g.cm.$^{-3}$)	Molecules/ unit cell
Glycyl-L-tyrosine $2H_2O$	Monoclinic	$P2_1$	$a = 11{\cdot}61$, $b = 10{\cdot}28$, $c = 5{\cdot}70$ Å	1·348	2·00
$NH_2.CH_2.CO.NH.CH(CH_2.C_6H_4OH).COOH.2H_2O$			$\beta = 97°\ 33'$		
Glycyl-L-tyrosine HCl. H_2O	Monoclinic	$P2_1$	$a = 14{\cdot}03$, $b = 9{\cdot}40$, $c = 5{\cdot}11$ Å	1·435	1·99
$NH_2.HCl.CH_2.CO.NH.CH(CH_2.C_6H_4OH).COOH.H_2O$			$\beta = 90°\ 55'$		
Glycyl-DL-leucine	Monoclinic	$P2_1$	$a = 15{\cdot}33$, $b = 5{\cdot}58$, $c = 6{\cdot}36$ Å	1·181	2·01
$NH_2.CH_2.CO.NH.CH(CH_2.CH(CH_3)_2)COOH$			$\beta = 101°\ 27'$		
Glycyl-DL-serine H_2O	Triclinic	$P1$ or $P\bar{1}$	$a = 4{\cdot}92$, $b = 11{\cdot}66$, $c = 15{\cdot}48$ Å	1·464	3·99
$NH_2.CH_2CO.NH.CH(CH_2OH)COOH.H_2O$			$\alpha = 69°\ 20'$, $\beta = 86°$, $\gamma = 77\frac{1}{2}°$		

Fischer & Otto (1903). Freedom from amino-acid contamination of the final peptide material was checked chromatographically—chromatograms of the peptide itself showed only a single spot and after hydrolysis two spots resulted corresponding to the constituent amino acids.

Crystals suitable for X-ray examination were in all cases obtained by isothermal evaporation of aqueous solutions. Unit-cell dimensions were derived from rotation photographs about the principal crystallographic axes. In the determination of the symmetry of the unit cell and the space group, information from stationary-film photographs was supplemented as required by zero- and n-layer moving-film photographs on an equi-inclination Weissenberg goniometer.

*Glycyl-*L*-tyrosine* readily yielded large prismatic crystals several millimetres across with {100}, {101} and {110} prominent. The only systematic absence observed was $0k0$ with k odd so that the space group is $P2_1$.

*Glycyl-*L*-tyrosine hydrochloride* also crystallized well but with a greater tendency to elongation along c. {100}, {110} and {011} were well developed. The same systematic absence was observed as in the case of the parent dipeptide so that the space group is again $P2_1$. Both materials contained water of crystallisation. Loss in weight on drying at 100° C. *in vacuo*:

Glycyl tyrosine, 12·9% (calculated for glycyl tyrosine. $2H_2O$, 13·1%);
Glycyl tyrosine HCl, 5·5% (calculated for glycyl tyrosine. H_2O, 6·1%).

*Glycyl-*DL*-leucine* yielded acicular crystals with b as the needle axis and with {100}, {001} and {201} prominent. They exhibited a pronounced cleavage parallel to 100. The only systematic absence observed was $0k0$ when k was odd so that the space group is apparently $P2_1$ with two molecules in the unit cell. As this space group excludes a racemic crystal it would appear that resolution occurred during crystallization, as already observed by Pasternak & Leonard (1952*a*, *b*) for DL-leucyl glycyine when attempting the preparation of racemic crystals from synthetic mixtures of the optical isomers.

*Glycyl-*DL*-serine* crystallized less well, generally in the form of rosette-like aggregates of very small crystals. A small fragment on which (100) and (001) were recognizable was employed in the X-ray examination. Water of crystallization was present in the unit cell. Loss in weight on drying at 100° C. *in vacuo*, 10·0% (calculated for glycyl serine. H_2O, 10·0%).

Weissenberg photographs revealed triclinic symmetry—the angle between the b and c axes was determined from measurements of the 011 spacing but the other two axial angles were read directly from the Weissenberg films and are of a lower order of accuracy. The space group is, therefore, $P1$ or $P\bar{1}$ with four glycyl serine and four water molecules in the unit cell.

The crystal structure of glycyl tyrosine hydrochloride is being examined in greater detail.

I am grateful to the Director and Council of the Wool Industries Research Association for permission to publish these results.

Thanks are due to Dr S. Blackburn of the Wool Industries Research Association for carrying out the necessary chromatographic tests on the synthetic peptides and for the gift of the glycyl-DL-serine.

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Structure of barium chlorate monohydrate, $Ba(ClO_3)_2.H_2O$.

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A series of isomorphous compounds of the type $A(BO_3)_2.H_2O$, where A is a divalent metal and B is a halogen, are known to exist. The most common among these being barium chlorate monohydrate, a complete structure analysis of the crystal has been undertaken and the results are given below.

Rotation and Weissenberg photographs gave the following data (Kartha, 1951):

$$a = 8{\cdot}86 \pm 0{\cdot}02,\ b = 7{\cdot}80 \pm 0{\cdot}02,\ c = 9{\cdot}35 \pm 0{\cdot}02\ \text{Å},\quad \beta = 93°\ 30',$$

whence the number of molecules per unit cell is four. The systematic absent reflexions were found to be hkl for $h+k+l$ odd and $h0l$ for h or l odd. Further, since the morphological studies (Groth, 1906–19, vol. 2, p. 114) showed the crystal to belong to the monoclinic prismatic class, the space group of the crystal is C_{2h}^6–I2/c with the above unit cell, which corresponds to the morphological axial ratios. By a transformation of axes this can brought to the standard orientation $C2/c$ as given in the *International Tables*.

The structure amplitudes were obtained from Weissenberg photographs (Mo radiation) using three films interleaved with silver foils. The crystals being elongated with c as neddle axis, the c-axis zero-level photograph was taken by the normal-beam method, whereas the a-axis and b-axis zero-level photographs were obtained by the anti-equi-inclination method. The intensities were estimated visually by comparison with standard intensity spots. They were corrected for Lorentz and polarization factors, according to Buerger & Klein (1945) in the case of the c-axis photograph and according to Kartha (1952) for a- and b-axis photographs. The relative sets of intensities thus observed were put on an absolute scale using the statistical method of Wilson (1942). This method also gave the temperature factors for the various zones.

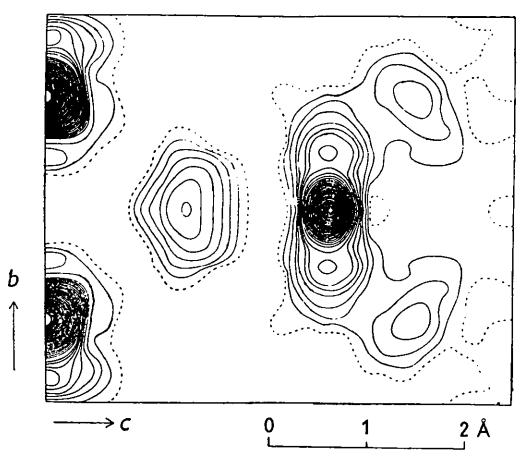

Fig. 1. The (100) Fourier projection showing one quarter of the unit cell. Contours at intervals of 2, 4 and 8 e.Å^{-2} around oxygen, chlorine and barium respectively.

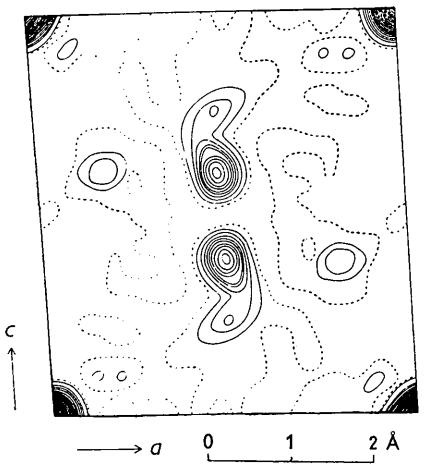

Fig. 2. The (010) Fourier projection showing one quarter of the unit cell. Contours at intervals of 10 e.Å^{-2} around barium and 5 e.Å^{-2} around other atoms.

The structure determination was based on two-dimensional Patterson and Fourier projections along three axes. The c-axis Patterson projection helped to fix the barium and chlorine positions in the projection. The signs of the combined barium and chlorine contributions to the $hk0$ reflexions were calculated and these signs were used in making the Fourier synthesis. After Fourier refinement a good set of x and y coordinates were obtained for those atoms which were well resolved in the projection. In the b projection, the projected unit cell is only a quarter of the complete unit cell and contains only one barium atom. The atomic number of barium being far more than that of any other atom in the unit cell, the heavy-atom method was used to obtain the Fourier projection. This projection after refinement gave the x and z coordinates. Patterson and Fourier projections were also made on the (100) plane. The a and b Fourier projections are given in Figs. 1 and 2 respectively, while Fig. 3 gives a perspective diagram of the unit cell.

The final values of the atomic coordinates were obtained by making use of all the projections. The values expressed as fractional coordinates, with the unit cell given above and with the origin at a centre of symmetry, are as follows: