

the values. The construction and use of the nomogram is best understood by some examples.

The construction of a nomogram

Two methods are possible: (1) draw a set of curves for different values of $|F|^2$; or (2) draw only the curve for $|F|^2 = 1$ and then use a logarithmic scale. The second alternative is the simpler as it requires very little time.

Suppose we are interested in the $|F|^2$ values from a photograph with $\mu = 11.2$ (Fig. 1(a)). Then we first draw a line parallel to the ξ axis at $\mu = 11.2$ in a chart of the old type. The points a , b and c correspond to a_1 , b_1 and c_1 , and the actual values are 0.95, 0.80, 0.20 and 1.05, 1.25, 5.0 respectively. In this way a nomogram can be constructed for every value of μ .

Use of the nomogram

In Fig. 1(b), if $|F|^2$ is a , where $a \neq 0$ and $a \neq 1$ the curve would be displaced by the distance $\log a$. This displacement is scaled off with the logarithmic scale, which is used for the reading of the $|F|^2$ values. However, the scale must have the same modul as the diagram.

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The crystal structure of hexagonal L-cystine. By BERYL M. OUGHTON and PAULINE M. HARRISON*, *Chemical Crystallography Laboratory, South Parks Road, Oxford, England*

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The structure of the hexagonal form of L-cystine [$-\text{S}-\text{CH}_2-\text{CH}(\text{NH}_2)\text{COOH}$] $_2$ has been determined from three-dimensional X-ray data. The unit-cell dimensions were measured accurately by the back-reflexion method (Farguhar & Lipson, 1946) and the values found differ

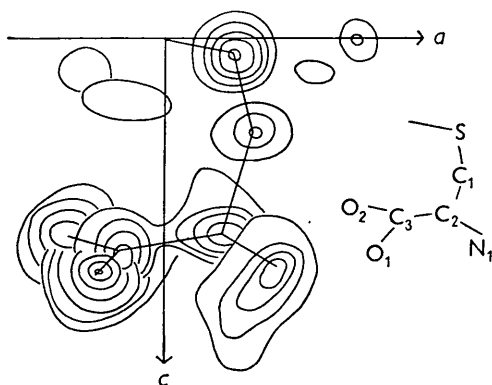


Fig. 1. The conformation of half the cystine molecule in hexagonal L-cystine, viewed down the twofold axis parallel to $[11\bar{2}0]$. The contours are those obtained from the three-dimensional sulphur-phased Fourier synthesis. Contours begin at the $1 \text{ e.}\text{\AA}^{-3}$ level and are at $1 \text{ e.}\text{\AA}^{-3}$ intervals, except for the S atom, which is contoured from the $5 \text{ e.}\text{\AA}^{-3}$ level in $5 \text{ e.}\text{\AA}^{-3}$ intervals. All peaks above $1\frac{1}{2} \text{ e.}\text{\AA}^{-3}$ are shown.

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Example 1

$$I = 3.5, \xi = 1.85; \text{ thus } |F|^2 = 1.2,$$

Example 2

$$I = 85, \xi = 0.80; \text{ thus } |F|^2 = 44.$$

The calculation of $|F|$

The method is identical with that outlined for $|F|^2$ above, the only difference being that the scale has a modul twice that of the nomogram. Consequently the square roots are obtained. However, care must be taken so that the correct figures are obtained.

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only slightly from those of Steinrauf & Jensen (1956). They are:

$$a = 5.4220 \pm 0.0005 \text{ \AA}, \quad c = 56.275 \pm 0.005 \text{ \AA}.$$

The space group is $P6_122$ with six molecules per unit cell. All the atoms are in general (12-fold) positions, the two halves of each cystine molecule being related by a twofold axis of symmetry parallel to a $[11\bar{2}0]$ axis.

The sulphur parameters were determined from the three-dimensional Patterson synthesis. A three-dimensional Fourier synthesis, calculated with phases based on the sulphur positions alone, gave a completely unambiguous picture of the whole structure (Fig. 1). F_c values for this structure were determined for all (hkl) reflexions with $F_o \neq 0$ and give $R = 21\%$. The three-dimensional refinement of the parameters is proceeding, but the general molecular conformation is already quite clear. Preliminary parameters are given in Table 1.

Table 1. Preliminary atomic parameters for hexagonal L-cystine (at the present stage of refinement)

x , y and z are as defined in *International Tables* (1952, p. 285) for space group $P6_122$

	x	y	z
S	-0.0317	0.1669	0.07943
C ₁	0.280	0.361	0.0592
C ₂	0.213	0.267	0.0336
C ₃	0.167	-0.035	0.0285
N ₁	-0.036	0.279	0.0229
O ₁	-0.068	-0.220	0.0230
O ₂	0.384	-0.059	0.0328

The approximately planar $-\text{CH}(\text{NH}_2)\text{COOH}$ groups lie almost perpendicular to the c axis, and are hydrogen-bonded together to form continuous sheets which are almost identical in structure with those found in glycine (Albrecht & Corey, 1939) (see Fig. 2). The structure of

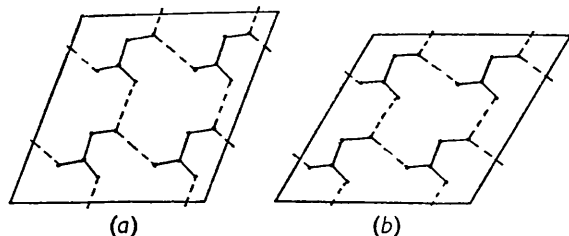


Fig. 2. Diagrammatic representation of (a) one layer of the glycine structure, (b) one layer of $-\text{CH}(\text{NH}_2)\text{COOH}$ groups in the hexagonal L-cystine structure.

hexagonal L-cystine may therefore be thought of as composed of parallel glycine-like sheets with the C-R bonds pointing alternately up and down in successive sheets, linked together in pairs by disulphide bridges. Adjacent sheets which are not linked by disulphide bridges are held together by $\text{N}-\text{H} \cdots \text{O}'_1$ hydrogen bonds.

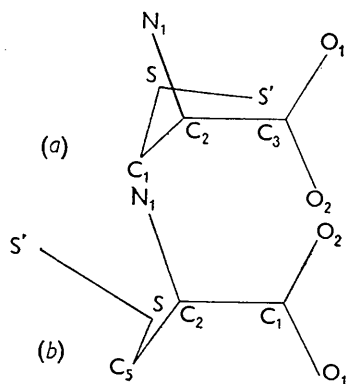


Fig. 3. Projection of one half of the cystine group on to the plane of the planar $-\text{CH}(\text{NH}_2)\text{COOH}$ groups in (a) cystine, (b) $N-N'$ -diglycyl-L-cystine dihydrate.

The conformation of the cystine molecule is different from that found in L-cystine hydrochloride (Corsmit, Schuyff & Feil, 1956) and the cystine group in $N-N'$ -diglycyl-L-cystine dihydrate (Yakel & Hughes, 1954) (Fig. 3).

The individual halves of the molecule are very similar in the two types of structure, with only small differences in the orientations of the S-C₁ and C₁-C₂ bonds relative to the planar $-\text{CH}(\text{NH}_2)\text{COOH}$ group. There is, however, rotation about the S-C₁, S-S' and S'-C'₁ bonds, and the disulphide bridge in L-cystine is the mirror image of that in the other two structures. Thus in L-cystine, the S-S' and C₂-C₃ bonds lie on the *same* side of the SC₁C₂ plane, whilst in $N-N'$ -diglycyl-L-cystine dihydrate and L-cystine hydrochloride the equivalent bonds lie on *opposite* sides of this plane.

It appears, therefore, that in the cystine group there is a preferred position of the S-C₁ bond relative to the planar group, with the SC₁C₂ plane approximately bisecting the angle N₁-C₂-C₃. There is also a preferred position of the S-S' bond, which makes an angle of approximately 83° with the SC₁C₂ plane, but the disulphide bridge can take up either of the two possible conformations, related by a mirror plane of symmetry perpendicular to the S-S' bond, which satisfy this condition.

We are much indebted to Dr J. S. Rollett and to members of the staff of the National Physical Laboratory who computed the three-dimensional Fourier synthesis and structure factors on 'Deuce', the N. P. L. electronic computer.

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Further refinement of the crystal structure of cycloserine hydrochloride. By J. W. TURLEY and R. PEPINSKY, *X-Ray and Crystal Analysis Laboratory, The Pennsylvania State University, University Park, Pa., U.S.A.*

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Recent advances in programming large electronic computers for crystallographic calculations have led to extensive refinement of many structures in three dimensions. When these methods of calculation became available to us, it was decided that a least-squares refinement of cycloserine hydrochloride (Turley & Pepinsky, 1956) in three dimensions might yield further information concerning the hydrogen-bond network in this crystal. Accordingly, the calculation was made using the IBM 704 Electronic Data-Processing Machine (Sayre, 1956), and the results are presented in this paper.

All data were placed on an absolute scale by comparing $|F_o|$ with the last set of $|F_c|$. The coordinates and crystal temperature factor resulting from the last IBM 604 calculation were used as beginning parameters. Six least-squares refinement cycles, refining on coordinates and individual temperature factors for all cycles, led to the coordinates and temperature factors shown in Table 1. The agreement factor, $R_1 = \sum ||F_o| - |F_c|| \div \sum |F_o|$, dropped from 15.9% to 14.4% ($F_o \neq 0$). For the last refinement cycle, all indicated shifts were less than 0.001 cell edge.