The Th–Bi distances are:

Th–4 Bi_I = 3·44; Th–1 Bi_{II} = 3·26; Th–4 Bi_{II} = 3·29 Å.

The smallest Bi–Bi distance is Bi_I–4 Bi_I = 3·18 Å.

The above mentioned compounds are isostructural with both U_3Bi_4 and UBi_2 (Ferro, 1952, 1953) and with Th_3As_4, $ThAs_2$ (Ferro, 1955) and Th_3Sb_4, $ThSb_2$ (Ferro, 1956) previously studied.

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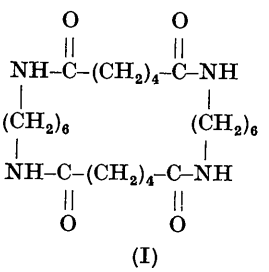
Elementarzelle des cyclischen Nylon-Oligomeren 1,8,15,22-tetra-aza-2,7,16,21-tetra-oxo-cyclo-octacosan.

Von Hans von Dietrich, Helmut Zahn* und Franz Schmidt, *Chemisches Institut der Universität Heidelberg, Deutschland*

(*Eingegangen am* 11. *März* 1957)

Das aus Nylon 66 isolierbare cyclische Oligomere (I)



(I)

kristallisiert aus Wasser in monoklinen Blättchen (Zahn *et al.*, 1956*a*; Brown, Hill & Youle, 1956; Zahn, Miro & Schmidt, 1957); Blättchenebene (010), Spaltbarkeit nach (001) angedeutet.

Die röntgenographische Untersuchung ergab folgende Daten:

$a_0 = 10{,}78 \pm 0{,}03$, $b_0 = 25{,}12 \pm 0{,}05$, $c_0 = 9{,}67 \pm 0{,}02$ Å, $\beta = 92° 22' \pm 6'$.

Nimmt man an, dass die Zelle vier Moleküle enthält, so ergibt sich die Dichte = 1,149±0,005 g.cm.$^{-3}$ (bei 25–27° C.). Gemessen wurde: 1,148 g.cm.$^{-3}$ (bei 28° C.).

Der aus Debye–Scherrer-Aufnahmen bestimmte Netzebenenabstand von 12,6 Å (Schmidt, 1956; Zahn *et al.*, 1956*b*), also gerade $\frac{1}{2}b_0$, lässt darauf schliessen, dass die Ausdehnung der Einzelmoleküle auch in Richtung der *b*-Achse höchstens 12,6 Å ist, was in Verbindung mit den übrigen Abmessungen der Elementarzelle eine starke Faltung der Ringe fordert. Bei völliger Streckung der Einzelmoleküle haben diese eine Länge von *ca.* 20 Å.

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A graphical method for the calculation of $|F|^2$ and $|F|$ from equi-inclination Weissenberg photographs.

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(*Received* 2 *April* 1957)

Introduction

In a given Weissenberg equi-inclination photograph the intensities of the spots obey the equation

$$I = C.\lambda^3.A\,\frac{1+\cos^2 2\theta}{\cos^2\mu\,\sin\gamma}.|F|^2 \qquad (1)$$

if the extinction is not taken into consideration. Here C is constant and A an absorption factor. The other symbols are identical with those used by Buerger (1942).

We can write (1) in the following way:

$$|F|^2 = \frac{I}{C.\lambda^3.A}\cdot\frac{\cos^2\mu.\sin\gamma}{1+\cos^2 2\theta}. \qquad (2)$$

Lu (1943) introduced the abbreviation

$$\alpha = \frac{\cos^2\mu.\sin\gamma}{1+\cos^2 2\theta}. \qquad (3)$$

If $C.\lambda^3.A = 1$, equation (1) becomes

$$|F|^2 = I.\alpha. \qquad (4)$$

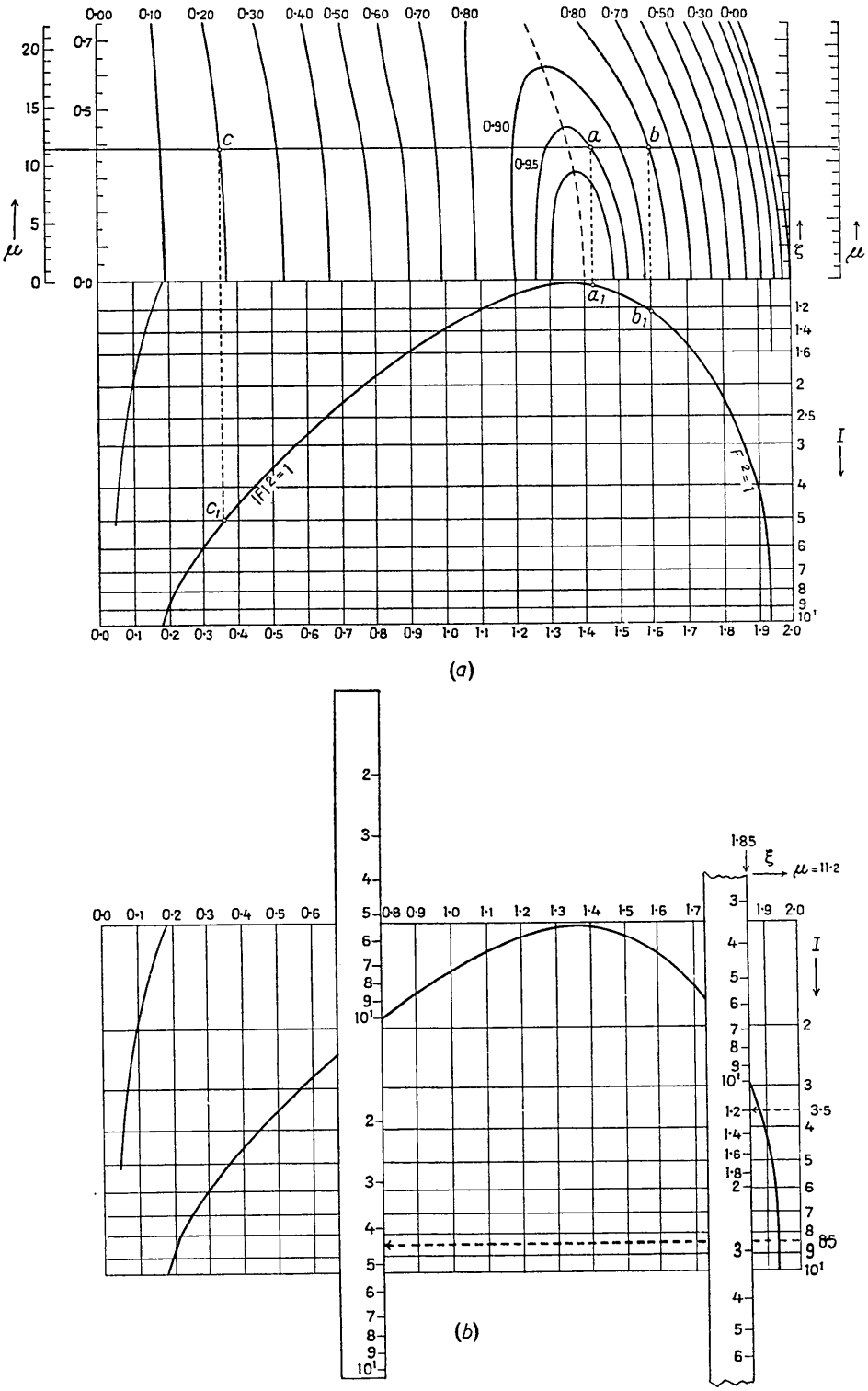

Fig. 1.

Lu (1943) and Cochran (1948) have constructed charts where α is a function of ξ and μ. These charts simplify the calculation of $|F|^2$.

However, it is possible to make a further simplification. If we plot I as a function of α, assuming $|F|^2$ constant, in a logarithmic diagram, we have a nomogram for the calculation of $|F|^2$. As the nomogram is logarithmic, it is convenient to use a logarithmic scale for the reading of

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 $\mu = 11{\cdot}2$ (Fig. 1(*a*)). Then we first draw a line parallel to the ξ axis at $\mu = 11{\cdot}2$ 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.

Example 1

$I = 3{\cdot}5$, $\xi = 1{\cdot}85$; thus $|F|^2 = 1{\cdot}2$,

Example 2

$I = 85$, $\xi = 0{\cdot}80$; 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.

The author wishes to convey his thanks to Prof. F. E. Wickman, Swedish Museum of Natural History, and Prof. G. Hägg, Uppsala, for their kind interest.

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The crystal structure of hexagonal L-cystine.

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(*Received* 13 *May* 1957)

The structure of the hexagonal form of L-cystine $[-S-CH_2-CH(NH_2)COOH]_2$ 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 only slightly from those of Steinrauf & Jensen (1956). They are:

$$a = 5{\cdot}4220 \pm 0{\cdot}0005 \text{ Å}, \quad c = 56{\cdot}275 \pm 0{\cdot}005 \text{ Å}.$$

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 (*hkil*) 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.

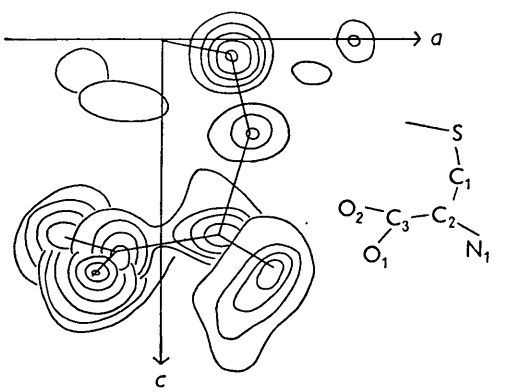

Fig. 1. The conformation of half the cystine molecule in hexagonal L-cystine, viewed down the twofold axis parallel to $[11\bar{2}0]$. The contours are those obtained from the three-dimensional sulphur-phased Fourier synthesis. Contours begin at the 1 e.Å^{-3} level and are at 1 e.Å^{-3} intervals, except for the S atom, which is contoured from the 5 e.Å^{-3} level in 5 e.Å^{-3} intervals. All peaks above 1½ e.Å^{-3} are shown.

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

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