

We further have  $E_0 = \frac{1}{2} |F(0)|^2 = \frac{1}{2} \left| \sum_{a=1}^s Z_a \right|^2 (E_0$

here and  $E_h$  above as well as all the other symbols not defined in this letter have the same significance as in Y.L.). Now let us combine Y.L. equation (2) and equation (4) and substitute the values of  $E_h$  and  $E_0$  given above in the resultant equation; we then obtain

$$E(q) = \frac{1}{2} \left| \sum_{a=1}^s Z_a \right|^2 \sum_{\mu=0}^{N/2} a_{\mu 0} \cos 2\pi q u_{\mu} + \sum_{\mu=0}^{N/2} \sum_{h=1}^{\infty} a_{\mu h} \frac{K_h}{c} \cos 2\pi q u_{\mu},$$

where  $u_{\mu} = \frac{\mu}{N}$ . If in the equation we replace  $q$  by

an integer  $k$  and substitute  $E(k)$  by  $\frac{K_k}{2c}$ , we have, after a transformation of terms, that,

$$c = \frac{K_k - 2 \sum_{\mu=0}^{N/2} \sum_{h=1}^{\infty} a_{\mu h} K_h \cos 2\pi k u_{\mu}}{\left| \sum_{a=1}^s Z_a \right|^2 \sum_{\mu=0}^{N/2} a_{\mu 0} \cos 2\pi k u_{\mu}}.$$

When  $k=0$ , we have,

$$c = \frac{2 \sum_{\mu=0}^{N/2} \sum_{h=1}^{\infty} a_{\mu h} K_h}{\left| \sum_{a=1}^s Z_a \right|^2 \left\{ 1 - \sum_{\mu=0}^{N/2} a_{\mu 0} \right\}}.$$

Since all the quantities on the right-hand side of the last two equations are known,  $c$  can be calculated by either of the equations. Consequently the absolute values of  $E(h)$  and so of  $|F(h)|^2$  are determined. The method might be an approximate one in general due to the approximation involved in Y.L. equation (5). Accordingly, if the absolute values of  $|F(h)|^2$  are determined by the existing experimental methods, the present method would provide a test of the approximation involved in Y.L. equation (5) for the crystal in question.

S. H. YÜ.

Metals Research Institute,  
National Tsing-Hua University,  
Kunming, Yunnan. April 14.

<sup>1</sup> Bragg, W. L., "The Crystalline State", 1, 219.

<sup>2</sup> Compton, A. H., *Phys. Rev.*, 9, 29 (1917).

<sup>3</sup> Yü, *NATURE*, 149, 638 (1942).

Yü's letter<sup>1</sup> on the determination of absolute from relative X-ray intensities suggests several interesting possibilities. His equations might be useful to anyone working with his synthesis<sup>2</sup>, but it is possible to devise a method not depending on the quantities  $a_{\mu h}$ , which are not yet available. The ideal intensity of the  $hkl$  reflexion is given by

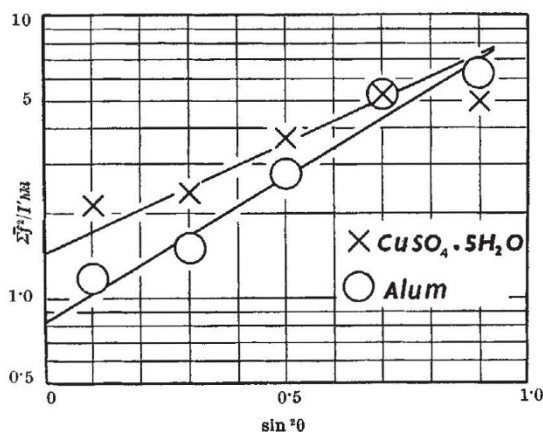
$$I_{hkl} = \sum_a \sum_{\beta} f_a f_{\beta} \exp\{2\pi i[h(x_a - x_{\beta}) + k(y_a - y_{\beta}) + l(z_a - z_{\beta})]\} \\ = \sum_a f_a^2 + \sum_{a \neq \beta} \sum_{\beta} f_a f_{\beta} \exp\{2\pi i[h(x_a - x_{\beta}) + k(y_a - y_{\beta}) + l(z_a - z_{\beta})]\}, \quad (1)$$

where the  $f$ 's are the structure factors and the  $x, y, z$ 's are the parameters of the atoms. Suppose that  $I_{hkl}$  is averaged for all reflexions in a given range of  $\sin^2 \theta$ . If  $\lambda/\sin \theta$  is small compared with the interatomic distances, the exponential terms in equation (1) will take on both positive and negative values, and their average over  $h, k, l$  will be practically zero. Then to a close approximation

$$\overline{I_{hkl}} = \sum_a \bar{f}_a^2, \quad (2)$$

where the  $\bar{f}$ 's are the atomic structure factors for the centre of the range of  $\sin^2 \theta/\lambda^2$ .

The experimental value of the intensity of the  $hkl$  reflexion,  $I'_{hkl}$ , will differ from  $I_{hkl}$  by two factors: a scale factor independent of  $\theta$ , and the temperature factor. The ratio  $I'_{hkl}/I_{hkl}$  for the group of reflexions will be the product of these. By dividing the reflexions into groups covering suitable ranges of  $\sin^2 \theta/\lambda^2$  and forming the ratio  $\Sigma \bar{f}^2/I'_{hkl}$  for each group, the factor  $1/c$  required to convert  $I'_{hkl}$  to  $I_{hkl}$  will be found as a function of  $\sin \theta/\lambda$ . If the usual form of the temperature factor ( $\exp\{-B \sin^2 \theta/\lambda^2\}$ ) is correct, the logarithm of  $1/c$  should be a linear function of  $\sin^2 \theta/\lambda^2$ .



In normal Fourier and Patterson syntheses it is usual to work only with a zone of intensities, say, the  $hk0$ 's. If two atoms are close together in the projection, they ought to be counted as a single atom with atomic factor equal to the sum of their respective atomic factors. Since in general such coincidences cannot be predicted, there will be an error tending to make the value of  $1/c$  too small. In special cases (for example, alum<sup>3</sup>, in which the potassium and aluminium atoms coincide in the  $hk0$  projection) certain coincidences can be predicted from the space group only, and allowed for.

To test the feasibility of the procedure, it has been applied to the  $hk0$  reflexions of alum<sup>3</sup> and copper sulphate<sup>4</sup>. The ranges of  $\sin^2 \theta$  used were 0.0–0.2, 0.2–0.4, . . . 0.8–1 (copper radiation), but little reliance can be put on the average for the 0.0–0.2 group. The values of  $\bar{f}$  were taken from the Internationale Tabellen<sup>5</sup>. The logarithm of  $1/c$  is plotted against  $\sin^2 \theta$  in the graph above. The points scatter somewhat, but lie fairly well on straight lines. Since the measurements<sup>3,4</sup> are 'absolute', the values of  $1/c$  for  $\sin^2 \theta=0$  should be 1. Actually they are about 0.8 and 1.5 respectively. Without further investigation it cannot be claimed that the method is capable of high accuracy, but even that indicated should be useful in much structure work.

A. J. C. WILSON.

Cavendish Laboratory,  
Cambridge. June 18.

<sup>1</sup> Yü, *NATURE*, 149, 729 (1942).

<sup>2</sup> Yü, *NATURE*, 149, 638 (1942).

<sup>3</sup> Lipson and Bevers, *Proc. Roy. Soc., A*, 148, 664 (1935).

<sup>4</sup> Bevers and Lipson, *Proc. Roy. Soc., A*, 146, 570 (1934).

<sup>5</sup> "Internationale Tabellen zur Bestimmung von Kristallstrukturen", 2, 571 (Berlin: Gebrüder Borntraeger, 1935).