

theoretical interest and warrants further study. It is hoped shortly to publish this work in detail.

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<sup>1</sup> See, for example, Elenbaas, W., *Phil. Res., Rep.*, 2, 20 (1947). Francis, V. J., *Phil. Mag.*, 37, 433, 653 (1946), and references given therein.

<sup>2</sup> Nelson, E. H., *G.E.C. J.*, 14, 73 (1946). Bourne, H. K., *B.T.H. Act.*, 19, 181 (1947).

### Radial Patterson Distribution Functions

It has been indicated in a previous paper<sup>1</sup> how a comparison between the structure factors ( $F(h,k,l)$ ) resulting from a given molecular configuration, and those actually observed by experiment, can be effected by comparing the Patterson maps resulting from the observations and from the proposed molecule. This suffers the disadvantage of requiring a knowledge, not only of the intra-molecular configurations, but also of the positional relationships between the molecules themselves in the unit cell. Another approach is suggested by a result obtained recently<sup>2</sup>. Since the Patterson synthesis, in a certain neighbourhood of the origin, depends mainly upon the intra-molecular configuration, a possible basis of comparison between a postulated molecular structure and a set of observations would lie in an investigation of the distribution functions resulting from each in Patterson space.

It is simple to obtain the radial Patterson function of a given molecule by the processes of elementary geometry. We now investigate very briefly the technique for deriving the same function from the observed  $|F(h,k,l)|^2$  values.

For a radially symmetric function  $T(R)$ , the corresponding radially symmetric function in the reciprocal space is

$$g(r) = 4\pi w \int_0^\infty R^2 T(R) \left[ \frac{\sin 2\pi rR}{(2\pi rR)} \right] dR,$$

where  $w$  is the total weight of  $g(r)$  and  $T$  is scaled to value unity at the origin. For a cylindrically symmetric function  $T(RZ)$ , the corresponding function in the reciprocal space is<sup>2</sup>

$$g(rz) = 2\pi w \int_{-\infty}^{\infty} \int_0^\infty RT(RZ) J_0(2\pi rR) \exp(-2\pi izZ) \cdot dRdZ.$$

Hence the three-dimensional radial Patterson function for a unit cell of volume  $V$  may be written

$$g_3(r) = (1/V) \sum_{\mathbf{h}} |F(h,k,l)|^2 \sin(2\pi rR_{\mathbf{h},k,l}) / (2\pi rR),$$

where  $1/R_{\mathbf{h},k,l}$  is the spacing of the plane  $(h,k,l)$ . The two-dimensional radial Patterson function for a unit cell of volume  $V$  may correspondingly be written

$$g_2(r) = (1/A) \sum_{\mathbf{h}} |F(h,k,0)|^2 J_0(2\pi rR_{\mathbf{h},k,0}).$$

Applications of the above methods to crystalline powders have been pointed out elsewhere<sup>3</sup>, but we wish to remark here their special suitability to work in proteins. In this field a number of theories have

been advanced for the structure of single molecules, and any check has been rendered difficult since it requires, not only a knowledge of the single molecule, but also of the relationship which this bears to its fellows in the unit cell. The present technique may permit a first comparison to be made without any consideration of intermolecular structure and with only limited computations. This is important since it will enable certain structures to be ruled out immediately. We wish to emphasize, however, that it can never establish the correctness of a given structure, but only its right to inclusion in the general class of possibilities.

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<sup>1</sup> Booth, A. D., and Wrinch, D., *J. Chem. Phys.*, 15, 416 (1947).

<sup>2</sup> Wrinch, D., "Fourier Transforms and Structure Factors", A.S.X.R.E.D. Monograph No. 2, 10 (1946).

<sup>3</sup> Booth, A. D., *Trans. Farad. Soc.*, 44, 37 (1948).

### A Mechanical Calculating Machine for X-Ray Structure Factors

A LARGE mechanical machine for calculation of X-ray crystallographic structure factors has now been completed in our laboratories and is running satisfactorily. The machine is of a tide-predictor type, and it deals with up to 24 harmonic components at a time.

The expression calculated is

$$F(hkl) = \sum_i f_i \cos 2\pi (h x_i + k y_i + l z_i).$$

During the calculation, for example,  $h$  and  $k$  are kept constant and the machine calculates  $F$  for all required  $l$  values at one setting. If there are  $N$  atoms per unit cell,  $N$  harmonic units are switched on; each unit has a phase dial on which is first set the value  $h x_i + k y_i$ . The values  $z_i$  are set on a multiplier bar, which at each stroke adds these through a clutch to the values on the dials with an accuracy better than 1:1,000. After  $l$  strokes, the dials thus read  $h x_i + k y_i + l z_i$ . Their angles are transferred to cosine arms, each of length  $f_i$ , the results of which are added together by means of a pulley belt differential with an accuracy better than 0.2 per cent of  $F(000)$ . An output pulley indicates on two geared-down dials the resulting values of  $F$ . The calculation assumes that the variation of  $f_i$  with index is the same for all the atoms; heavy atoms must thus be treated separately.

The machine has provision for calculation of Booth corrections<sup>1</sup>  $\epsilon$  from the derivatives of  $R$ . For this purpose the errors  $F_0 - F_c$  are copied from a drum and thus fed into the machine. The machine is run again, but with  $\pi/2$  added to the angles of the phase dials of the harmonic units, so that their arms produce sines instead of cosines. There is an arrangement which multiplies these by  $W(F_0 - F_c)$ . The weights  $W$  are chosen according to the formula for  $R$  used<sup>2</sup>, and according to whether  $x$ ,  $y$  or  $z$  co-ordinates are to be corrected. The products are summed up on the  $\epsilon$  dials for all  $l$ . After completing the run, the  $\epsilon$  dials read the corrections by which the co-ordinates should be altered to decrease  $R$ . The cycle of calculations is represented in Fig. 1.