elliptic paraboloid by the method of Ladell & Katz, which in turn affect the determination of (x_0, y_0), ε, and θ.

(iii) The influence of the other peaks in the projection on the electron-density values in the vicinity of the compound peak. If a reliable atomic profile has been obtained, as mentioned under (i) above, then this effect may be corrected for.

The basic approximation involved in the method can, of course, be improved by including additional terms in the expansion of ln cosh u; but taking into account only the next term, namely $-u^4/12$, and dealing only with the simple case in which the electron density has been computed at the points of a square mesh, the required correction term to equation (8) is much too cumbersome to be of any practical value. In any event, in view of the other sources of error present, it is doubtful whether any such attempt at correcting (8) would be worth while.

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An X-ray investigation of air-dried lysozyme chloride crystals. II: correction.

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If the Wilson (1942) method of obtaining the scale factor is to give a reliable value, the Patterson peak at the origin must not contain any contributions arising from the spreading out of near-by peaks. In an earlier communication (Corey, Donohue, Trueblood & Palmer, 1952), which dealt with the interpretation of the Patterson function of air-dried lysozyme chloride, we described briefly a procedure for modifying the Wilson method for application to cases in which a very large temperature factor results in a considerable overlapping of peaks arising from short interatomic distances with the Patterson peak at the origin. The procedure, of course, involves the estimation of the total height contributed by these peaks at the origin in Patterson space. Our attention has been called (Crick, 1953) to an error in our treatment. It is the purpose of this note to correct this error, to restate the problem, and to indicate a method for its possible solution. Since our original treatment contained several minor ambiguities with regard to notation, we now define the following terms:

R = distance from the center of a Patterson peak to the origin.

$P_{ij}(r)$ = height of a Patterson peak (due to atoms i and j) at a distance r from the center of the peak (spherical symmetry assumed).

$P(u, v, w)$ = value of Patterson function at point (u, v, w).

Thus the height of the Patterson peak at the origin is the sum of two terms:

$$P(0, 0, 0) = \sum_i P_{ii}(0) + \sum_i \sum_j P_{ij}(R) .$$

As before,

$$P_{ij}(r) = Z_i Z_j (2\pi/B)^{3/2} \exp\left[-2\pi^2 r^2/B\right] ,$$

so that

$$\sum_i P_{ii}(0) = (2\pi/B)^{3/2} \sum_i Z_i^2 ,$$

and

$$\sum_i \sum_j P_{ij}(R) = (2\pi/B)^{3/2} \bar{Z} \sum_i Z_i \int_0^\infty \exp\left[-2\pi^2 x^2/B\right] dN(x) ,$$

where $N(x)$ is a function which gives the number of atoms within a distance x of each atom. Our previous treatment was in error in that $N(x)$ was assumed to be uniform (equal to $0{\cdot}25x^3$), that $N(x)dx$ was used instead of $dN(x)$, and that $\sum_i Z_i^2$ was used in place of the always smaller $\bar{Z} \sum_i Z_i$. Since the value of the Patterson function at the origin is also given by

$$P(0, 0, 0) = \frac{1}{V} \sum_{hkl} k|F'|^2_{hkl} + \frac{1}{V} |F|^2_{000},$$

where F'_{hkl} are the observed relative structure factors, and k is the scale factor, we may equate the two expressions, and solve for k, provided that both $N(x)$ and B can be evaluated from other considerations. $N(x)$ can, in principle, be obtained from a (non-uniform) radial distribution function derived from some appropriate model.

The function $N(x)$ must be evaluated for values of x extending from zero to a maximum value beyond which there is no significant overlap of the $P_{ij}(R)$ with $P(0, 0, 0)$. If B is small, as for ordinary crystals, there is no overlap; if B is large, then the maximum value of x will be so great that the function $N(x)$ may be, in practice, difficult to evaluate. The accuracy of the scale factor will depend upon the accuracy with which B and $N(x)$ have been estimated.

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