The study of this claim in the light of the experimental vector map forms the subject of another communication.

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A contribution to the determination of signs in the Fourier analysis of crystals.

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In the preliminary analysis of a crystal structure it may become clear from symmetry or packing that the electron density is low and nearly uniform over certain planes. The writer, in analysing a long-chain fatty acid, was able to conclude from the possible packing that the density was low and nearly uniform over the three bounding planes of a suitably chosen unit cell. A two-dimensional projection of such a cell parallel to one of the axes will have low, uniform density along its bounding lines. The existence of uniform or zero density over certain lines and planes must determine certain relations between the coefficients of the Fourier series giving the density, and this may help to determine their signs.

Consider a two-dimensional projection on the *bc* plane, having a centre of symmetry which is also the origin of coordinates. If (v, w) are the fractional coordinates of a point in the projection in terms of 2π, the density, $\sigma(v, w)$, is given by

$$S\sigma(v, w) = A(0, v) + A(l, v)\cos lw + B(l, v)\sin lw \quad (1)$$

(James, 1948), S being the area of the unit projection, with

$$\left.\begin{aligned} A(0, v) &= F(000) + 2\sum_1^k F(0k0)\,.\cos kv\,, \\ A(l, v) &= 2F(00l) + 2\sum_1^k \{F(0kl) + F(0\bar{k}l)\}\cos kv\,, \\ -B(l, v) &= 2\sum_1^k \{F(0kl) - F(0\bar{k}l)\}\sin kv\,. \end{aligned}\right\} \quad (2)$$

Suppose $\sigma(v, w)$ to be constant along a line $v =$ const. in the projection throughout the range $w = 0$ to $w = 2\pi$. Then, in the Fourier series (1) $A(l, v)$ and $B(l, v)$ must vanish, while $A(0, v)$ must be constant. If the density is very small or zero, $A(0, v)$ will be small or zero also. We consider the case in which the density is constant along the line $v = 0$. Equations (2) then give

$$\tfrac{1}{2}F(000) + \sum_1^k F(0k0) = \text{constant}\,, \quad (a)$$

$$F(00l) + \sum_1^k \{F(0kl) + F(0\bar{k}l)\} = 0 \text{ for any value of } l. \quad (b)$$

We can draw no conclusions from the vanishing of $B(l, v)$ since $\sin kv$ is itself zero.

If the density is uniform or zero along the line $w = 0$, we have the analogous relations

$$\tfrac{1}{2}F(000) + \sum_1^l F(00l) = \text{constant}\,, \quad (a')$$

$$F(0k0) + \sum_1^l \{F(0kl) + F(0k\bar{l})\} = 0, \text{ for any value of } k\,. \quad (b')$$

If the absolute values of F have been determined, conclusions about the signs of the coefficients may be drawn, provided that some of them are already known. In one example many of the signs of $F(00l)$ were fairly certainly known. Equations (*b*) allowed other signs to be determined. One such equation ran

$$\begin{array}{ccccc} F(005) + & F(015) + & F(0\bar{1}5) + & F(025) + & F(0\bar{2}5) \\ -7\cdot9 & \pm2\cdot3 & \pm2\cdot7 & 0 & 0 \end{array}$$

$$\begin{array}{cccc} +F(035) + & F(0\bar{3}5) + & F(045) + & F(0\bar{4}5) = 0\,, \\ 0 & 0 & 0 & 0 \end{array}$$

from which it is fairly clear that both $F(015)$ and $F(0\bar{1}5)$ are positive.

Prof. R. W. James has pointed out to me that the results can be extended to three dimensions, and to planes of uniform density that do not pass through the origin. For example, if the density is uniform over the plane $w = 0$,

$$F(hk0) + \sum_1^l \{F(hkl) + F(hk\bar{l})\} = 0$$

for any pair of indices h and k. Each such equation corresponds to the sum of the structure factors along any row of reciprocal-lattice points perpendicular to the plane of constant density. If the density is not zero, the row through the origin must be excluded.

Reference

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