and $n = 0$, $m = \pm 1$ terms are most important. They yield, on the right, U_{H+K} and U_{H-K}, so this series inequality is closely related to the well known 'sum and difference' inequality of Harker & Kasper.

The validity of the derivation requires that q_j shall be a positive constant. This in turn requires that the atoms shall all have a common shape factor multiplied by their appropriate magnitude factors and that the shape factor shall have a Fourier transform that is positive within the range of the data required to make the series effectively converge.

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Note on the sign determination by optical-transform methods.

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It is reported (Lipson & Taylor, 1951; Hanson, Lipson & Taylor, 1953; Lipson & Cochran, 1953; Pinnock & Taylor, 1955) that the signs of the structure factors for a given arrangement of atoms may be quickly determined by means of optical-transform methods. They state that in optical-transform of a centrosymmetrical structure (1) the positive and negative regions are separated by nodal lines, and (2) by adding an extra hole at the centre of symmetry of a structure, the positive regions of the original transform are enhanced and the negative regions are depressed. These criteria have been proved powerful in solving a number of organic structures.

It has become common to use a mask in which some holes are displaced by a lattice translation in order to avoid overlapping, or several holes are placed at integral multiples of lattice translations in order to give appropriate weights to the scattering factors for particular atoms. As the number of such holes increases, the whole transform will become so modulated that criterion (1) will no longer be applicable, and that intensities only at reciprocal-lattice points will have a significant meaning.

Let us confine ourselves to the intensities of the optical transform at reciprocal-lattice points. In this case, criterion (2) must be used with caution, as will be explained in the following.

The Fourier transform of a centrosymmetrical structure consisting of holes of equal size can be given by

$$F(R) = f(R)g(R)\,, \qquad (1)$$

where $f(R)$ is the Fourier transform of a single hole and $g(R)$ is the geometrical structure factor $\sum_i \exp 2\pi_i r_i R$, r_i being the positional vector of the ith hole and R a vector in reciprocal space.

When an extra hole is added at the centre of symmetry of the same structure, the transform will become

$$F'(R) = f(R)\{1+g(R)\}\,. \qquad (2)$$

Since both $f(R)$ and $g(R)$ are real, the increment in intensity is proportional to

$$F'(R)^2 - F(R)^2 = f(R)^2\{1+2g(R)\}\,. \qquad (3)$$

Hence, the regions for which $g(R) > -\frac{1}{2}$ are enhanced and those for which $g(R) < -\frac{1}{2}$ are depressed. It follows that intensities weaker than $\frac{1}{4}f(R)^2$ are always enhanced so that signs of their corresponding Fourier coefficients cannot be determined.

The sign determination can be extended to those weak reflexions $> \frac{1}{4}f(R)^2$ in the following way. Prepare three photographs which correspond to the following three quantities:

$$A = f(R)^2 g(R)^2\,, \qquad (4)$$

$$B = f(R)^2\{1+g(R)\}^2\,, \qquad (5)$$

$$C = f(R)^2\{1+g(R)^2\}\,. \qquad (6)$$

A is the optical transform of a given centrosymmetrical structure. B is the optical transform of the same structure plus an extra hole added at the centre. C is the superposition of A and the optical transform of a single hole, and can be prepared by exposing the mask of the structure and a single hole in succession. By subtracting C from B, we get

$$B - C = 2f(R)^2 g(R)\,. \qquad (7)$$

The sign of (7) is exactly the same as that given by (1). Thus the original transform is positive if B is stronger than C, and is negative if B is weaker than C. This criterion can be applied throughout the whole optical transform observed at reciprocal-lattice points.

Further improvement can be made by comparing B with D, which is another photograph corresponding to the optical transform defined by

$$D = f(R)^2\{-1+g(R)\}^2\,. \qquad (8)$$

D can be prepared by exposing the mask of the structure and a central hole, the latter being covered with mica which retards the phase of the incident light by π. The difference in intensity between B and D is

$$B - D = 4f(R)^2 g(R)\,, \qquad (9)$$

which is twice as much in magnitude as that given by (7).

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