with $S(\mathscr{F}_1) \neq S(\mathscr{F}_2)$ may be strong but the number of such reflexions is limited owing to the small probability of condition (8) being satisfied. Thus $|x_-|^2$ will represent the correct roots for most reflexions. The change of sign however can occur more frequently if scattering length for one of the energies, say E_2, is negative [*i.e.* $b_2(r)$ is negative and further for the sake of discussion we shall assume again that $b_2(r) < b_1(r)$]. The conditions to be satisfied for such a change are

$$|b_2(r)\mathbf{x}| > |F_N(H)| \quad \text{if} \quad S(N) = S(x)$$

or

$$|b_1(r)\mathbf{x}| > |F_N(H)| \quad \text{if} \quad S(N) \neq S(x)\,.$$

In practice it seems advantageous to choose the neutron energies such that $b_1(r)$ and $b_2(r)$ are of the same sign.

For structures with large 'heavy atom' ratio, the position of the anomalous scatterer can be determined by an ordinary Patterson synthesis or synthesis with $|F_1(H)|^2 + |F_2(H)|^2$ (Ramaseshan, 1966). The latter is known to contain only $A-A$ and $N-N$ vectors if the neutron energies are chosen so that $b_1(r) = -b_2(r)$. As the 'heavy atom' ratio decreases, an increasing background is provided by the $N-N$ vectors. For a small 'heavy atom' ratio, $A-A$ vectors can hardly be distinguished from the $N-N$ vectors. It is in such cases that the present method is particularly useful. Further for a structure with small 'heavy atom' ratio, cases with $S(\mathscr{F}_1) \neq S(\mathscr{F}_2)$ are not many and $|x_-|^2$ represents the correct root for most reflexions.

Equation (4) has coincident roots if E_1 and E_2 are chosen so that $b_1(r) = b_2(r)$ and $b_1(i) \neq b_2(i)$. The roots are then given by

$$|x_+|^2 = |x_-|^2 = Q/P\,.$$

Thus there is no ambiguity in the determination of $|x|^2$. However in such a case the signs of the reflexions cannot be determined [see equation (9)].

A Patterson synthesis with $b_1^2(r)\,|x_-|^2$ as coefficients will yield the positions of the anomalous scatterers. A comparison of the calculated $|x|^2$ values with those obtained from equation (4) will indicate the cases in which a wrong solution has been chosen. Once such corrections have been made $|x_-|^2$ values from equation (4) can be used to refine the thermal and the positional parameters of the anomalous scatterers.

The sign determination

On subtracting equation (3) from (2) we get,

$$2F_N(\mathbf{H})\,\{b_1(r) - b_2(r)\}\mathbf{x} = \{|F_1(H)|^2 - |F_2(H)|^2\} - [\{b_1^2(r) + b_1^2(i)\} - \{b_2^2(r) + b_2^2(i)\}]\,|x|^2\,. \quad (9)$$

Thus, $\mathbf{x}$ being known, $F_N(\mathbf{H})$ can be determined. With this all the information necessary for solving a structure is complete. A Fourier synthesis with $F_N(\mathbf{H})$ as coefficients will reveal the position of the normal scatterers.

As pointed out in the previous section, the choice of two neutron energies such that $b_1(r) = b_2(r)$ and $b_1(i) \neq b_2(i)$ leads to unique solution of $|x|^2$. However on letting $b_1(r) = b_2(r)$ in equation (9) the term containing $F_N(\mathbf{H})$ vanishes and equation (9) becomes an identity. Thus $F_N(\mathbf{H})$ cannot be determined under these conditions. However, from equation (2) or (3), both of which are identical under the condition $b_1(r) = b_2(r) = b(r)$, we get

$$|F_N(\mathbf{H})| = -b(r)\mathbf{x} \pm [b^2(r)|x|^2 + \{|F_1(H)|^2 - (b_1^2(r) + b_1^2(i))\,|x|^2\}]^{1/2}.$$

These two roots correspond to the two cases (i) $F_N(\mathbf{H})$ having the same sign as $b(r)\mathbf{x}$ and (ii) $F_N(\mathbf{H})$ having a sign opposite to that of $b(r)\mathbf{x}$. However this ambiguity cannot be resolved.

Thus an attempt to combine the data at two neutron energies to give $|x|^2$ leads to two possible solutions [equation (5)]. The correct roots can be chosen indirectly and a Patterson synthesis with these will give the position of the anomalous scatterers. Equation (9) can then be used to determine $F_N(\mathbf{H})$.

Equation (6) leads to a unique solution for $b_1(r) = b_2(r)$ and $b_1(i) \neq b_2(i)$ but $F_N(\mathbf{H})$ cannot be determined from equation (9). This situation is similar to that encountered in the noncentrosymmetric case (Singh & Ramaseshan, 1968*b*) wherein such a choice of radiation gives $|x|^2$ unambiguously but the ambiguity in the phase remains unresolved.

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The crystal structure of iodine monobromide, IBr.

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In an earlier article under this title (Swink & Carpenter, 1968) we neglected, through an oversight, to refer to a more recent powder diffraction study (Cheesman & Hawes, 1959) covering the entire composition range of iodine–bromine mixtures. The discrepancy between the cell constants reported in the latter paper for a 50 at.% powder and those reported by us for single crystals of the same composition remains unexplained, despite rechecking of original photographs in both laboratories (Cheesman, 1968).

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