use of constant structure amplitudes and by attributing the sign of the heavy atom to them, that is, with a structure factor contribution of the form $\Delta F_{\mathbf{h}} \sim \text{sign}(\cos 2\pi \cdot \mathbf{h} \cdot \xi)$, where $\xi = (x/a, y/b, z/c)_{\text{Th}}$. This can be seen as follows: if we introduce the Fourier expansion of

$$\text{sign}(\cos\alpha) = 4/\pi \sum_{m\geq 0} \frac{(-1)^m}{2m+1} \cos(2m+1)\alpha$$

we find that our

$$\Delta F_{\mathbf{h}} \sim 4/\pi \sum_{m} \frac{(-1)^m}{2m+1} \cos(2\pi \cdot \mathbf{h} \cdot (2m+1)\xi)$$

corresponds formally to a structure factor contribution from atoms at sites $(2m+1)\xi$ with their numbers of electrons proportional to $(-1)^m/(2m+1)$.

The next question was, how can such a $\Delta F_{\mathbf{h}}$ arise in our observed amplitudes? We propose the following explanation: in our data collection we rejected a reflexion as unobservable if the measured intensity (essentially scan count minus background count) was smaller than its standard deviation (essentially the square root of the sum of scan count plus background count). Any such criterion is biased – it tends to reject measured intensities with negative random errors and to retain those with positive random errors. Since we had relatively weak intensities (because of our small crystal) against a high background count, this bias must have affected a large percentage of our weak high-order reflexions. This could be confirmed by remeasuring a sample of 49 weak reflexions. Of these, 13 were twice accepted, 10 twice rejected and 26 switched sides. On average, this bias acts like adding a positive term, ε, to the observed structure amplitudes and therefore, when ε is multiplied by the heavy-atom sign, it produces the pattern described above. Unfortunately, this kind of bias will be present with any rejection procedure and cannot be completely eliminated, but it was argued that it should be possible to reduce it by throwing out data with large standard deviations in the structure amplitudes, F. Since $\sigma(F) \sim \sigma(I)/\sqrt{I}$, this would reduce both the average value of ε and the number of marginal data (the weakest reflexions tend to have the highest estimated standard deviations). Indeed, when such a stronger rejection criterion was applied, reducing the number of observed reflexions from 2037 to 1407, the hole-peak pattern almost completely vanished from our difference electron-density map.

Our example corresponds to the simplest possible case. Higher symmetries and more than one heavy atom complicate the pattern considerably, but it can be worked out by similar methods.

As a conclusion we would like to point out that it can be imprudent to suppress negative electron densities in the electron-density map: holes may furnish crucial information for the identification of spurious peaks. Moreover, one can miss genuine atomic peaks if they coincide by chance with a hole produced by the described heavy atom effect.

Acta Cryst. (1969). A **25**, 717

The role of intensity measurement projects: Correction.

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(*Received* 29 *May* 1969)

A correction to *Acta Cryst.* (1969), A **25**, 264

Owing to a slip in proof correction, an error was introduced into the acknowledgment, p. 273, of the original paper (Mathieson, 1969). The necessary change in the first sentence of the relevant paragraph is '... my colleagues, Drs J. K. Mackenzie and V. W. Maslen ...' and in the third sentence '... my Commission colleagues, Drs S. C. Abrahams and W. C. Hamilton ...'.

Reference

Mathieson, A. McL. (1969). *Acta Cryst.* A **25**, 264.