Let

$$|F(\mathbf{h})|^2 = \frac{KI(\mathbf{h})}{\mathrm{Lp}\,t(\mathbf{h})}$$

assuming negligible background counts and where I(h) is the total counts accumulated in time $t(\mathbf{h})$. Define

$$R(\mathbf{h}) = \frac{I(\mathbf{h})}{t(\mathbf{h})} \, .$$

The variance of $F(\mathbf{h})$ due to counting statistics is

$$\sigma_1^2(\mathbf{h}) = \frac{|F(\mathbf{h})|^2}{4R(\mathbf{h})t(\mathbf{h})} \,.$$

It has been suggested (e.g. Grant, Killean & Lawrence, 1969; Killean & Lawrence, 1969a) that additional terms must be added to this variance to give a satisfactory weighting scheme for least-squares analysis but it is open to question whether these terms represent mainly random or mainly systematic errors in the data. The subsequent analysis does not involve these terms since they are independent of $t(\mathbf{h})$ and consequently their form is unimportant for a priori optimization. Let these terms be denoted by $A(\mathbf{h})$. The variance of the structure factor may be estimated as

and

$$\sigma^{2}(\mathbf{h}) = \sigma_{1}^{2}(\mathbf{h}) + A(\mathbf{h}) = \frac{|F(\mathbf{h})|^{2}}{4R(\mathbf{h})t(\mathbf{h})} + A(\mathbf{h})$$
(2)

$$\sigma^{2}(\varrho) = \frac{1}{2} \left(\frac{2}{V}\right)^{2} \sum \left\{\frac{|F(\mathbf{h})|^{2}}{4R(\mathbf{h})t(\mathbf{h})} + A(\mathbf{h})\right\}.$$
 (3)

The measuring time for the diffractometer experiment, ignoring circle setting time, is

$$T = \sum t(\mathbf{h})$$

and the *a priori* optimal time for any $t(\mathbf{h})$ is given by solving

$$\frac{\partial \psi}{\partial t(\mathbf{h})} = 0$$

for $t(\mathbf{h})$, where

$$\psi = \langle \sigma^2(\varrho) \rangle - \lambda \{T - \sum t(\mathbf{h})\},\$$

i.e.

$$t(\mathbf{h}) = \left(\frac{1}{\mathrm{Lp}}\right)^{1/2} \left(\frac{K}{4\lambda}\right)^{1/2}.$$
 (4)

The fraction of the experiment time to be spent on any reflexion is

$$\frac{t(\mathbf{h})}{T} = \frac{\left(\frac{1}{\mathrm{Lp}}\right)^{1/2}}{\sum \left(\frac{1}{\mathrm{Lp}}\right)^{1/2}}$$
(5)

and the time spent measuring each reflexion is independent of the magnitude of the reflexion but depends on the geometry of the diffractometer and the wavelength of the Xradiation.

Define

$$G^{2} = \frac{\sum \sigma_{1}^{2}(\mathbf{h})}{\sum |F(\mathbf{h})|^{2}} = \frac{1}{4\mathrm{T}} \cdot \frac{\left\{\sum \left(\frac{1}{\mathrm{Lp}}\right)^{1/2}\right\}^{2}}{\sum \frac{R(\mathbf{h})}{\mathrm{Lp}}}$$
(6)

and, assuming that the random errors are due only to counting statistics

$$T = \frac{\sum |F(\mathbf{h})|^2}{2\langle \sigma^2(\varrho) \rangle V^2} \cdot \frac{\left\{ \sum \left(\frac{1}{\mathbf{Lp}} \right)^{1/2} \right\}^2}{\sum \frac{R(\mathbf{h})}{\mathbf{Lp}}}.$$
 (7)

In order to evaluate T for a given $\langle \sigma^2(\varrho) \rangle$ it is necessary to estimate the average variation of $R(\mathbf{h})$ with (\mathbf{h}) and the height of the origin of the Patterson function $(\sum |(F(\mathbf{h})|^2))$.

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References

CRUICKSHANK, D. W. J. (1949). Acta Cryst. 2, 65.

- CRUICKSHANK, D. W. J. (1960). Acta Cryst. 13, 774.
- GRANT, D. F., KILLEAN, R. C. G. & LAWRENCE, J. L. (1969). Acta Cryst. B25, 374.
- HAMILTON, W. C. (1967). Abstract E6, ACA Summer Meeting, Minneapolis, Minnesota, U.S.A.
- KILLEAN, R. C. G. (1967). Acta Cryst. 23, 1109.
- KILLEAN, R. C. G. & LAWRENCE, J. L. (1969a). Acta Cryst. B25, 1750.
- KILLEAN, R. C. G. & LAWRENCE, J. L. (1969b). Acta Cryst. A 25, 603.
- SHOEMAKER, D. P. (1968). Acta Cryst. A 24, 136.

Acta Cryst. (1972). A28, 658

On the diffraction enhancement of symmetry. Erratum. By HITOSHI IWASAKI, The Institute of Physical and Chemical Research, Rikagaku Kenkyusho, Wako-shi, Saitama 351, Japan

(2)

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A correction is given to Iwasaki, H. (1972). Acta Cryst. A28, 253.

In a previous paper of the above title (Iwasaki, 1972), equation (25) (p. 256) should read:

Reference

 $I_{n}(hkl) = I_{n}(khl).$

IWASAKI, H. (1972). Acta Cryst. A 28, 253.

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