groups $P1$ and $P\bar{1}$, and their results will be used below. In the following formulae, $z = I_{min.}/I_{av.} = F^2_{min.}/F^2_{av.}$ is the ratio of $I_{min.}$ to the average I over a shell of constant $\sin^2\theta$, and $N(z)$ is the cumulative distribution function.

$P1$

$$N(z) = \int_0^z e^{-t}dt$$

$$\begin{aligned}\mu(z) &= \int_0^z te^{-t}dt/N(z)\\ &= 1-ze^{-z}/N(z)\\ &\approx z/2\end{aligned}$$

$$\begin{aligned}\sigma^2(z) &= \int_0^z t^2e^{-t}dt/N(z)-\mu^2\\ &= 2\mu-\mu^2+z(\mu-1)\\ &\approx z^2/12\end{aligned}$$

$P\bar{1}$

$$\begin{aligned}N(z) &= \operatorname{erf}(z/2)^{\frac{1}{2}}\\ &= \frac{1}{\sqrt{(2\pi)}}\int_0^z e^{-\frac{1}{2}t}t^{-\frac{1}{2}}dt\end{aligned}$$

$$\begin{aligned}\mu(z) &= \frac{1}{\sqrt{(2\pi)}}\int_0^z e^{-\frac{1}{2}t}t^{\frac{1}{2}}dt/N(z)\\ &= \sqrt{\left(\frac{2}{\pi}\right)}z^{\frac{1}{2}}e^{-\frac{1}{2}z}/N(z)\\ &\approx z/3\end{aligned}$$

$$\begin{aligned}\sigma^2(z) &= \frac{1}{\sqrt{(2\pi)}}\int_0^z e^{-\frac{1}{2}t}t^{3/2}dt/N(z)-\mu^2\\ &= 3\mu-\mu^2+z(\mu-1)\\ &\approx 4z^2/45\end{aligned}$$

From the definition of z we have $\mu(I_{min.}) = I_{av.}\mu(z)$ and $\sigma^2(I_{min.}) = I^2_{av.}\sigma^2(z)$, and thus, for the two cases above, we have approximately

$P1$	$P\bar{1}$
$\mu \approx I_{min.}/2$	$\mu \approx I_{min.}/3$
$\sigma^2 \approx I^2_{min.}/12$	$\sigma^2 \approx 4I^2_{min.}/45$

For practical purposes, these values may be taken as the proper ones for all acentric and centric space groups for all but the very finest refinements.*

Each unobserved reflexion must, to be consistent with the least-squares motivation, be entered into the refinement with its appropriate mean value and weight, as determined from the theoretical distribution. It is a mistaken notion that only those unobserved reflexions which have $F^2_{calc.} > F^2_{min.}$ at a particular refinement stage should be entered in the succeeding refinement. Even in the event that all the calculated structure factors are less than the minimum observable values, these reflexions must properly be included in the next refinement to obtain reliable estimates of error, which is one of the most useful features of the least-squares procedure.

References

Howells, E. R., Phillips, D. C. & Rogers, D. (1950). *Acta Cryst.* **3**, 210.

Rogers, D. (1950). *Acta Cryst.* **3**, 455.

* The average intensity for a group of special reflexions may differ by an integral multiple from that for general (*hkl*) reflexions. These multiples depend on the symmetry elements present and may be as great as twelve; a table of their values for all the space groups is given by Rogers (1950). For such reflexions, z must accordingly be defined with the local average being taken over the group characterized by the same multiple, or, better, as the appropriate multiple times the local average for the non-special reflexions. However, to the approximation considered above, this factor does not enter the expressions for the mean values or variances of the *intensities*. For example, the next term in the series expansion for the variance in the acentric case is $-z^4/240$, so that the variance of the intensity to this degree of approximation is $I^2_{min.}/12-z^2I^2_{min.}/240$. In the present application, z will invariably be considerably less than unity, so that the second term is very unimportant. In the very rare case where it is large enough to be significant, use of the correct multiple is of course necessary.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

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The Battelle Memorial Institute announces that sets of indexing charts for the tetragonal, hexagonal and orthorhombic systems are available. The tetragonal and hexagonal charts cover c/a ratios from 0·2 to 5·0. The orthorhombic charts cover the range of b/a from 0·99 to 0·70 and c/a from 0·2 to 5·0. The set is available upon request for 'Battelle Indexing Charts for Diffraction Patterns of Tetragonal, Hexagonal and Orthorhombic Crystals' to Battelle Publications Office, 505 King Avenue, Columbus 1, Ohio, U.S.A.