17.5—4   THE VARIANCES AND COVARIANCES OF MEASURED INTENSITIES IN PRECISE LATTICE-CONSTANT DETERMINATION BY THE BOND METHOD. By E. Gałdecka, Institute for Low Temperature and Structure Research, Polish Academy of Sciences, pl. Katedralny 1, 50-950 Wrocław, Poland.

Precision of measurements on the Bond diffractometer depends on several factors as discussed in my papers (Urbanowicz E., (1981). Acta Cryst. A37, 364-368 and 369-373). In theoretical considerations it is often assumed that the variance of measured intensity is equal to number of counts. This result from Poisson statistics and from the assumption that the only source of statistical errors is counting statistics and all the other factors are negligible. In present paper beside counting statistics the following parameters which influence the statistical errors are taken into account:
a) $\sigma(V)/V$ – fluctuation of the power voltage,
b) $\sigma(\omega)_M$ – statistical angle-reading error,
c) $\sigma(\Delta\omega)$ – the error in positioning of the angle by stepping motor.
As a result, the following formula for the variance of measured intensities was derived:

$$\sigma^2(h_i) = e_1 h_i + e_2 h_i^2 + \sigma^2(\omega_i)(h_i')^2$$

where: h_i – the number of counts in i-th position of the sample (i = -p,...,p and 2p + 1 – the number of the scanning points),
ω_i – angle position of the sample,
h_i' – the first derivative $\partial h/\partial\omega$ in the i-th position,

$$\sigma^2(\omega_i) = e_3 + i^2 e_4, \quad e_1 = 1, \quad e_2 = \sigma^2(V)/V^2,$$

$$e_3 = [\sigma^2(\omega)_M + p\sigma^2(\Delta\omega)]/2,$$

$$e_4 = [\sigma^2(\omega)_M - p\sigma^2(\Delta\omega)]/(2p^2).$$

An analysis of the covariances of angle positions ω_i of the sample leads to the conclusion that in the case of automatic scanning the covariances between the values ω_i and ω_j (i,j = -p,...,p and i ≠ j) cannot be neglected, as their values given by the formula

$$cov(\omega_i, \omega_j) = e_3 + ije_4 - |i - j|e_5 ,$$

where $e_5 = \sigma^2(\Delta\omega)/2$,

are comparable with the values of the variances.

Covariances between ω_i, ω_j (angle positions) result in correlations between measured intensities h_i, h_j:

$$cov(h_i, h_j) = h_i' h_j' cov(\omega_i, \omega_j)$$

The model of variances and covariances of the measured intensities has been verified on the basis of several series of experimental data. Experimental conditions were discussed when:

1) we can take $\sigma^2(h_i) = h_i$,
2) fluctuations of the power voltage are essential,
3) dispersion of position angles of the sample cannot be neglected.

17.5—5   PSEUDOTRANSLATIONS AND STATISTICS. By G. Cascarano, C. Giacovazzo & M. Luić, Dipartimento Geomineralogico, University, 70121 Bari, Italy.

Pseudotranslation symmetry frequently occurs in crystal structures. Their effects on the structure factor statistics has been studied by different authors in some aspects and in few space groups. It seems interesting to describe a general theory which provides the distribution of the structure factors in any space group for any combination of the pseudotranslations.
An important complementary problem is that of deriving, from the observed statistical effects, information about the pseudotranslations : for example the nature of the pseudotranslations, the percentage of atoms which are related by the pseudotranslations, ... Such an information is of primary importance in the field of direct methods, where the particular features of the structure have to be taken into account.

17.5—6   EFFECT OF HEAVY ATOMS ON INTENSITY STATISTICS OF X-RAY DIFFRACTION FROM CRYSTALS. By D. Pradhan, S. Ghosh and G. D. Nigam, Department of Physics, Indian Institute of Technology, Kharagpur-721 302, India.

It is well known that if the unit cell contains one or few heavy atoms in addition to a large number of light atoms, the distribution of x-ray intensities usually deviate considerably from those inferred by Wilson statistics. In such cases, strong correlation between atomic positions results from the finite radii of atoms, which prevents complete randomness in the distribution of atoms in the unit cell.
A modified cumulative distribution function of normalised intensities is derived for a triclinic cell when heavy atom occupies special position in the unit cell. The distribution being considered, the remaining light atoms would no longer be randomly distributed in the midst of heavy atom in the whole unit cell. It corresponds, in fact, to an inaccessible volume, which is assumed spherical, around the heavy atom with radius equal to the sum of the radius of heavy atom and the average radius of light atoms. This inaccessible volume would modulate the average intensity and the distribution parameter as a function of s. Numerical study is made to investigate the effect of the inaccessible volume on the cumulative distribution function. The results are compared with experimental distributions for rubidium di-o-nitrobenzoate and potassium hydrogen di-o-nitrobenzoate.