17.5–1 EFFECT OF STATISTICAL FLUCTUATIONS AND SYSTEMATIC ERRORS ON INTENSITY DISTRIBUTIONS. By A.J.C. Wilson, Crystallographic Data Centre, University Chemical Laboratory, Cambridge CB2 1EW, England.

Depending on the assumptions made, one or more of the following representations of an ideal probability distribution of intensities of reflexion (or structure factors) may be practicable:

(1) An expression in closed form.
(2) A series expansion in orthogonal polynomials.
(3) A Fourier (Barakat) series.
(4) A steepest-descents approximation.

[For recent references see A.J.C. Wilson, Proc. Ind. Acad. Soc. Chem. Sci., 92, 335-339, 1983.] Observed distributions, even if the underlying distribution is ideal, are distorted by statistical fluctuations and systematic errors in the intensity measurements, and a valid comparison of a calculated and an observed distribution must take these distortions into account. In principle the distribution of the statistical fluctuations will be fully predictable [for a discussion of several cases see A.J.C. Wilson, Acta Crystallogr., A 36, 929-936, 1980], but little is known of the distribution of systematic errors -- often no more than the first and second moments, sometimes even less. An attempt is made to modify each of the four representations in the light of limited knowledge of the fluctuations and errors. Closed forms are rarely obtainable; known moments are readily incorporated in orthogonal-polynomial expressions; full knowledge is required for Fourier representations.

17.5–2 A STATISTICAL PERSPECTIVE ON ABSORPTION ANALYSIS EXPERIMENTATION: PROBLEMS IN ESTIMATION AND DESIGN. C.M.O'BRIEN, Department of Statistical Science, University College London, Gower Street, LONDON WC1E 6BT, England.

For many years crystallographers have been concerned with both the theoretical calculation and experimental estimation of attenuation coefficients. The adoption, in the latter case, of the method of least squares for the estimation of these coefficients - along with the implicit assumption of multiplicative homoscedastic error - in problems involving exponential absorption of particle beams by matter represents only one statistical approach to the problem of unknown parameter estimation.

A number of alternative approaches to problems of parameter estimation have recently found favour within the areas of growth model development, time series analysis and pharmacokinetics. These are adapted within the context of increasingly complex but defendable model assumptions and presented for the analysis of data obtained from absorption measurements.

An analogy is made between this design/analysis possibility and current research into statistical aspects of activation analysis experimentation, where there is also a large but finite data base involved (O'Brien & Stone: Nuclear Instruments & Methods in Physics Research (1984): in the press). However, the fact that the absorption exponentials are thickness-dependent rather than time-dependent alters the way in which model fitting procedures may be utilised.

The possibility of using the knowledge for each element of the variation of attenuation coefficient with incident particle energy and type is discussed with a view to the non-destructive composition determination of chemical specimens.

The application of these ideas to absorption measurements made by R.C.Henriques (Ph.D. Thesis, London 1971) will be illustrated. In these experiments (Io) is the intensity of a Laue reflection from a diamond crystal acting as a radiation analyser, and (I) is the intensity of the same reflection when the incident beam is intercepted by a specimen plate of thickness x, so that absorption coefficients and/or chemical composition can be estimated from an analysis of many ratios (I/Io), the analyser orientation being optimised for the problem in hand.

We also intend to adapt these statistical approaches for designing experiments yielding new measurements of absorption coefficients obtainable by using X-radiation produced in a scanning electron microscope, where many elements not available in conventional X-ray tubes can be used as targets.

17.5–3 APPLICATION OF DIGITAL FILTER TECHNIQUES TO THE EVALUATION OF WEAK X-RAY INTENSITIES. By H. Bondza, K. Hümmer and H. Burzlaff, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Loewenichstr. 22, Universität Erlangen-Nürnberg, FRG.

For some problems (Powder diffraction, superstructures) it is important to measure weak X-Ray reflections with good accuracy. The bad signal-to-noise ratio, however, leads in most cases to very poor results. To improve this situation the application of a digital narrowband filter technique is proposed.

The profile of a reflection is recorded by a usual step scan. In addition to the normal evaluation the correlation between succesive steps is used as a base for the input signal of the filter. Simulated computational models gave indication for a remarkable improvement in the signal-to-noise ratio of the output without increase of measuring time.

The procedure will be applied to experimental weak intensity measurements. The result will be reported.