factor. There is therefore an obvious need to extend the earlier intensity measurement project to a second stage in which the effects of differences between individual crystals are diagnosed and minimized. To reduce measurements from different crystals to a more or less common base, it is necessary that corrections be applied, not only for simple absorption but also, and probably more importantly, for extinction. Correction procedures for simple absorption are relatively straightforward but there is no single preferred procedure for the estimation of extinction effects. Since theoretical F_c values are dependent on the particular model adopted, reference to such values as a guide or measure of experimental accuracy is questionable. It seems therefore more appropriate to test, as far as possible, *experimental procedures which are intended to diagnose and correct for extinction.*

There are a number of feasible procedures for the estimation of extinction which are essentially experimental. These involve either measurements on the one specimen or measurements on two (or more) specimens – for example:

(*a*) with a single specimen,
  (i) measurements with a polarization analyser, *e.g.* Chandrasekhar *et al.* (1969);
  (ii) measurements made at two or more wavelengths, *e.g.* DeMarco & Weiss (1962);
  (iii) measurements of integrated intensity with varying path lengths as achieved, for instance, by rotating about the scattering vector, *e.g.* Willis (1962).

(*b*) with more than one specimen,
  (i) comparison with measurements on powdered specimens of the same material, *e.g.* Stewart & Jensen (1969);
  (ii) measurements on single crystals of different size, or extinction condition, and appropriate extrapolation, *e.g.* Cochran (1953).

Any other suitable procedure not specified above, but of an experimental nature, may be used.

The Commission welcomes the cooperation of crystallographers in this project. Its successful operation will obviously depend critically on their willingness to participate. It is recognized that the proposed project is not a simple straightforward one but, just as phase I focused attention on the potential gross effect of specimen variation, so phase II could be most valuable and instructive in highlighting the magnitude and significance of intensity-dependent factors in experimental measurements and should assist in assessing the scope of operational procedures for estimating extinction.

Any individual crystallographer or group wishing to have further details should contact the Chairman – Dr A. McL. Mathieson, Division of Chemical Physics, C.S.I.R.O., P. O. Box 160, Clayton, Victoria 3168, Australia.

References

ABRAHAMS, S. C., HAMILTON, W. C. & MATHIESON, A. McL. (1970). *Acta Cryst.* A**26**, 1.

CHANDRASEKHAR, S., RAMASESHAN, S. & SINGH, A. K. (1969). *Acta Cryst.* A**25**, 140.

COHRAN, W. (1953). *Acta Cryst.* **6**, 260.

DEMARCO, J. J. & WEISS, R. J. (1962). *Acta Cryst.* **15**, 1125.

STEWART, R. F. & JENSEN, L. H. (1969). *Z. Kristallogr.* **128**, 133.

WILLIS, B. T. M. (1962). *Pile Neutron Research in Physics*, p. 455. Vienna: I.A.E.A.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M.M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

Thermal neutron diffraction. Proceedings of the International Summer School at Harwell 2-5 July 1968. Edited by B. T. M. WILLIS. Pp. xiv.+229. London: Oxford University Press, 1970. Price 65 *s.*

The booklet contains the proceedings of the International Summer School, held in July 1968 at Harwell, with the dominant theme of accurate determination of neutron intensities and structure factors. There are three main divisions, *A*, *B* and *C*, dealing respectively with the experimental methods and corrections, with nuclear crystallography and finally with magnetic scattering.

The four chapters of the experimental part (*A*) describe the collection and correction of data (Cooper and Rouse) with special emphasis on the correction of intensities for thermal diffuse scattering (Cooper) and the most important experimental methods: the two- and three-axis goniometry (Caglioti) and time of flight diffractometry (Turberfield).

The main part *B* (100 pages) is devoted to neutron crystallography and its connexions with solid state physics and chemistry. There is a delightful introductory chapter by C. A. Coulson on *Molecular Objectives in Elastic Neutron Scattering* where crystallographers may learn that the difference between the charge centroids (the so called 'atomic positions' seen by X-rays) and the nuclei (seen by neutrons) may be as high as 0·1 Å for H and for heavier atoms like N as high as 0·04 Å. These differences are much greater than the precision nowadays attainable on the 'atomic positions' (0·005 to 0·01 Å) and it even raises the question of the definition of the bond-length. The knowledge of the true positions of charge centroids and of nuclei will be very essential for the comprehension of the chemical bond and of lattice vibration problems. Coppens considers more specifically structural and chemical problems of small organic molecules where X-ray and neutron data are compared in difference Fourier syntheses and isotopic effects (H–D) may be detected. There are four chapters in part *B* with a strong emphasis on thermal aspects, on rigid body motion as examplified by hexamethylenetetramine (Dawson), on anharmonicity in BaF_2 (Willis, Dawson), on constraints (mainly thermal) used in structure refinement (Pawley) with a generalized treatment for thermal motion written by C. K. Johnson. One feels surprised by the importance of anharmonicity which in a cubic crystal like BaF_2 gives rise to intensity differences of 20% at room temperature and of more than 100% at 600°C for the 'equivalent' lines 11, 1, 1 and 5, 7, 7 ($h^2+k^2+l^2=123$). It is also gratifying to state that anharmonicity explains these differences quantitatively (Willis).