

**International tables for X-ray crystallography. Vol. IV.** Edited by J. A. IBERS and W. C. HAMILTON. Pp xi + 366, Figs. 10, Tables 39. Birmingham: Kynoch Press, 1974. Price £ 10.

Volume IV of *International Tables* contains updated values for much of the numerical information in Volume III and also extra material concerning certain aspects of crystallography which have been extensively developed since the earlier volumes were published. The choice of the latter topics was partly due to the personal preferences of the editors and although important topics have been omitted, crystallographers will welcome the authoritative treatment of important subjects which is presented in the later sections.

Section 1 contains tables of X-ray wavelengths, one collated according to the atomic number of the elements and a second table collated in increasing wavelength. This section gives a much more extensive tabulation than is found in Volume II.

Section 2 begins with tables of X-ray cross sections and attenuation coefficients. These are followed by tables of X-ray scattering factors. New in this volume are a table of coefficients for an analytical approximation to the scattering factors giving maximum and mean errors, and a table of X-ray scattering factors of unfilled orbitals which may be used for aspherical atoms. The table of dispersion corrections for X-ray scattering factors gives what are apparently more accurate values than in Templeton's tabulation in Volume III, but no indication of accuracy or variation with  $\sin \theta$  is given. The electron scattering factor tables are much more extensive than in Volume III, occupying more than one hundred pages.

Section 3 is devoted to diffractometer geometry. A series of excellent sub-sections by the late W. C. Hamilton deals with the mathematical aspects of the calculation of setting angles, the determination of an orientation matrix and measurement procedures.

Section 4 by the same author, gives a table for *R*-factor ratio significance tests and tables for analysing least-squares weights for consistency. The accompanying discussion is very valuable.

Section 5 contains mathematical articles by C. K. Johnson and H. A. Levy on the thermal motion of independent atoms and rigid bodies. The correction of interatomic distances and angles for thermal motion is also covered. A final sub-section deals with the site symmetry restrictions on the coefficients of thermal-motion tensors.

In Section 6, J. Karle discusses the solution of the phase problem by direct methods. Tables for assisting origin specification along with examples of choices of phases for the different space-group types are included. The following two sub-sections include discussions on the normalization of structure factors and phase-determining formulae. The final sub-section discusses the symbolic addition method of application of these formulae in X-ray and neutron diffraction. It is a pity that greater recognition is not given to the computer applications of the formulae that have developed in the last ten years. Although Section 6 contains some very useful material, the clarity of presentation of the textual material is not up to the high standard of the previous sections.

In sum, Volume IV is a fine addition to the other volumes. The earlier volumes of the pre-computer era now look rather dated. One hopes that Volume IV sets a stan-

dard that will be followed by future volumes in this series.

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**Molecular structure by diffraction methods. Vol. 2.**

By G. A. SIM and L. E. SUTTON (Senior Reporters). Pp. xiii + 513, Figs. 92, Tables 27. London: The Chemical Society, 1974. Price £17.50.

This second volume in the series is arranged according to the same format as Vol. 1 with three parts: *Electron Diffraction*, *Neutron Diffraction* and *X-ray Diffraction*. All three parts review papers published between April 1972 and March 1973 but the period covered is extended to August 1973 for the neutron diffraction section and to mid-autumn 1973 for the electron diffraction section. Because of the shorter period reviewed than in Vol. 1 and because the electron diffraction section is this time confined entirely to structural results, Vol. 2 is considerably shorter than the 824 pages of Vol. 1. It is a measure of the inflation of book prices, however, that the smaller Vol. 2 costs more. The reduction in size does not correspond to a reduction in the number of references in all sections. The electron diffraction part discusses 139 references (compared with 464 in Vol. 1), the part on neutron diffraction reports 72 references (96 in Vol. 1) and that concerned with X-ray diffraction has 741 references on organic structures, 168 on globular proteins and 1128 on inorganic structures. (The corresponding X-ray figures for Vol. 1 were 631, 146 and 1228.)

Throughout Vol. 2 there are useful references to Vol. 1. Diagrams are used liberally to supplement descriptions in the text and the many tables provide valuable numerical correlations. The team of Reporters is practically the same as for Vol. 1 and they are to be congratulated on having discussed so much factual information in a way which is concise and yet readable. There seem to be remarkably few errors. Every reader is bound to find some sections of the book which are particularly fascinating for him. For the reviewer, one of the most interesting features is the way in which hydrogen bonding and other forms of intermolecular interaction keep cropping up in a volume which is largely devoted to intramolecular geometry. Exciting developments are reported in the globular protein section where the high-resolution structures of a fragment of an immunoglobulin and a Bence-Jones protein are briefly described. The reporter comments that these results might represent the most significant contribution of crystallography to medicine. Readers who found Vol. 1 interesting will certainly be rewarded by continuing their studies in Vol. 2. Besides being a must for every scientific library, many individual scientists concerned with structural chemistry will want to have their own copies.

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