Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

New Co-editor of *Acta Crystallographica*

The Executive Committee of the International Union of Crystallography has approved the appointment of Professor G. A. Jeffrey as a Co-editor of *Acta Crystallographica* Professor Jeffrey will take up this work on 1 August 1973. His address is given in the list of Co-editors on the inner front cover of this issue.

Conference on Anomalous Scattering, Madrid, Spain, 22–26 April 1974

This specialist inter-Congress conference, organized by the Commission on Crystallographic Apparatus of the International Union of Crystallography, will take place at the Consejo Superior de Investigaciones Cientificas, Madrid. The purpose of this Conference is to assess the experimental and theoretical errors that arise in the measurement and interpretation of anomalous scattering of X-rays, neutrons and electrons. Topics under consideration include the accuracy of anomalous-scattering measurement using characteristic X-radiation, continuous X-radiation, X-radiation at an absorption edge, neutrons, and electrons; the effects of dispersion corrections on atomic parameters and the accuracy of the dispersion corrections; the application of anomalous scattering to structure determination; the probability of error in absolute-configuration determination; the relation of absolute atomic arrangement to macroscopic tensorial properties; novel uses of anomalous scattering, such as Mössbauer effect and electron scattering; other applications of anomalous scattering. It is proposed to publish the proceedings of the Conference. Participation in the Conference, which will be limited to a total attendance of about 125 specialists for optimum discussion and interaction, is by invitation only. Further information may be obtained from Dr S. C. Abrahams, Bell Laboratories, Murray Hill, New Jersey 07974, U.S.A.

U.S.A. Inter-Congress Symposium on Intra- and Intermolecular Ferces, Pennsylvania State University, 14–16 August 1974

This meeting, which is sponsored by the International Union of Crystallography, will be held immediately prior to the meeting of the American Crystallographic Association at the Pennsylvania State University 19–24 August 1974. The topics of the symposium are (i) theoretical and experimental determination of nonbonded interactions, (ii) models for calculation of molecular conformation, (iii) molecular and ionic packing in crystals, (iv) vibrational and spectroscopic analyses, (v) nonbonded interactions in polymers and (vi) conformational calculations for proteins and other biological macromolecules. It is intended that the programme will appeal to non-crystallographers with an interest in intra- and intermolecular forces, as well as to crystallographers. Copies of the First Circular and further information may be obtained from Professor D. E. Williams, Chemistry Department, University of Louisville, Louisville, Kentucky 40208, U.S.A.

Tenth General Assembly and International Congress of Crystallography Preliminary Announcement

At the invitation of the Stichting voor Fundamenteel Onderzoek der Materie met Röntgen- en Elektronenstralen the Tenth General Assembly and International Congress of Crystallography of the International Union of Crystallography will be held at the R.A.I. Congress Centre, Amsterdam, The Netherlands, 7–15 August 1975.

The first formal announcement will appear in *Acta Crystallographica* at the end of 1973 or early in 1974 and will give the address from which copies of the First Circular can be obtained. In addition, copies of this First Circular will be sent to all National Committees for Crystallography.

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.

Early papers on diffraction of X-rays by crystals. Vol. II. Edited by J. M. BIJVOET, W. G. BURGERS and G. HÄGG. Pp. xix + 484. Utrecht: Oosthoek, 1972. Price £10·80.

This work is of particular interest to the reviewer, because it is a collection of the publications he and his colleagues read and discussed during the years 1933 to 1936 when he was one of Professor Linus Pauling's graduate students in the Chemistry Department of the California Institute of Technology. The fundamental discoveries necessary for the development of the science of X-ray crystallography had been made by about 1930; the papers collected in the five chapters of the first volume of this work cover this subject matter beautifully. The second volume, which is the subject of this review, contains an intelligent selection of papers from which the early growth of the science of crystal structure determination can be traced.

Chapter VI, the first in Volume II, contains selections from the works which eventually led to the symbols for space groups and the tables of their symmetrically related

points that we use today. Some papers are included which describe how space groups could be found from X-ray diffraction patterns, and how molecular symmetry could sometimes be inferred from the space group of a crystal and the atomic content of its unit cell. Chapter VII presents most of the classic papers in which the ionic and covalent atomic radii are defined and stated. (Metallic radii were also much used in the 1930's, but no paper about them is included.) Then follows some material describing the early work on the structures of ionic crystals, together with some mention of the hydrogen bond. Chapter VIII contains papers, or fragments of papers, describing the various techniques for collecting data on the directions and intensities of X-rays diffracted by crystals, crystalline powders, and partially crystalline fibers. The Laue, powder, rotation, and Weissenberg techniques are described, and some of the structural results so obtained are presented. Chapter IX deals in a similar way with the classic works on solid solutions, random stacking of layers, and rotating groups. Some of the early work on alloys and their structures is also included in this chapter. Chapter X presents a collection of pioneering papers on crystal-structure determination. Early uses of symmetry, cell dimensions, diffracted intensities, chemical intuition, trial and error, and isomorphous replacement are all described. The increasing complexity of the structures studied during the period 1920 to 1935 is clearly brought out. The chapter ends with the first papers on X-ray diffraction by crystalline proteins. Chapter XI is a group of papers in which is traced the history of the use of Fourier series in crystal structure determination. It starts with the working out of the electron density in alkali halides, continues with the use of signs from trial structures, and ends with the heavy-atom method. Chapter XII contains only one paper: the famous 1935 paper fully explaining the Patterson method, then – tacitly – limited to finding the projections of interatomic vectors onto lines or planes.

The names of the authors of all these great papers are not quoted above; to do so would have made this review too long. The distinguished names are all in the book, of course, and most of them are familiar to every physical scientist.

An interesting example of the discovery, loss, and rediscover of an important idea appears on the title page of Chapter XII. P. P. Ewald pointed out in 1921 that the squared magnitudes of the structure amplitudes of the X-rays diffracted by a crystal depend on the interatomic vectors and not the atomic positions. No use seems to have been made of this fact until it was rediscovered by A. L. Patterson in 1934.

By carefully reading the material in this book, a student could learn more than three quarters of what a modern X-ray crystallographer should know, and at the same time get a feeling for the excitement that existed among investigators of crystal structures in those thrilling days. He would also discover how incorrect ideas are sometimes held by very distinguished scientists, and how subsequent thought and experiment changes these ideas into others. Eventually the current ideas are evolved; these are the ones we think are correct.

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Crystal structure determination. By HERBERT A. HAUPTMAN. Pp.xii + 407. New York: Plenum Press. 1972. Price $ 23.00.

Significant advances in the practical use of formalized direct methods for determining more and more complex atomic structures bring not only a sense of achievement but also a feeling of loss. The thrill of searching for an intricate atomic pattern guided primarily by the investigator's intellect will never return. Computer-controlled diffractometers and powerful computers on which the modern methods for solving the problem of structure analysis are being programmed allow automation of the whole process of the determination of the atomic structure of crystals. With structure determination turned into a routine process mineralogists, chemists, physicists and specialists in molecular biology can use structure analysis as an effective method in their everyday research.

In recent years the number of structures established by direct methods has steadily increased. In these methods two approaches can be considered as the most effective ones: symbolic addition and the multiple-solution method.

The subject of this monograph is concerned with a third approach which is based on the systematic use of structure invariants and seminvariants. At the present time this approach does not seem to have as many successes to its credit as the other two, but the examples of its practical use as presented in the final chapters of H. A. Hauptman's book give a good idea of the potential development of this method.

The monograph is divided into three parts: in the four chapters of the first part an attempt is made to expound the theoretical bases of the method. The treatment of the algebraic formulae for deriving structure seminvariants is given fully. This section of the book closes with an account of the probability approach to the phase problem in structure analysis. The techniques of implementation of the theoretical methods described in the first part of the monograph are thoroughly discussed in the second part. The algorithm for solving the phase problem is divided by the author into three more-or-less independent stages – the calculation of cosine seminvariants from the values of the moduli of normalized structure amplitudes, the determination of phases of a small number of the basic structure amplitudes, and finally the establishment of the phases of a sufficient number of structure amplitudes sufficient to reveal an approximate structure in an E map.

The sections in which the criteria for selecting the structure enantiomorph are given attract the reader's particular attention. This new approach to enantiomorph discrimination is based not by fixing the phase of one selected reflexion, but through the selection of two groups of reflexions for such an identification. This idea seems useful for any of the variants of direct methods.

The most important stage in applying direct methods is the establishment of the phases of a small number of basic structure amplitudes. A least-squares method is here described by which a set of phases in best agreement with the derived cosine seminvariants is readily selected.

The application of the tangent formula for refining and extending phase information is now a generally accepted procedure in direct methods. Hauptman discusses possible modifications of this technique and gives a number of examples which illustrate the advantages of the proposed modifications. A good part of the book is devoted to the