

The magnetic scattering part *C* is introduced by Lomer who calls the attention of the experimentalists to the significance of accurate intensity measurements for the determination of radial *d*- and *f*-electron densities and also of magnetic structures. The chapter by P. J. Brown considers the problem of extinction in polarized neutron work and the quite modern topic of analysing the orbital part of the magnetization. Magnetic moment distributions are reviewed by Forsyth including spin pairing effects of electrons (Yosida) and magnetic moment transfer to ligands. A chapter by Rimmer on covalency in magnetic salts illustrates the Marshall-Hubbard theory in which the covalency parameters  $A_G^2$  and  $A_N^2$  are directly related to the spin reduction observed in magnetic scattering.

From the point of view of mathematics the book is quite readable with the exception perhaps of the more sophisticated but excellent treatment by C. K. Johnson of thermal motion. There is some criticism on the lack of consideration of up-to-date topics like statistical- and Fourier-choppers or the possibility of polarization analysis (Moon, Riste, Koehler) for which however references are indicated.

To summarize, the collection of papers edited by Dr B. T. M. Willis is not meant to be a complete text book, but it is remarkably well suited as an introduction for the X-ray crystallographer and also for the neutron diffractionist who will find there about three hundred references to dig deeper.

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### Early papers on diffraction of X-rays by crystals.

Edited by J. M. BIJVOET, W. G. BURGERS and G. HÄGG. Pp. xvi + 372. Published for the International Union of Crystallography by A. Oosthoek's Uitgeversmaatschappij N.V., Utrecht. Price *f.* 48, \$ 13.50, £ 5.14 s. (£ 5.70).

The birth of a wholly new science is a rare event. The birth of the 'New Crystallography' is exceptional in that it can be dated exactly, and that its importance was immediately recognized and developed by a nucleus of young scientists of outstanding ability, of varied nationalities, many of whom are still living. Their recollections of those early days have been put on record.\* Succeeding generations will want to know how the ideas were presented and explained at the time in the published papers that gave them definite form. Nowadays it is only the older workers who remember these papers as the immediate source of their own knowledge, whether sought out directly by their own reading or reported verbally by teachers who had gone to the originals. From the late nineteen-thirties, this situation began to change as intermediaries became available: the presentation of the ideas to younger scientists has been shaped through an ever-increasing supply of text-books and incorporation in formal University courses, in constantly changing perspec-

tive as they bring in factual evidence not available in the earlier days. By now, the basic concepts of crystallography have permeated thinking in physics and chemistry to such an extent that it often requires an effort of the imagination to realize that what appear to present-day scientists as intuitively acceptable postulates were once controversial innovations based on modes of thinking quite alien to the older conventional disciplines.

In attempting a compilation of original papers, editors are always faced with a dilemma: shall they try to include everything that later historians would judge relevant, or shall they concentrate on what will help scientists of the present day? Professor Bijvoet, Professor Burgers and Professor Hägg have taken a clear stand for present education rather than future history. They quote Professor Guinier's definition of the objective: 'Il ne s'agit pas seulement d'honorer ceux qui ont fait oeuvre original, mais aussi nous voudrions que le livre soit utile pour la formation et la culture des jeunes cristallographes'. At the same time, their own firsthand knowledge of the subject from its early days, their involvement in its growth and their own major contributions to it, ensure that what they present to young crystallographers is neither a routine nor a trivial choice, but is informed by a real understanding of the impact of such papers on the progress of scientific thought.

The task of selection was not easy – the amount of important material is so large. Limitations of date and of subject matter were necessary so that the volume could be shaped as a coherent whole. Only papers up to 1935 were considered for inclusion (except for some later review-type quotations used as chapter headings). Most crystallographers would probably agree that, so far as one is entitled to divide up the history of diffraction crystallography into separate periods, one era ended and another began with the publication of Patterson's two papers in 1934–5. As regards subject matter, diffraction crystallography has from the very beginning advanced on two fronts – the study of diffraction processes on the one hand, of the structures revealed by diffraction analysis on the other. The two are not, of course, wholly distinct: each provides ideas necessary to the other, and the same worker may be actively interested in both simultaneously. In a given piece of work, however, one aspect or the other is likely to predominate, and this has served the editors as a basis for classification. The present volume, they say, 'apart from the very first papers, deals with the intensity of X-ray diffraction in the kinematical and the dynamical theory. The development of X-ray crystallography in the 'trial-and-error' period and the (re-)birth of the Fourier method are planned for a second volume'.

The papers chosen for inclusion are not quoted in their entirety. Passages are of very varied length, ranging from what appear to be complete papers (one could only check this by reference to the originals, as omissions are not marked) to short extracts ten or twelve lines long. They are not grouped primarily by date, but by topic, into chapters and sections; within each section, they are ordered to show the progressive development and clarification of thought. Short extracts are mixed effectively with the longer ones, short and long ones from the same paper being sometimes included in different sections where they are most relevant.

Chapter headings are: (I) The discovery of X-ray diffraction by crystals, interpretation and some of the first structure determinations, (II) The reciprocal lattice, (III) The intensity factors of the kinematical theory, (IV) The dynamical theory, (V) The *f* factor continued, extinction, anomalous

\* See, for example, *Fifty Years of X-ray Diffraction*, edited by P. P. Ewald and with the same publishers as the present volume; also the recent numbers of *Acta Crystallographica* honouring P. P. Ewald (1968, A24, Part 1 and B24, Part 1) and W. L. Bragg (1970, A26 Part 2 and B26 Part 3).

scattering. In (I) we have the original paper of Laue, Friedrich and Knipping; the early work of the Braggs; Friedel on symmetry. (III) includes the first treatments of atomic scattering factors, and the theories of thermal motion by Debye, by Waller, and by Darwin. (V) covers rather later work on atomic scattering factors – the experimental studies of Bragg, James and Bosanquet, Hartree's self-consistent field principle (in very short extracts), the problem of imperfections and mosaic texture, and the theory and applications of anomalous scattering.

Altogether, there are 83 numbered passages taken from 73 papers by 31 different authors (if we arbitrarily count only the first name in a collaboration as that of the author). The longest passage (19 pages) is from Laue's 1931 paper on the dynamical theory; nearly the shortest (11 lines) is from W. H. Bragg's Bakerian Lecture in 1915, where he foresees the use of Fourier methods. Most of the long passages (as we should expect) are from the work of Laue, Ewald, W. H. Bragg and W. L. Bragg: others are by Darwin (two 1914 papers), Debye & Scherrer (1918), and Coster, Knol & Prins (1930). A histogram of the dates is interesting: 41 of the numbered references are for the years 1912-14, 5 for 1915-18, 7 for 1921-23, 19 for 1925-28, and 11 for 1930-34. All extracts are reprinted in their original language, of course, but page headings provided by the editors are in English throughout. These headings are a welcome help to the reader who may want to refer to a particular point without re-reading the whole of a long text to find where it comes.

The technical production of the book deserves praise. The printing is clear and attractive, with pleasant paragraph spacing, and the quotations which serve as introductions to chapters (or sections) are set out invitingly in italics. As a help for reference, chapter numbers and serial numbers of excerpts are printed at the top of every left-hand page. The whole appearance and design of the book, in fact, invite the reader's attention and create an expectation of enjoyment.

This is a book which ought to be in every library, and which many teachers, having once seen, will want on their own shelves. Its selection and arrangement reflect the editors' experience in the ways of thought that are being presented to the reader, and make the old work come alive in a new perspective. Besides its general interest, it will be of particular value to teachers preparing lecture courses and, on occasion, as formally recommended reading for their classes; and in any case, enterprising students wanting to know how discoveries looked to the discoverers and their contemporaries should be encouraged to browse in it.

My one substantial criticism is that the subject matter of this volume represents only half the story. Students as well as teachers will want to hear of the growth of ideas about what structures are actually *like* – for example, W. L. Bragg's original introduction of the idea of atomic radii in 1920 and Bernal & Fowler's tetrahedral picture of the water molecule in 1933. This field, even more than diffraction theory, is one where the origins of our present knowledge are obscure to younger physicists and chemists – and sometimes to crystallographers too – and incentives to new thinking are thereby weakened. A companion volume covering structural studies and Fourier methods is promised, if interest in the present volume warrants it. The proviso is a little dangerous: it is only too easy for the appreciative reader to forget to take active steps to record his interest; and in any case this is the sort of book whose value will be discovered by an

increasing circle of readers over a period of years, rather than all at once. It is to be hoped, however, that as many as possible *will* write to the publishers asking for the second volume.

The International Union of Crystallography, who sponsored the book (on the recommendation of their Teaching Commission), are to be congratulated on the success of their undertaking, as are the three editors who have given it reality.

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**N.M.R. basic principles and progress. Volume 1. N.M.R. studies of molecules oriented in the nematic phase of liquid crystals.** By P. DIEHL and C. L. KHETRAPAL. **The use of symmetry in nuclear magnetic resonance.** By R. G. JONES. Editors: P. DIEHL, E. FLUCK and R. KOSFELD. Pp. 174. New York: Springer Verlag, 1969. Price: cloth \$ 10.80, DM. 39.

This is the first volume in a series devoted to authoritative reviews, plus progress reports and original work, in nuclear magnetic resonance spectroscopy. The main aim, as stated by the editors, is to publish articles which take the reader from the introductory stage to the latest development in the field. The descriptions 'introductory' and 'basic principles' are used in a restrictive sense in that a good knowledge of at least the fundamentals of n.m.r. is prerequisite. The concept, however, is a good one and should offer a useful and different approach from the Advances-Progress-Annual Review type of publication.

The first article, by Diehl & Khetrpal, describes the results of studies on molecules oriented by solution in nematic liquid crystal solvents, a method which is receiving increased attention as a means of obtaining information on molecular geometry, the anisotropy of chemical shifts, the absolute signs of indirect coupling constants, and the magnitudes of small quadrupole coupling constants. The basic principles and theory receive a brief concise treatment and the major part of the article is devoted to an extensive catalogue of results. Details of experimental methods are sparse. The authors have achieved the remarkable feat of including the literature data available to mid-1969 (and beyond with the inclusion of unpublished material from various sources). The molecules discussed are classified for this purpose on the basis of their spectral notation and tables of transition frequencies and intensities are given in a number of cases. A vast amount of information is presented in tables but no index is provided. The authors appear to have placed a limitation on the article in that it is essentially a survey of the available data, commendable for its comprehensive nature, but devoid of critical comment or comparison. For example, there is no discussion of the significance of the results on the anisotropy of chemical shifts, and, although this article places a major emphasis on structural information, the influence of molecular vibration and the comparison between molecular geometry determined by this and by other techniques receive only limited discussion. The important effects of vibrational anharmonicity are not discussed at all.

Symmetry plays a fundamental role in the analysis and