Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1981). A**37**, 270

Modern X-ray analysis on single crystals. By PETER LUGER. Pp. xiii + 312. Berlin, New York: Walter de Gruyter, 1980. Price DM 96.00.

For anyone starting on X-ray crystal structure determination, this book is a 'must'. It takes the reader through all the stages in the process, from selection of the crystal and the X-radiation to the final calculation of the molecular geometry and the representation of the structure in diagrammatical form. The essential theory is given at every stage but it never overwhelms the practical bias of the book. This excellent balance is largely achieved by the fact that three typical structure determinations – those of potassium hydrogen tartrate (KAMTRA), ammonium tetrasulphurpentanitride oxide (NITROS), and sucrose (SUCROS) – are followed in detail through all the various stages described in the book. KAMTRA belongs to the space group $P2_12_12_1$ and the solution of its structure by the Patterson heavy-atom method is described. NITROS belongs to the centrosymmetric space group $C2/m$ and SUCROS to the non-centrosymmetric $P2_1$ and their structure solutions by direct methods are explained, including the use of the *MULTAN* suite of computer programs. At every point, the techniques described are up-to-date and commonly used, so the reader is taught good standard crystallographic practice. With a few exceptions, the explanations of theory and descriptions of practical techniques are clear and they read very easily in spite of not being written in the author's native language. (He is Professor of Crystallography at the Freie Universität Berlin.) The author acknowledges the help of Professor G. A. Jeffrey in the linguistic revision of the English manuscript, and Professor Jeffrey should be congratulated on the general high standard of the text. A few infelicities in the English have escaped his attention but the meaning is always obvious. There are also a few typographical errors.

The first chapter of the book explains all the mathematics needed for crystallographic theory, particularly matrices and determinants and basis transformations, and then goes on to discuss Fourier series and transformations and diffraction theory in relation to the reciprocal lattice. Readers who, like the reviewer, are not mathematically inclined should not be put off by this rather difficult chapter and should skip when the going gets too hard. Mastery of the mathematics is only necessary for those who wish to understand the proof of every relationship. It is not necessary for the understanding of the rest of the book and for the application of crystallographic relationships in practice.

Chapter 2 explains the film methods of recording X-ray diffraction patterns and the interpretation of these patterns. It then goes on to discuss the generation and absorption of X-rays, with practical application in the selection of the most appropriate target material and filter, and of the voltage and current settings. Chapter 3 is concerned with all the various types of symmetry that may be associated with a crystal structure and with an X-ray diffraction pattern, the practical application here being, of course, the determination of space groups. It also includes a discussion of the Fourier-series representations of electron densities in crystals and of structure factors. Chapter 4 explains the operation of a four-circle diffractometer and includes discussions of the statistics of intensity counts and of the choice of crystal and scanning mode.

Chapter 5 is an excellent one on methods of solving the phase problem. It gives detailed and practical acounts of the Patterson and direct methods and even goes through, in detail, the beginning of a sign-determining process for a centrosymmetric crystal. Chapter 6 gives the theory of least-squares refinement of structural parameters and then outlines various practical considerations in applying the method. Finally, it discusses molecular-geometry calculations and the pictorial representation of crystal structures.

It is remarkable how much theory, practical application, and detailed example have been incorporated in the 312 pages of this excellent book. The price is rather high for anyone buying this as their first crystallographic book but it is not unreasonably high, since it will serve all the crystallographic needs of many of its readers. The printing and binding are also of a high quality. In fact, the only aspect of the book that can be seriously criticized is the title – X-ray analysis, these days, suggests the techniques of X-ray fluorescence spectroscopy and X-ray photoelectron spectroscopy, which this book is definitely not about. The book can be strongly recommended as a sound practical guide for the novice in crystal structure determination and as a handy compendium of theory and practical hints for those already familiar with the techniques.

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Acta Cryst. (1980). A**37**, 270–271

Lattice dynamics and statics of alkali halide crystals. By J. R. HARDY and A. M. KARO. Pp. IX + 314. New York: Plenum Press, 1979. Price US $32.50.

This theoretical book presents an extensive review of a variety of lattice dynamic models that have been used for the study of dynamical and static properties of alkali halide

crystals. The authors have given strong emphasis to predictions of many physical properties related to the phonon frequency spectrum, calculated by means of lattice-dynamical phenomenological models whose parameters can be determined from macroscopic data.

The book is written by two physicists engaged in theoretical research work on lattice dynamics of alkali halide crystals. Consequently, the data presented are largely the result of their long collaboration in this area.

The opening chapter offers a historical background of the subject permitting the reader to follow the development of ideas and to realize the contributions some individual scientists have made to the progress of this field.

The next two chapters are devoted to the general theory, introducing the normal coordinates and describing the macroscopic and microscopic theories of long-wave optical vibrations of cubic ionic lattices. In this part, the authors also give a detailed description and justification of various dipolar models, including a derivation of the dipolar coupling coefficients.

In chapter IV, a very interesting comparison of theoretical and experimental single-phonon data, such as Debye–Waller factor and specific heat, is presented. The remainder of the chapter is devoted to reviewing the technique of inelastic neutron scattering for determining the normal modes of a crystal lattice and to comparing the measured and calculated dispersion curves for almost all alkali halides. The side-band spectra of fundamental infrared absorption and the second-order Raman spectra of alkali halides are carefully discussed in chapter V.

Chapter VI deals with the static behaviour of alkali halides, specifically the manner in which these materials respond to the presence of point imperfections. The theory of impurity vibrations is used to calculate the various physical effects of impurity mismatch. The later part of the chapter discusses the use of techniques employed in the study of dynamical problems, suitably modified, to treat static problems that arise in connection with the study of lattice imperfections.

In conclusion, the authors have presented a very useful book which should be recommended to the research worker in lattice dynamics and statics of alkali halide crystals.

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Acta Cryst. (1981). A**37**, 271

N-dimensional crystallography. By R. L. E. SCHWARZENBERGER. Pp. iv + 139. London: Pitman, 1980. Price £6.50.

After introductory chapters (I: *Symmetry in the plane*, II: *Groups of affine transformations*) the central theme of this book appears in III: *Space groups*. Their *Determination* (VI) is preceded by IV: *Point groups*, and V: *Lattices*. The last chapter is VII: *Deformations*.

Both the title and the flap text seem to suggest that, apart from mathematicians, crystallographers will be interested by this book. Indeed the chapter titles could well be those of an introduction for them – but the reader will soon discover that this a research note in mathematics, period. Even the explanatory appendices turn out to be addressed to old-fashioned mathematicians rather than crystallographers of whatever fashion. The appealing first chapter, too, does little more than express what we all know in terms of formal algebra; at least that is how the author's 'geometrical approach' will be judged by most members of our picture-prone profession (actually there are some well-meant attempts at illustration). When even just a hint of true modern algebra enters in chapter II one feels one should either stop or get hold of the relevant books (which unfortunately are not specified) and take some weeks' leave. The reviewer has done neither, and has continued browsing. Though the meaning of many words and symbols has to be derived from the context, more of the book is readable than appears at first sight, and certainly more than in most of the existing literature of this level.

The strategy for deriving n-dimensional space groups is well explained. Since most of the text deals explicitly with the cases $n = 2$ and 3, either fully or in examples, there is much to be recognized and, sometimes, reappraised. Often one has the sensation of reading a foreigner's account of a journey through one's home country. This fellow notices features overlooked by most of the inhabitants: in the present case, the all-important rôle of arithmetic classes and of colour groups is perhaps foremost among them. Topological and other mappings of Bravais types, lattices, orthogonal groups and even space groups onto certain other sets are sometimes very difficult, but so fascinating that one makes a try anyhow to grasp the essence. This is also true for what appears to be the author's most personal contribution: derivation of orthogonal spacegroups by using their equivalence to graphs. On the negative side there are a deplorable number of printing errors, both misprints and mere vacancies, some of them quite nasty for the uninitiated. Mathematical rigour, too, is lacking surprisingly often. On p. 4 the shift vector (differing from ours in an interesting way) is said to be 'non-zero' in a case (*e.g.* m in cm) where it can actually be chosen zero. Except for $\bar{3}m$, all holohedral groups are assumed on p. 60 to contain m's normal to all rotation axes and the assumption is never dropped ($m3m$!). Orthogonal point groups are defined so as to include 222 but that group is forgotten in the list (p. 55) and in counting them. So the autochthones can feel satisfied: the foreign traveller himself is not perfect either. They should be grateful, however, for the publicity given to their beloved country, as well as for the impulse to look at their problems in this unusual, often very revealing light.

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