

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). A37, 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 tetrasulphurpenta-nitride 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 practice, 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 accounts 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.

S. C. WALLWORK

*Department of Chemistry
University of Nottingham
Nottingham NG7 2RD
England*

Acta Cryst. (1980). A37, 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