

Das erste Kapitel (50 S.) 'Symmetry and the solid state' bringt nach einer kurzen historischen Einführung Definitionen und Sätze der Gruppen- und Darstellungstheorie über Punktgruppen und Raumgruppen. Kapitel 2 (30 S.) 'Symmetry-adapted functions for the point groups' beschäftigt sich mit den irreduziblen Darstellungen und den angepassten Kugelfunktionen der Punktgruppen. In Kapitel 3 (90 S.) findet man Angaben über Raumgruppen, Bravais-Gitter, reziprokes Gitter, irreduzible Darstellungen der Translationsgruppen sowie Symmetrie-Operationen und Darstellungen der Raumgruppen. Kapitel 4 (55 S.) ist den Beziehungen der Darstellungen einer Gruppe und denen ihrer Normalteiler gewidmet (und geht erheblich über die Grenzen kristallographischer oder kristallphysikalischer Probleme hinaus). Kapitel 5 (193 S.) enthält die Tabellen der eindeutigen Darstellungen der Raumgruppen, Kapitel 6 (151 S.) diejenigen der zweideutigen Darstellungen der Punkt- und Raumgruppen. Kapitel 7 (113 S.) schliesslich beschäftigt sich mit den Schwarz-Weiss-Gruppen und ihren Darstellungen. Ein kurzer Anhang und 52 S. Literaturverzeichnis sowie ein ausführliches Register beschliessen den Band.

Die im Titel angekündigte systematische Theorie der Symmetrie der Festkörper findet sich in dem Band leider nicht. Es handelt sich eher um eine Beschreibung der Symmetrie durch Matrixgruppen als um eine geschlossene Theorie. Zwar finden sich viele einzelne Angaben zu dem Thema, doch ist die Darstellung wenig zusammenhängend und nicht genügend durchgearbeitet. Der Hauptwert liegt in den Teilen, die zur Darstellungstheorie Beziehung haben und in den umfangreichen Tabellen. Hier führen theoretischer Teil und Beispiele zum Verständnis und zur Anwendung. Wertvoll ist ferner das umfassende Literaturverzeichnis, das zu den Quellen führt. Ein ausgezeichnetes Register erleichtert das Zurechtfinden.

HANS WONDRATSCHEK

*Institut für Kristallographie
der Universität
Kaiserstrasse 12
D-75 Karlsruhe
Deutschland (BRD)*

The structures of non-molecular solids. By GRAHAM M. CLARK. Pp.v + 365, 193 Figs., 55 Tables. London: Applied Science, 1972. Price £9.00.

To anyone interested in structures, any book which attempts to classify and relate the vast number now known in the solid state is of considerable importance, and this one is no exception. The emphasis in this book, which virtually excludes the simple packing of molecules, is on structural descriptions based on the linking of polyhedra, where classification depends solely on the geometry of the structure and not, for example, on the type of chemical bonding.

The first part of the book deals briefly with fundamental principles relating to structure, such as the closest packing of spheres, the prediction of shapes of complex ions by valence-shell electron-pair repulsion theory, crystal-field theory, the linking of polyhedra, and defects in the solid state. No attempt is made to deal with structure determination; the only direct reference to classical crystallography is a two-page treatment of crystal symmetry.

The larger part of the book then classifies and describes structures on the basis of the linking of polyhedra involved.

Each chapter deals with a particular type of linking, for example with structures containing polyhedra sharing only edges, or those sharing vertices and edges; within a chapter classification is on the basis of tetrahedra, octahedra and other polyhedra, and then on the number of linkages involved. The final chapter considers crystal energetics, with a useful discussion of the influence of lattice energy compared with that of radius ratio on the structures adopted by the alkali metal halides.

There is a list of references at the end of each chapter, a general bibliography and separate formula and subject indexes. The book has numerous diagrams, some of which would benefit in clarity from shading, to increase the three-dimensional impression; a particular example is the structure of Mo_8O_{23} , which is almost incomprehensible to anyone unfamiliar with this type of representation.

The linked polyhedra approach leads to some fascinating insights into structures not previously described in this way. However, the almost exclusive use of this treatment, although sometimes accompanied by a close packing of spheres description, does lead to some peculiarities. Thus a description of sodium chloride in terms of octahedra linked through edges and vertices, although precise, appears rather artificial and not as useful as the more often encountered 'ball and stick' picture.

Despite some factual errors the book is recommended reading for those interested in the classification of inorganic structures, although, in the reviewer's opinion, it by no means provides a definitive answer to the problem of such classification.

A. J. EDWARDS

*Department of Chemistry
The University of Birmingham
P.O. Box 363
Birmingham B15 2TT
England*

Thermodynamics of crystals. By DUANE C. WALLACE. Pp.xviii + 484. New York: John Wiley, 1972. Price £8.85.

As the title suggests, this book should prove useful to anyone interested in understanding and/or calculating the thermodynamic properties of crystals from atomistic lattice models. The first four chapters outline the basic theory necessary to calculate the equilibrium thermodynamic properties of a perfect crystal from the interatomic potential function in the absence of externally applied electric or magnetic fields. Although, as the author admits, this is a 'well-worn trail' much traveled since Born & Huang's (1957) classic, the literature is full of niggling points left unresolved in Born's work. One example is the correct formulation of the thermodynamics of strained crystals; while Born & Huang state that the method of long waves is applicable only to zero-pressure crystal configurations, it has since been shown that this method can also yield the elastic constants appropriate for the propagation of elastic waves in a pre-stressed crystal. Because the literature on this point is scattered, it is useful to have the basic theory presented in a way which resolves this difficulty as well as the associated problem of reconciling the methods of long waves and homogeneous static deformation. Similarly, it is useful to have recent anharmonic formulations, the re-normalized and self-consistent phonon theories, presented in concert with the basic theory.

In chapters five and six, the problem of formulating a physically motivated interatomic potential function is confronted. Although the author claims the book to be self-contained, these chapters are not a good place to learn the quantum theory of solids. For the investigator with a strong quantum background, who would like to have a go at the thermodynamic properties of crystals, these chapters develop the basic mechanics necessary to such an approach. In specific, elementary band theory, and the pseudopotential theory of metals are developed in the framework of the first four chapters, but little feeling is given for the nature of the approximations or the physics of the bonding.

The final two chapters and the appendices discuss the details of actual lattice-model calculations and the procedures for data-fitting. The concrete examples of these final chapters are a necessary complement to the rather formal development of the earlier chapters. The anharmonic analysis is of particular interest.

Anyone who has attempted lattice-model calculations of thermodynamic properties quickly realizes that, even if he understands the basic procedure, the practical matters of first lattice summation, and then proper selection and weighting of wave-vectors in the thermodynamic sums can be formidable obstacles. Realizing this, the author has devoted an appendix to the complete description of these procedures, detailed to the extent of a computer program to determine wave vector weighting factors for a number of Bravais lattices. Although this is an extremely useful chapter, a word of warning is in order; in attempting thermodynamic calculations on the face-centered cubic lattice, this reviewer found several errors in the Brillouin-zone boundary weighting factors given by the author on page 456. I have not checked the other lattices.

In summary, the strong point of this book is that it puts recent developments in the thermodynamics of strained crystals, anharmonicity, elementary band theory, and pseudopotential theory into a single, consistent framework. Its weakest point is that very little background and virtually no references to the vast literature on these topics are given. The author has picked a logical trail through this literature, but has given few hints to those who would like to gain additional insight from peripheral reading.

C. G. SAMMIS

*The Pennsylvania State University
College of Earth and Mineral Sciences
Department of Geosciences
201 Mineral Sciences
University Park
Pennsylvania 16802
U.S.A.*

X-ray crystallography. By G. H. W. MILBURN. Pp.217, 70 Figs., 13 Tables. London: Butterworths, 1972. Price £6.00.

The author states his intention that the book should provide the reader with the basic knowledge needed to solve crystal structures by X-ray diffraction methods. In particular it should be a textbook of interest to final-year science students or to first-year postgraduate crystallographers.

The subject is divided into four parts. The first chapter of Part 1 outlines in 25 pages, including long tables and figures, the basic concepts of the crystal lattice, Miller indices and symmetry, the reciprocal lattice and its relation to X-ray

diffraction and Fourier transform theory. The reviewer feels that no inexperienced reader can get a real understanding of the subject from just a list of statements without any proof. Some misleading statements must also be pointed out, as for instance: (i) the recombination of the scattered rays into an image corresponds to a Fourier transformation not only in the case of X-rays as stated on page 17; (ii) the definition of the structure factor as the 'resultant of j waves scattered in the direction of the reflection hkl by the j atoms in the unit cell', is, to say the least, confusing without a previous explanation of the real process of interaction between X-rays and crystals.

The second chapter of Part 1 and Part 2 deal with the practical aspects of structure determination. The choice and the setting up of the crystal, the use of oscillation and Weissenberg methods, the determination of the unit-cell parameters and symmetry are described in some detail. In Part 2 the measurement of intensities is treated with reference both to photographic and diffractometer techniques, with more emphasis on the latter. This section is nothing more than a list of recipes the reader should follow to get data and very little effort is made to give an explanation of the physical facts beyond the experimental procedures. Four types of four-circle diffractometers are described in much the style of the commercial brochures which one can get free of charge from the manufacturers.

Part 3 deals with the treatment of the measured data and with methods of overcoming the phase problem. In the introduction the author emphasizes the need for 'a computer with large store' to carry out a crystal-structure analysis, but one feels very sorry for the British electronic industry seeing that a 1972 book quotes only the somewhat outdated KDF9 and Atlas computers. Formulae are given for the Lorentz-polarization and spot-shape corrections and reference is made to some of the methods for correcting for absorption and extinction (in the latter only old work by Zachariasen is quoted and not his recent developments). The very unusual order, where the Patterson synthesis, comes first, then the Fourier synthesis and finally structure factors, does not help the clarity very much. The use of the Patterson function in connexion with heavy atoms is described in detail and I think it is the clearest part in the book. The section on vector-search methods is very ambitious in the sense that in three and a half pages it tries to give an account of the work by Buerger, Tollin, Jacobson, Rossman & Blow, Hoppe *etc.* (even the double Patterson is mentioned) on the interpretation of the Patterson function. Fourier and least-squares techniques to complete and refine a structure are described with some practical examples. The chapter on direct methods illustrates, after a short historical and theoretical introduction, some of the procedures used for sign determination in centrosymmetric structures. An account is also given of the application of direct methods to non-centrosymmetric structures; I am afraid that the use, in this paragraph, of the quasi-normalized structure factors to derive phase relationships will cause confusion to the reader unaware of the statistical basis of direct methods. Several misprints, that a cursory examination of the proofs should have revealed, make this chapter difficult to read. An account of isomorphous replacement and anomalous-scattering methods concludes Part 3.

Part 4 is a description of some computer programs used in Crystallography. For each program the purpose and the kind of input-output data expected are illustrated.