

A format for a File of Inorganic Crystal Structure Data

The increased rate of publication of crystal structure determinations has led to a number of statistical surveys of structure and bonding, each of which has resulted in its author building up a large file of crystal structure data (usually atomic coordinates and cell constants). FICS-FORM is a format which allows such files and the programs which read them to be exchanged between workers as well as providing a method of file management.

A tentative version of FICS-FORM (FICS-FORM-73) is now available. The definitive version should be ready about the time of The Tenth International Congress of Crystallography but files written in FICS-FORM-73 should be compatible with later versions. Ultimately, it may be possible to edit the various users' programs and files into a single file. In the meantime, the use of FICS-FORM will ensure that these programs and files can be exchanged privately.

Copies of FICS-FORM and further information may be obtained from Dr I. D. Brown, Institute for Materials

Research, McMaster University, Hamilton, Ontario, Canada L8S 4M1. Periodic news letters describing files and programs that are available as well as changes in the definition will be sent to those who ask to be placed on the mailing list.

Index of French laboratories producing mineral crystals

The Montpellier Documentation Centre has just issued a new index of French industrial and university laboratories which produce mineral crystals. This index supersedes the index prepared in 1967.

This index may be obtained by sending the sum of three francs (postage stamps) or four international reply coupons to Professor Vergnoux, Centre de Documentation sur les Synthèses Cristallines, Université des Sciences et Techniques du Languedoc, Place Eugène Bataillon, F-34060 Montpellier Cedex, France.

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.

Molecular structures and dimensions. Vol. A1. Interatomic distances 1960-1965. Edited by OLGA KENNARD, D. G. WATSON, F. H. ALLEN, N. W. ISAACS, W. D. S. MOTHERWELL, R. C. PETERSON AND W. G. TOWN. Pp. xix + 637. Utrecht: Oosthoek's. Price £24.50 (personal price £17.50)

This volume is of such obvious value to crystallographers and others interested in structural chemistry, and it has been prepared with such thoroughness, that it is difficult at first sight to venture any criticism. Nearly 1300 organic and metal-organic compounds, in 86 different classifications, have been listed, cross-referenced in terms of authors, chemical names and formulae. Where possible, each entry contains the name, formula, structural formula, stereo illustrations, publication references, bond lengths, bond angles and torsional angles. The structural details have been recalculated and compared with published values, and in many cases errors in published values have been cited.

Looking ahead to the publication of future editions of this series, one wonders whether it will be possible to devote as much space to each compound, in view of the increasing publication rate. Structural organic chemists will still require a complete list of bond distances, bond angles and torsion angles, but a reduction of type size would be tolerable, and would effect a substantial saving in space. One hesitates to recommend the elimination of the stereo illustrations with their obvious usefulness, but perhaps they could be dispensed with for simple structures and for those where steric features are obvious or of little importance. With the present style of presentation, one feels a little cheated by the omission of such things as water molecules, heavy ions and intermolecular hydrogen bonds. In many instances, these features represent the main purpose of the

investigation. With the current tendency to present stereo illustrations in original publications, such features would be quickly ascertainable, and could perhaps be included in cases where they were judged to be of sufficient importance. Finally, a cross-index according to space group would be of value to many users, and would add little to the preparation time or volume size.

In conclusion, those responsible for the planning and compilation of the volume are to be commended for its general excellence and clarity. The criticisms and suggestions above are relatively minor, in the category of suggestions requested in the preface. Features deserving of praise are so numerous as to be impossible to list, but one in particular should be mentioned. In the few cases where a check was made, the elimination of redundant publications was found to have been thoroughly carried out. Such a policy will be of even greater importance in future volumes.

J. McCONNELL

*Department of Physics
University of York
Heslington
York YO1 5DD
England*

Crystal structures - a working approach. By HELEN D. MEGAW. Pp. xviii + 563. Figs. 208, Tables 42. London: Saunders, 1973. Price £8.30

The results of a crystal structure analysis can be summarized in a set of data (space group, lattice parameters, atomic coordinates, *etc.*) which usually constitute an essential part

of an original paper. The data are given together with a discussion of the methods used, of the reliability of the results and with a description of the structure as seen from the point of view of the author in its relation to the particular chemical, physical or purely crystallographic problem which led to the research. But it is possible to obtain a variety of views of a crystal structure, starting from the same fundamental data. To do this it is necessary to know how to interpret the conventional symbols and to be trained in dealing with crystal geometry. That is what the author of the book wants to teach and that is what the subtitle 'a working approach' means. Indeed the purpose of the book is to show how crystal structures ought to be looked at in order to obtain from them the particular information in which one is interested. The importance of this is self-evident since a knowledge of crystal structure is fundamental in interpreting many aspects of modern solid state physics and chemistry.

The plan of the book is developed for that purpose. The first three chapters are introductory in character and deal with general concepts of crystal-structure building, interatomic forces in crystals and the lattice nature of crystals. In the third chapter a number of simple fundamental structures are examined applying the concepts previously introduced. Theoretical aspects of geometrical crystallography are more deeply considered in the following six chapters in which the main aspects of lattice geometry and crystal symmetries are treated. In the successive three chapters

all these concepts are systematically applied to the description of the most relevant and representative types of crystal structures, *i.e.* oxides, 'families of structures', hydrogen-containing compounds. In the last two chapters thermal effects and phase transitions are treated mainly from the geometrical and lattice-dynamical point of view.

At the ends of the chapters are summaries emphasizing the main points and there are well chosen exercises which can be used to test how well the concepts have been learned. The references given at the end of the book allow the reader to extend his knowledge about many topics and to become acquainted with original works.

The book is particularly well written, clear, logically developed and provides stimulating reading. All the subjects have been treated exhaustively and rigorously within the imposed framework. The reviewer was particularly pleased to note how well the author has succeeded in putting over her experience as an outstanding researcher in the field. The book, which is recommended to all who are directly or indirectly interested in crystals, will certainly contribute to the spread among non-crystallographers of a better knowledge of modern crystallography.

M. NARDELLI

*Istituto di Chimica Generale ed Inorganica
Università degli Studi di Parma
Via M. D'Azeglio 85
43100 Parma
Italy*