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Book Reviews


This book contains the proceedings of the International Summer School on Crystallographic Computing, which was held in Prague, Czechoslovakia, 28 July–5 August 1975. It covers three main topics: (A) structure solving methods; (B) computational aspects of protein crystallography; (C) miscellaneous crystallographic computer applications and techniques.

*Acta Crystallographica: Change in Editorship*
Professor A. J. C. Wilson will resign as Editor of *Acta Crystallographica* and Chairman of the Commission on Journals on 31 December 1977 and will be succeeded by Dr S. C. Abrahams, Bell Laboratories, Murray Hill, New Jersey 07974, USA. Professor J. Wyart and Professor H. Lipson will also resign on 31 December 1977 as Co-editors of the journal. A more detailed report of these changes will be published in the January 1978 issue of Section A of *Acta Crystallographica*.

Offprints of articles published in
*Acta Crystallographica*
As a result of changes in the printing of *Acta Crystallographica* and in order to keep production costs for offprints at a reasonable level it has been necessary to change the arrangements for printing offprints. Offprints will be printed exactly as the article appears in the journal. Extracts of the preceding or subsequent article will not be ‘blanked out’ nor will the pages of the article be rearranged for the printing of the offprint. Offprints of articles which do not commence at the top of a right-hand page in the journal will include the last part of the preceding article, whilst offprints of articles which do not finish at the bottom of a left-hand page in the journal will include the first part of the subsequent article. These changes took effect for offprints for *Acta Crystallographica*, Section B, from the September 1977 issue onwards and will also apply to Section A commencing with the January 1978 issue.

It is hoped that the termination of the expensive practice of rearranging the printed articles for the production of offprints will make it possible to continue the provision of free offprints, and that authors will understand the necessity of introducing this new format for the offprints.
Of the more recent developments in direct methods this book contains a remarkable contribution by Main, who introduced into MULTAN, as a systematization of older theories, a procedure that makes use of molecular structure. Apart from this there are some preliminaries on entirely new methods that we may expect in the near future: magic integers (Woolfson), matrix methods (Main) and a heuristic theory on the concept of neighborhoods (Hauptman).

A number of papers in both sections A and B cover the subject of partial structure, phase refinement and phase extension in proteins. Sayre's method (Sayre), the maximal-determinant method (Tsoucaris) and the methods that modify the electron density (Gassmann, Simonov, Collins et al.) all seem to show a capability of improving the resolution of protein electron-density maps, starting from about 2.5 Å resolution.

Section B contains papers on protein crystallography which are also very informative to the general crystallographer: data collection (Bassi), the handling of protein data (Dodson), isomorphous replacement (Dodson, Kartha, Ashida) and anomalous scattering (Srinivasan). The increasing importance of Patterson search procedures, especially for the larger protein structures and viruses, is reflected in papers by Tollin, Blow, Bricogne, Colman et al. (see also, for ordinary structures, a paper by Kutschabsky and Reck on the convolution-molecule method in section B). The use of molecular structure and of non-crystallographic symmetry, which have always been the basic ingredients of these methods (contrary to direct methods until recently), combined with data from isomorphous replacement, seems to be very effective in phase refinement and extension at lower resolution, especially in direct-space procedures.

Papers on coordinate refinement, with constraints, by least-squares or Fourier methods (Diamond, Steigemann et al.; Jensen, Freer et al.), on phase refinement at higher resolution by direct methods (mentioned above) and on model building (Diamond, Nagano) show the immense computational problems inherent in these methods, which have become highly important since more high-resolution data have become available.

Four major subjects can be distinguished in section C. The first is a study on electron diffraction of polycrystalline material by Imanov. Five papers give good insight into the problems and developments in the field of small-angle scattering. Special attention is given to collimation corrections (Schmidt, Walter), evaluation of scattered intensities from models of macromolecules (Soiber), and acquisition of neutron data (Klesse). Fedorov introduces large-angle scattering.

Studies on Fourier syntheses and least-squares refinements permanently hold the attention of the crystallographer. The papers on symmetry considerations (Larson), anomalous dispersion (Larson) and fast Fourier transforms will assist every programmer in getting optimum efficiency in his programs. Rollett gives remarkable conclusions on convergence in least-squares techniques.

In the last part of this chapter, developments in program design and data-handling techniques have been gathered. Owing to the rapid developments in computer design during the last decade large program systems and data systems have been set up, and are at the disposal of the modern crystallographer. A great variety of information on program design for large computers is given by Sukarai, Hall, Stewart, Sasvari, Ahmed and Morimoto. Trends in minicomputer techniques are discussed by Sparks and Gabe, and the Cambridge data base by Motherwell.

The reviewer is pleased to recommend this book to crystallographers with interest in direct methods and protein crystallography. The subjects contained in the third part are of general interest to most crystallographers. As a continuation of the proceedings of foregoing Summer Schools it is a valuable book; it provides very useful information on principles and developments in crystallographic computing.

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The title could have been '60 Years of Low Temperature X-ray Crystallography'. It may seem surprising that, although the first low-temperature measurements were made in 1917, the technique is still not regarded as standard in all laboratories. Some people, who have had their fingers frozen in the first attempt and have not tried again, may be encouraged to do so by studying this book.

There is a contrast between the, literally, hundreds of devices for cooling specimens for diffraction measurements and the rather small number of models of single-crystal goniometers, cameras and diffractometers or powder cameras and diffractometers now in use. If the solutions to a problem are many and various it does not mean that the problem is easily solved!

This book is comprehensive from 1945 and gives selected references to earlier work. There is an introductory chapter on the applications showing why, despite the difficulties, crystallographers wish to make low-temperature measurements. There is then a 74 page section on the gas-stream method and 54 pages on all the other methods, this division reflecting the relative preponderance of the former method. The ingenuity displayed is tremendous, from the complete enclosure of the X-ray output and detector at one extreme, to the use of minute cryogens at the other. While the book is about equipment for X-ray diffraction there has been considerable spin-off from neutron diffraction where the normal excellent engineering facilities found in atomic energy establishments and the greater size of neutron diffractionists have enabled a whole new range of devices to be made and later adapted for X-ray work. In general the smaller the equipment and cold chamber, the more economical it will be. There are numerous diagrams, some in Imperial and some in metric units and copious references to the original literature. There is a section on sample preparation and on how to collect the intensities and apply corrections, for example for absorption. In the 34 pages of the appendices details are given of methods of measuring temperatures, behaviour of cryogens, safety aspects and names of equipment manufacturers.