Journal of
Synchrotron Radiation

ISSN 0909-0495

book reviews

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Structure Determination by X-ray Crystallography. By Mark Ladd and Rex Palmer. Pp. xlii + 819. New York: Kluwer Academic/Plenum, 4th ed., 2003. Price (paperback) GBP 41, ISBN 0-306-47454-9.

I was very surprised when I was asked by the Editors to write a book review of this Fourth Edition to find that there was no book review for the former editions in the IUCr journals, since 'Ladd & Palmer' is a very famous and fundamental book on the subject of crystal structure determination. Therefore, I accepted to write the review, although this edition was published about three years ago. Currently, intensity data are collected automatically within two or three hours using a diffractometer with a two-dimensional detector, and the crystal structure can be solved automatically using a convenient software package. The crystal and molecular structures will be drawn on the display of the personal computer. Moreover, all of the crystallographic data and the details of the structure determination are formatted in a crystallographic information file (CIF). It may be possible to submit a report of the crystal structure analysis without any knowledge of crystallography. However, the number of such ideal crystals whose structures are determined automatically is gradually decreasing. We must often analyze the structures of twinned crystals and crystals with disordered groups, solvate molecules or false symmetry. Deep knowledge of crystallography is necessary to overcome such difficult problems. This book is well adapted not only for the beginner but also for the researcher if they want to know the basis of crystallography.

In addition to basic crystallography, the following three chapters were added in this edition: X-ray Structure Determination with Powders (chapter 9); Proteins and Macromolecular X-ray Analysis (chapter 10); and Computer-Aided Crystallography (chapter 11). Recently the structure determination of organic and macromolecules using powder diffraction data has been extensively developed. In addition to an explanation of the methods of data collection, indexing and the assignment of the unit cell and space group, an outline of how to build the model structure is described. Not only the reciprocal-space method but also the several direct-space methods are explained in detail. Several examples analyzed by powder diffraction are shown.

There are many books on protein crystallography. However, I think it is adequate, as the authors suggest in chapter 10, that, although there are definite distinctions between large and small molecules in the crystallographic arena, there is no reason to exclude one from the other, and that there are many advantages of being familiar with both. The chapter includes the methods of crystallization, data collection and processing, phase determination using isomorphous replacement, molecular replacement and multiple-wavelength anomalous dispersion, and structure refinement such as density modification, simulated annealing and least-squares methods.

Computing is an essential feature in any modern crystallographic investigation. The basic computation programs for single-crystal and powder structure determinations are explained in chapter 11 using several examples. The programs and data are supplied on a CD which is attached inside the back cover of the book. The reader can easily analyze and display the structures operating the programs.

This is a remarkable text. A wide variety of crystallography can be surveyed with this book only. The exercises at the end of each chapter are very instructive for beginners in crystallography. The many references to the primary literature offer entry points for further study. However, it is regrettable to say that recent requirements for structure determination are missing. In order to submit the analyzed structure to the *Acta Crystallographica* IUCr journals, some requirements should be satisfied; for example, in the structure analyses of small molecules, the maximum diffraction angle, 'completeness' in data collection, the number of reflections more than ten times of the number of parameters, and the least-squares refinement on F^2. I think it is essential to explain the reason why such requirements were introduced in the journals. Information on CIFs is very important although no explanation is given in the book.

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