Book Reviews

Crystal Structure Analysis for Chemists and Biologists; Edited by J.P. Glusker, M. Lewis and M. Rossi. VCH: New York, 1994; xvii + 854 pp. DM 120.00. ISBN 0-89573-273-4

It is not an easy task to write a book on crystallography for chemists and biologists if the intention is to do this without too much reference to the underlying mathematics and physics. Why should one do that at all? The obvious reason, is that so many structures based on crystallographic methods are now produced both in chemistry and in biology that students and researchers in these fields, even if they do not have crystallography as their main subject, very often will have to read and understand original research papers dealing with structural information based on crystallography. Also for the researcher working with crystallography it is so much easier to communicate with his fellow chemist or biologist on important structural projects if some basic knowledge of fundamental concepts in crystallography is at hand. And frankly, knowledge of structure is so important that chemistry and biology would not be what it is today if structural information as the basis for understanding fundamental issues was not available.

However, it is not easy to write a book like this one. If the authors could rely on the fact that the reader would have as much insight into mathematics and physics as they have themselves then the task would be much easier, and in fact not necessary at all as many books have been written on this subject for specialists. J.P. Glusker has tried this challenge before in an earlier much shorter book, so she is experienced in conveying difficult concept in words rather than in formulae. This much larger book is very successful in solving the demanding task of informing students who will never again read crystallography as their main subject.

The first half of the book follows a rather traditional lay-out of chapters starting with descriptions of crystals, introducing diffraction and symmetry of crystals, giving the Fourier transform, explaining how to obtain data, pointing out the phase problem, describing how to obtain electron density maps and how to refine structural models. The other half contains chapters not normally found in expert textbooks and is devoted to how results are interpreted. It contains interesting chapters on conformation, atomic displacement, chirality, packing in crystals and how to use databases when comparing structures. The book ends with two very interesting and useful chapters on molecular recognition and structure/activity relationships. All chapters have at their end a summary extracting the main concepts of the subject of the chapter, a very useful glossary where many terms are explained in short (or sometimes long) paragraphs and very extensive references. Terms found in the glossary are very conveniently highlighted by boldface in the text.

The book has a very delightful introduction to crystal structure analysis. It is actually a full historical account of important developments of science based on structural results. The work of von Laue and Bragg was of course fundamental to modern crystallography. However, the determination of the structure of hexamethylbenzene by Kathleen Lonsdales so wonderfully demonstrated how structural results are able to stop endless theoretical discussions and focus them on some important new aspects. The Kekulé formulation (and many other more bizarre formulations) for benzene and the discussions on the valency of carbon had to be reformulated into the delocalized electron on the basis of Lonsdales results.

The underlying attitude of minimal use of mathematics goes well with some of the chapters in the first half of the book. Description of crystals can be understood by text and figures, although stereographic projections in themselves are not very easy to understand. Symmetry and chirality are nicely dealt with in large figures with representative molecules and left and right hands. Schoenflies notations are used along with the crystallographic Hermann Mauguin notations, probably to create a logical link to chemists trained in spectroscopy. Physical properties of crystals are described to an extent and to a depth not usually found in expert textbooks.

On the other hand chapters on diffraction by crystals and on Fourier series are not easy to write mainly referring to figures. In fact diffraction theory starting with light scattering from slits and masks are almost as difficult to grasp for (at least continental European) students, as their training in physics do not make them very familiar with diffraction patterns. The more formalistic way of introducing diffraction theory used by Lipson and Cochran in their 1966 textbook does rely on vector algebra, but can then on very few pages derive Bragg's equation, Laue conditions, the atomic scattering factor, the molecular transform and diffraction from crystals. Vector algebra is creeping into the text anyway in the chapter on Fourier series when summing waves by means of a vector diagram. It is also unavoidable in describing isomorphous replacement for phase determination. Vectors are also found in the second half of the book where calculation of a torsion angle has to use rather advanced vector algebra.

The chapter on estimation of relative phase angles gives very good introductions to all the presently used methods for solving the phase problem. Very appropriately direct methods are now dealt with first as this is the most widely used method in small molecule crystallography and also recently has been used successfully for small proteins. The classical Patterson methods are still in use not only for small molecules with one or a few heavy atoms, but also increasingly for proteins, where prior knowledge of the structure of parts of a molecule or a complex is used in molecular replacement. Isomorphous replacement is still the method of choice for experimental phase determination of protein or nucleic acid structures.

The chapter on electron density maps suffers from very little information on modern computer graphics programmes much in use in protein crystallography compared to the rather extensive description of the 'Richard's box' which is not in use anymore. Chapters on least-squares refinement are always chapters where mathematics is really unavoidable. And one has to introduce matrices. Restrained refinements and simulated annealing are such an integral part of many refinements today that they both deserved a few equations.

The chapter on conformation is very good and introduces most of the concepts that a chemist or biologist will ever want to know. It is especially good in the extensive explanation of amino acid and nucleic acid conformations. It even describes folding units and folding patterns of proteins. The chapter on chirality and absolute structure starts with an excellent overview of all the different systems of notations of chiral molecules. Pro-chirality is also well described. The use of anomalous dispersion in determining absolute structures is described in some details. Somewhat disappointingly the modern use of multiwavelength anomalous dispersion is not mentioned with one word.

This book is very good and is highly recommended as a first introduction to crystal structure analysis. It will also serve nicely as a reference book for specialists not least because of its excellent glossaries and extensive references to the original literature.

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