

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication

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Correlations, transformations, and interactions in organic crystal chemistry. (IUCr Crystallographic Symposia No. 7.) Edited by D. W. JONES and A. KATRUSIAK. Pp. xiii + 325. Oxford: International Union of Crystallography/Oxford University Press, 1994. Price £50.00. ISBN 0 19 855826 0.

This book is the proceedings of the eighth in a series of relatively small crystallographic symposia sponsored by the Adam Mickiewicz University under the leadership of the late Professor Zygmunt Kałuski. It contains 20 papers divided into four sections. Despite a valiant attempt by one of the editors to introduce a unifying theme, the papers are a motley crew. Some are mini-reviews of methods, some describe research on specific compounds or types of compounds. They vary in level of sophistication, in length and typography. Few would be accepted in the refereed journals of the IUCr without major revision.

Part I contains three papers: powder diffraction by synchrotron X-rays and pulsed neutrons; a review, growing crystals *in situ*, useful tips; molecular motion in crystals, a popular essay.

Part II contains three papers: solid-state isomerization, a long paper with examples which introduces the concept of the *reaction cavity*; proton transfer reactions; transformations and motion in 1,3-cyclohexanediones.

Part III is concerned with structure correlations and structure-activity relationships. It contains three mini-reviews with examples and one relating to benzeneselenazoles.

Part IV is concerned with conformation, packing and bonding. Two papers are concerned with hydrogen bonding and salt bridges. The remainder report the results of specific studies: cytidinium and 2-deoxycytidinium salts; tartaric acid esters and amines; ribofuranosyl nucleotides and related

imidazoles; superflexible silahydrocarbons; 6-methyl uracil; some metal aldoxides and oxoaldoxides.

This is not a book to be read from cover to cover; rather it is a useful reference if one of the topics happens to be of interest to the reader. Most of the review papers have material that has appeared previously and the substance of the research papers will surely be published elsewhere. For this reviewer, it raises this question: Why burden our over-extended library budgets with one more book? The great advantage and principal purpose of these small meetings is to provide the opportunity to meet fellow crystallographers and have interesting and often productive conversations. The best science takes place outside the lecture halls. This is particularly true in this case where ten of the contributors were Russian crystallographers and 13 were from Poland – colleagues we don't see so often.

The last chapter 'Whither organic crystallography?' is the report of a panel discussion which seems to be concerned with whether organic X-ray crystallography will become extinct, as has Crystallometry. The importance of a knowledge of the atomic structure of matter as a start for understanding properties and function makes this unlikely. The present advances in automation have made it possible for organic chemists to do their own crystal structure analyses with only a small chance of embarrassment. At the same time, however, crystallographers can use the methods developed by spectroscopists to study problems peculiar to the crystalline state and by theoreticians to predict structure. What we lose on the roundabouts, we can gain on the swings.

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Crystal structure analysis for chemists and biologists.

Edited by JENNY P. GLUSKER, MITCHELL LEWIS and MIRIAM ROSSI. Pp. xviii + 854. New York: VCH Publishers, Inc., 1994. Price \$69.95. ISBN 0-89573-273-4.

There have been some landmark events in the history of the publication of books on crystal structure analysis, in which attention has been focused on molecular (or organic)

rather than inorganic structures. Each book, in many ways, represented the 'bible' for a whole generation of practitioners, still holds a place in their hearts, and, most likely, continues to influence their scientific thinking even though events and other books have overtaken it. At the risk of exhibiting my own prejudices, and exposing myself to considerable criticism, I would say that the first in this category was *Organic Crystals and Molecules*, which resulted from the Baker Lectures that J. M. Robertson delivered at Cornell in 1951. The standard during the late 50's and most of the 60's was Lipson & Cochran's *The Determination of Crystal Structures* (in three

editions), which was the third volume in a series entitled *The Crystalline State*. In 1968, the first edition of Stout & Jensen's *X-ray Structure Determination – A Practical Guide* became the well worn standard no legitimate crystallography laboratory could be without. Dunitz's (1979) book, *X-ray Analysis and the Structure of Organic Molecules*, also resulting from a Baker Lectureship, linked applications of crystallography, symmetry, databases and analytical techniques to chemical problems, much in the tradition of Robertson, his mentor, while adding considerably more mathematical rigor to the crystallographic aspects of the book and, of course, updating the coverage by 30 years. There have been many other excellent books along the way, but to this reviewer at least, these have been the trend setters. In addition to their overall high quality and the unquestioned status of the authors in the crystallographic community, much of their success lay in the fact that they managed to capture the mood and direction of organic chemical crystallography at the time of their publication.

Albeit with some minor reservations, given below, I would suggest that the book under review is an excellent candidate to become the 'bible' of the next generation of chemical and biological crystallographers. It contains a wealth of information, with sufficient detail to provide the essence of almost any aspect of 'chemical' or 'biological' crystallography that a current practitioner might encounter. For additional depth of coverage the reader is provided a very complete bibliography at the end of each chapter, including references to many of the classic papers on the subjects covered. For that purpose it is also helpful that the authors have chosen to follow the citation practice, more common in the biological than in the chemical sciences, of including the title in a reference.

The book contains 18 chapters. Those relating to crystal structure analysis have a style similar to that of Glusker & Trueblood's *Crystal Structure Analysis – A Primer*, but generally are considerably expanded and more rigorous here, in concert with the intentions of this book. There is a very readable historical introduction as part of chapter 1 (and also in chapter 2) and there is an excellent chapter 5 on physical properties of crystals. This and chapter 1 are somewhat reminiscent of the *Historical Atlas of Crystallography*, edited by Lima-de-Faria, to which Glusker contributed the chapter on the history of organic chemical crystallography. I must admit to a weakness for historical accounts of this sort; others might find the material somewhat irrelevant, but I believe that it demonstrates the continuity and dynamism in the subject of crystallography, which indeed has a long and proud tradition of drawing from a variety of disciplines in order to develop and progress. Given Glusker's Oxford background, it is not surprising that chapter 5 has some of the flavor of C. W. Bunn's wonderful, but unfortunately largely forgotten, book, *Chemical Crystallography*. What makes that book and this chapter so appealing are the examples relating physical properties to detailed structure – the types of relationships that are of interest to chemists and biologists. Almost all the 'traditional' chapters on crystals, diffraction and crystal structure solution and refinement contain considerable material on the macromolecular crystallographic aspects of the subject, thus delivering on the promise of the title. In addition, there are chapters on 'Interpreting x, y and z (Atomic Coordinates)' – which will save me quite a few hours explaining the subject to my colleagues and their students – 'Conformation', 'Atomic

and Molecular Displacements', 'Chirality and Absolute Structure' (with a very nice summary of the current terminology in the field), 'Packing in Crystals', 'Comparison of Structures', 'Recognition and Receptors' and 'Structure-Activity Results'. All of these will serve chemists and biologists equally well.

There were a number of details which I found particularly well executed. I mention just a few of them here to demonstrate some of the attractive features of the book. There are some very well thought out summary figures and tables: e.g. Fig. 4.14, p. 129 (packing and symmetry operations); Fig. 7.17, p. 254 (the orientation matrix); Fig. 8.10, p. 298 (procedures in direct methods); Table 8.3, p. 332 (phase determining methods). Other noteworthy stylistic features include the use of boldface in the text when introducing an important concept. The casual browser, or one looking for a refreshing explanation will find this a particular convenience. Following the laudable practice used in the Glusker and Trueblood primer, each chapter closes with a glossary of the boldfaced terms. The pedagogical compromise of having a glossary at the end of each chapter rather than at the end of the book is compensated for by having a 'Glossary Index'. An excellent addition, moreover, is a summary at the end of each chapter, giving its essence. In a number of cases the summary is accompanied by a useful table or chart, which also helps to put much of the material covered into proper context and perspective. All these features would make the book a good textbook, although it is both more and less than that. It is certainly more than a candidate for a textbook, because it contains considerably more material than can be covered in a one semester graduate course on crystallography, but it is less than that because there are no exercises or problems. However, a student introduced to the book, if it indeed is used as a text, will no doubt continue to make use of it long after the course is over.

In spite of my general enthusiasm for the book, there is some room for improvement. The publishers are to be commended for keeping the price within the range graduate students can afford. However, this may have been accomplished by compromising somewhat on the technical aspects of the production. The size of the book has been kept to 850 pages by the use of rather dense print, which some, students in particular, may find intimidating. While the content of the figures is generally excellent (e.g. Fig. 3.9 on 'Conditions of Diffraction'), the quality of a quite a few could be significantly improved. Fig. 5.6 on birefringence is brilliantly conceived – I can't recall seeing anything like it elsewhere – but it loses much of its impact because of the poor resolution and contrast of the photographs. Some other examples: in Fig. 2.16 many lines are not reproduced (at least in my copy); Figs. 5.2, 8.1, 8.3, 9.16 and 13.2 are somewhat crude in execution with what appear to be lines drawn freehand; and many of the photographs are poorly produced [e.g. Fig. 2.4, 7.15(b) and Fig. 8.24(a)]. In the last (halftone) one must know that the purple (*sic*) chrome alum crystal is inside the larger potash alum. In Fig. 3.13 the captions (or the figures) are reversed, and the caption to Fig. 13.7(f) mentions a numerical example which is not included.

I have a very high regard for Glusker's ability to write clear expository prose. However, there are a few rough spots which apparently evaded her sharp editorial eye (e.g. the second sentence on p. 296, the opening sentence of the penultimate paragraph on p. 318, and the opening sentence on p. 523). The caption to Fig. 8.3 is uncharacteristically opaque, and that

to Table 8.1 has a statement '*i.e.* certain classes of Bragg reflections that have an average intensity higher than the average' – presumably that should be completed with 'of all the reflections'.

However, in the end, these are but minor blemishes on what, overall, is a highly commendable work. It most likely will become the first book I recommend to my students, and I am

sure it will become very well worn with use in both my office and my laboratory.

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