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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Crystallographic computing 5: from chemistry to biology. (IUCr Crystallographic Symposia No. 5.)

Edited by D. MORAS, A. D. PODJARNY and J. C. THIERRY. Pp. xiv + 479. Oxford: International Union of Crystallography/Oxford University Press, 1991. Price £40.00. ISBN 0-19-855384-6.

This International School on Crystallographic Computing was held at the Bischenberg Congress Center, near Strasbourg, from 29 July to 5 August 1990. According to the preface, this was 'the twelfth such school organized since 1960 under the auspices of the IUCr Commission on Crystallographic Computing'. Like others in recent years, it was held as a satellite meeting to an IUCr Congress, this one the XVth in Bordeaux. Again, as for the others, the papers presented at the meeting are now published in book form: a proceedings of a sort. This one contains 35 papers and 20 abstracts of posters.

In earlier years, the 1960s for example, when the practice of crystallography on computers was developing, these meetings served to bring together the current expertise to reveal, discuss, evaluate and dispute improvements in procedures and optimum methods for computation. As the practice of crystallography on computers has matured (and grown almost to exclude other forms of practice) and as crystallographic practitioners have grown in number and diversified, the principal purpose of these meetings has come to be to train younger crystallographers in the current methods of crystallographic computation and to provide hands-on workshop experience under the tutelage of experts. In both respects, in fact, recent meetings continue an excellent record of service and achievement.

The publication of papers presented at a School of Crystallographic Computing is meant, it seems, to serve several purposes. One appears to be to serve simply as a repository of notes of lectures presented at the school. This is a lesser purpose, I believe. Another is as a reference work, documenting the latest in computational advances. Still another is as a forum for more detailed or more explanatory presentations of difficult subjects. Yet another might be as an organized discourse on a topic of current interest. These are all higher purposes in my view. At one time or another, publications of papers presented at these schools have served some or all of these roles simultaneously.

The emphasis of the Bischenberg meeting was almost exclusively on crystallographic applications to structure studies of macromolecules of biological interest and the book mirrors that emphasis. Not all of the topics of current interest were covered; however, those covered, and they were the majority, received careful attention. The sections of the book on data collection and analysis, with emphasis on synchrotron applications, and on refinement, with coverage of molecular-dynamics issues, are two examples. The section on solutions to the phase problem, particularly the subtopics on anomalous dispersion and maximum entropy, is another and especially strong example. With only a few exceptions, the written contributions are carefully crafted to offer the reader new insight, a deeper understanding or a broader appreciation of the import of the subject. Several individual contributions are especially noteworthy in a field of papers of very high quality: those of Hajdu and co-workers on Laue applications, of Roth on phasing at low resolution and of Bricogne on maximum entropy. I recommend the book as a solid contribution to the crystallographic literature and as of special interest to macromolecular crystallographers. I also compliment the organizers and editors for the work they did to make both the school and the book successful.

The strength of this book comes from the contributions that make it more than a compendium of lecture notes, although not all the contributions do so. This is an expensive book and it can appear disappointing at first glance if one of the lesser contributions is encountered. I strongly urge the reader to take a second look in this case. But I wonder if it is worthwhile continuing to include contributions whose only purpose seems to be to provide a superficial outline of a subject. This does not seem fair to the majority of the authors who have worked hard to provide value to the readers, or to the readers, the majority of whom must seek more than sketchy outlines of lectures they did not attend. The Thirteenth School on Crystallographic Computing is planned for 1994. Perhaps it is time for the IUCr Book Series Committee to conspire with the organizers of the School and the editors of *Crystallographic Computing* 6 to end the automatic publication of lecture notes and to eliminate papers or topics that do not provide value. This would allow the editors to concentrate contributions in one or two areas so as to maximize the impact in terms of depth of coverage, insight, discourse and, if you please, synergy.

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Kristallphysik und Symmetrie.

By I. S. ZHELUDEV. Pp. 224. Berlin: Akademie Verlag, 1990. Price £10.00. ISBN 3-05-500688-7.

This book is a German translation of a Russian text originally published in 1987. It provides an interpretation of some of the phenomena of crystal physics in terms of symmetry.

The opening chapters give a very full account of symmetry groups, including those not normally discussed in textbooks on the subject. Thus, for example, the sphere with mirror planes is discussed separately from that in which those elements have been removed, and the rotating cylinder and cone are similarly distinguished from their stationary counterparts.

There follows a treatment of scalars, vectors and tensors that concentrates particularly on their relationships with the point groups.

A chapter on the symmetry of space and time includes a brief account of the symmetry theory of elementary particles as well as a discussion of the relative motions of galaxies in terms of space-like and time-like intervals. These highly theoretical topics of modern physics may seem out of place in a book bearing such a title as this one, but they serve to underline the thesis that all phenomena determined by conditions of symmetry are dependent on invariance with respect to the inversion of time. The stability of elementary particles is further discussed in an Appendix.

The book goes on to consider phase transitions in crystals. The symmetry relations that determine these are discussed in detail, as are the phenomena of pyroelectricity and piezoelectricity. Finally, some aspects of the optical properties of crystals form the subject of a separate section.

Throughout the book, the treatment is very theoretical and relies greatly upon fundamental considerations. The point is made strongly that natural phenomena can occur only if symmetry relationships permit them, but that not all changes so allowed will necessarily happen in practice. The exposition is clear, and the book should be useful to those wishing to gain an insight into this fascinating subject.

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Quasicrystals, networks and molecules of fivefold symmetry. Edited by I. HARGITTAI. Pp. xiii + 314. New York, Weinheim, Cambridge: VCH Publishers, 1990. Price £55.00. ISBN 0-89573-723-X.

This expensive but attractive book is a collection of 19 short specialist essays, connected by the single theme of fivefold symmetry.

Fivefold symmetry will always have a certain fascination for crystallographers. It is the symmetry governing two of the five regular polyhedra of Plato and it is a symmetry extremely common in biology, yet it is the first 'forbidden' symmetry for crystals. Only in the past ten or so years has this situation rather suddenly changed, for we now know that fivefold symmetry *can* fill space, only not periodically.

This change began quietly enough around the 1950s, on the far periphery of crystallography, in the mathematics of tiling (two-dimensional space filling), and advanced most notably when Penrose's paper of 1974 on 'The role of aesthetics in mathematical research' (a discussion with no apparent relevance to crystals) produced the paradigm 'Penrose tiling'. All this was abstract mathematics, even when Mackay, in 1981, generalized this nonperiodic tiling into three dimensions. But when Schectman and his colleagues in the US Bureau of Standards published electron diffraction pictures of fivefold symmetry obtained from micrometre-size grains of an aluminium alloy, crystallographers had to take notice. That was in 1984. Since then, about a thousand research papers have followed 'directly from the stimulus of that discovery' (Mackay's comment).

Not everything has changed, of course. The great majority of solids remain periodic, but the incidence of fivefold symmetry in certain special cases, forming 'regular' if not periodic solids, able to give high-quality diffraction, is important. These solids are now properly called quasicrystals. Hence the title of this book. This development has enormously spurred theoretical work on the mathematics of lattices in general – for 5-, 7-, 9- and 12-fold symmetries, in N-dimensional spaces, and so on – during the past decade. It is clear that good-quality quasicrystals are not easy to produce. They require quite special shapes of the packing polyhedra, they come only from certain special alloys, they require long annealing to be more than micrometre sized and they come with compositions such as $Al_{63.5}Cu_{24}Fe_{12.5}$. These restrictions and isolated cases of apparent fivefold symmetry observed since the earliest days of crystallography have led some researchers, notably and most recently Pauling, to argue that they could be explained by specific types of twinning associated with an unusually large cubic unit cell. Pauling's explanation has been very carefully tested by Dunlap and his collaborators at Dalhousie University and their findings (reported in detail in Chapter 6 of this book) show that it is definitely inferior to analyses based on true quasicrystallinity. We may take it that quasicrystals are real; they are also exciting, especially to theorists.

For crystallographers who wish to get up to date with these developments, Professor Hargittai of Budapest has provided this album of specialist essays. Hargittai himself has contributed only the six-sentence Preface; but he has assembled no fewer than 37 distinguished authors (from 9 countries) who have supplied 19 separate articles to cover as much as possible of this exotic field.

The first 12 essays focus on quasiperiodicity: tilings of all sorts, with fivefold and other symmetries; whereas the next 6 are concerned with fivefold symmetry in isolated molecules, principally the new icosahedral molecule C_{60} (which is the subject of four essays on its history, energy levels and vibrational modes). The final chapter is a short essay on the fusion of five-membered carbon rings – essentially an essay in organic chemistry and somewhat removed in tone from the rest of the book.

Each one of these essays is quite brief. There is little unity among them other than that they are all involved with fivefold symmetry of one sort or another; their order in the book does follow their subject orientation. A great variety of tilings and elaborate theoretical discussion are much in evidence, both in the text and in the numerous diagrams. A highlight is the essay by E. J. W. Whittaker and his coauthor R. M. Whittaker on fivefold symmetry in higher-dimensional spaces, for which there are six colour plates showing, stereoscopically, stick models that are three-dimensional projections of various four-dimensional structures. The principal highlight for this reviewer is the chapter exhibiting real quasicrystal specimens. This is a 14 page article by Denoyer, Heger & Lambert, of Université de Paris-Sud and CEN-Saclay. It shows a visibly pentagonal dodecahedral quasicrystal of a few tenths of a millimetre in diameter and another of triacontahedral symmetry, glued to a glass fibre, plus superb pictures of precession-type X-ray diffraction by these same specimens.