

and EM images and, in addition to these, reproductions of the title pages of nearly 100 of the most important crystallographically related publications from the 16th century through to the 19th. There are bound to be minor criticisms of the selections that have been made. For example, there can be no good reason why Kathleen Lonsdale has been omitted from the portraits; and what of C. G. Darwin, Nishikawa or Zhdanov...? But it is idle to pursue this sort of thing.

It is beyond argument that this book is a mine of information. Its lack of unity in the manner of presentation is a real defect but by no means a damning one. The fact is that most of this book is absorbingly interesting to read. Crystallography is one of the most central of all the sciences. Crystals constitute a bridge between the atomic level and the macroscopic world. The slow development, over the past five centuries, of our understanding of what crystals are and what they tell us is a paradigm of the growth of modern science. Sadly, because of the burgeoning superfluity of facts, techniques and theories, we give little attention these days to the history of the development of our modern competence in science, even in our universities. However, wherever the historical dimension is dealt with, this book should be on hand for study and for reference. This book is not one we should expect to see on the shelves of the individual crystallographer but it is a 'must' wherever the history of science is taught, particularly the history of crystallography and it should certainly be available in every respectable library of general science.

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**Neutron and X-ray scattering – complementary techniques.** Edited by M. C. FAIRBANKS, A. N. NORTH and R. J. NEWPORT. (*Institute of Physics Conference Series No. 101.*) Pp. vii + 252. Adam Hilger, Bristol, 1990. Price £30.00. ISBN 0-85498-057-1.

In the worlds of neutron and X-ray scattering, lip-service is being increasingly paid to the concept of 'complementarity'. The advent of central facilities has further pointed up this concept, as storage rings such as the SRS at Daresbury produce bright X-ray beams and high-flux reactors such as the ILL at Grenoble and pulsed spallation sources such as ISIS at RAL increase the potential of neutron scattering studies.

What does complementarity mean, however, specifically with respect to the exploitation of X-rays and neutrons? I had, perhaps, naively, considered it in terms of more than one technique being applied to a single problem, the information obtained from each technique being 'complementary' in giving different but complementary information on a single system; the sum of the information gained would be greater than that obtained from either technique separately. An example might be small-angle scattering from a two-component system, where the different scattering lengths of the components with respect to X-rays and neutrons would result in different contrasts being observed

by the two techniques. This I would regard as true complementarity. Many of the chapters in this book, however, deal with what I would prefer to call comparability, a related, but not identical, idea. For a given problem, we consider the advantages and disadvantages of both neutron and X-ray methods: we then choose the technique that would suit us best.

Comparability is relatively well developed: at its most trivial, it boils down to choosing the best technique in a particular case, a procedure in which you might expect any reasonable experimentalist to be competent. Complementarity is, however, despite the lip-service paid to it over many years, exploited relatively rarely. It was therefore highly appropriate, with ISIS following a full experimental programme (within its limited available funding) and the high-brightness lattice at the SRS fully operational, for a meeting to be held in Britain in early 1989, at the University of Kent. Its intention was to place '... emphasis ... on the complementary information available by using both techniques to gain a more complete understanding of the system under investigation'. Clearly complementarity, not comparability. This volume is a record of the proceedings.

The result is successful, but disappointing. There are good reviews of the well recognized and well explored complementary areas involving large-scale structures (small-angle scattering and the much newer but powerful techniques of neutron and X-ray reflection). The battery of X-ray and (inelastic and elastic) neutron techniques available to throw light on proton conductors are described in a chapter from Jones and Roziere in Montpellier. The use of X-ray and neutron techniques in ion and water location in fibres is discussed by Watson Fuller's Keele group and the joint potential of the very new technique of deep inelastic neutron scattering and X-ray Compton scattering is explored. However, many of the chapters really exemplify comparability rather than complementarity, with several papers describing studies using either an X-ray or a neutron technique almost exclusively, although sometimes results from the other technique are included for comparison.

A potentially promising area of complementarity of particular personal interest is liquid structure studies, where much lip-service has been paid to the potential value of both X-ray and neutron techniques arising from the different scattering lengths for the two probes. Here, there is a thoughtful and imaginative chapter from Delft which describes the use of both X-rays and neutrons in a careful and truly complementary study to extract the Si-Si partial pair-correlation function from vitreous silica, together with a good essay from Steve Gurman (and pipe) on conditioning for isotope substitution, neutron scattering and anomalous dispersion X-ray scattering. The controversially named reverse Monte-Carlo technique – a method which is increasingly seen as very powerful in interpreting liquid diffraction and crystal disorder data – is put forward clearly as one which is ideally suited to constructing models consistent with both neutron and X-ray results on the same system and hence one which will be increasingly used in complementary work. Perhaps it is a reflection of the attendance that there is nothing on *X-N* methods that have been used successfully for many years by crystallographers, both in joint structure refinement and electron density studies – an unfortunate omission.

The book contains some good papers exploring the potential and problems of exploiting complementarity and

I am pleased to have a copy, but the inclusion of many 'comparability' papers detracts. Their inclusion perhaps shows we have a long way to go in exploring – let alone usefully exploiting – the full potential of X-ray/neutron complementarity. Tighter selection would have resulted in a slimmer volume, but one which would have been focused more on the central issues of complementarity. Space would then have been available for a useful editorial review to summarize the current state and encourage possible fruitful ways forward.

It is the reviewer's privilege to make a couple of minor gripes and I am no exception in asserting this right. Firstly, it would have helped finding my way through the book if each page had carried the running title of the appropriate chapter rather than that of the book. Secondly, I was just a little surprised to find some of my own unpublished results in print without my being asked. Perhaps if the results had been ready for publication, I wouldn't have minded so much . . . .

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**X-ray structure determination, a practical guide.** By GEORGE H. STOUT and LYLE H. JENSEN. Pp. xv + 453. John Wiley and Sons, New York, 1989. Price US \$44.00. ISBN 0-4716-0711-8.

The first edition of this book, published in 1968, was intended to enable the average chemist to perform crystal structure analyses for himself. Automatic data collection and structure-determination packages have made the experimental and computational aspects a great deal quicker and more routine than they were in 1968, and it is tempting for the chemist/crystallographer to use them without much understanding of the processes or critical judgement. The authors would deplore such an approach and have provided a new edition of their book as a countermeasure. It covers a large amount of appropriate fundamental material, X-rays, diffraction, unit cells and space groups and their determination, intensity measurements, structure factors and Fourier series, followed by structure solution and refinement. Every stage is carefully and thoroughly explained, with illustrative examples and many diagrams as well as a lot of practical detail and advice on strategy. For the chemist who is prepared to read the book purposefully or for anyone else doing single-crystal structure determination, there is enough information to carry out and understand every stage of a structure determination. Sometimes the detail is a little excessive: for example, a cell constant is derived from an oscillation film using an angle in radians and a second time using the angle in degrees; in the instructions for loading an oscillation camera it is suggested that, for practice, a first trial should use a dummy piece of film! In contrast, instructions for radiation safety, though some are given, are not adequate, at least by modern European standards. The presentation is one which will appeal to many chemists; equations are accompanied by

an extensive explanation in words, rather than the more formal, elegant approach that is characteristic of a physicist's treatment.

The structure of the book is very similar to the earlier edition. The most notable exception is in the section on methods of solution of the phase problem; direct methods have, very properly, been given the first and most important position and their treatment expanded a little. A great deal of the earlier edition remains. In part this is a reminder that the fundamentals were all familiar 20 years ago – much of what has changed is in the implementation and the automation of the computations. In most chapters where it is relevant, new material has been added, rather concisely presented, together with useful references. The examples are mostly those of the earlier edition; they often provide good illustrations, but are probably not ones that would now be chosen on writing a new text book.

There are other more serious criticisms. It is not clear what kind of structures the book is meant to be most relevant to: the treatment is very good for small and medium-sized organic molecules; it is also appropriate for organometallics, but could be more helpful on problems associated with the presence of a few very heavy atoms (refinement strategies, residual peaks due to absorption errors *etc*). It discusses multiple isomorphous replacement, least-squares refinement with energy minimization, low-resolution refinement, all of which will normally only be relevant in protein studies, but it is not remotely adequate as a practical guide for protein crystallography. The treatment of anomalous dispersion is essentially unchanged since 1968; it is more relevant to proteins than to other types of structure (since it assumes that structure amplitudes will normally be available for crystals with and without the anomalous scatterer present), but it is not presented in the form commonly used in protein crystallography. (Also there are discrepancies between terms used in the text,  $F_H$ ,  $\Delta F'$ , and in the figures,  $f_H$ ,  $\Delta f'$ , on, for example p. 302.) Oscillation, precession and Weissenberg photographs are described in detail, including both their fundamental geometry and practical use; diffractometers get much briefer treatment and some of the description is in terms of Weissenberg geometry, not the most helpful approach for today's chemists who may well meet a diffractometer before a Weissenberg camera. Also, it would be much more helpful if, on pp. 101–102, in relation to the orientation of crystals, all the diagrams had the goniometer head and spindle in the same orientation. In other parts too, the balance of material reflects the 1960s rather than the 1990s; for example, considerable space is devoted to refinement by differential Fourier series, which, to my knowledge, is not in current use. Misprints are few, but the quality of paper and print is poorer than in 1968.

Despite these criticisms, the book does contain an immense amount of information, practical guidance and wisdom and is extremely readable. A copy of it should be available wherever a diffractometer system is generating structural data for chemists and it should help this process to be done with more understanding and judgement.

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