# Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.*

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**International tables for crystallography: Brief teaching edition of Volume A: Space group symmetry.** Edited by T. HAHN. Pp. viii + 119. Dordrecht: Reidel, 1985. Price Dfl27.50, US $8.50, £7.60.

This is a slim volume consisting of 24 selected space-group descriptions and several pages of the basic text sections from Volume A of *International tables for crystallography*. The declared purpose of the *Teaching edition* is:

(i) to provide a handy and inexpensive tool for researchers and students to become familiar with the use of the space-group tables in Volume A;

(ii) to be used in classroom teaching;

(iii) to serve as a laboratory handbook, because the 24 examples include most of the frequently occurring space groups, for both organic and inorganic crystals.

The basic text section consists of material found in chapters 1, 2, 3 and 5 of Volume A: namely *Symbols and terms used, Guide to the use of the space-group tables, Space-group determination and diffraction symbols*, and *Transformations in crystallography*.

I approve strongly of the idea of bringing out an introductory book on the excellent, but detailed, Volume A, as there is a serious need for material which can be read and understood by beginners and non-specialists. I was therefore delighted to hear that the International Union of Crystallography had, at last, brought out such a text. However, I am sorry to say that, when I opened my review copy, I felt somewhat surprised and, even, disappointed. The title had suggested a digestible and specially written account, which could be recommended to someone meeting, for the first time, the beauty and mysteries of crystallographic symmetry. Instead of the elementary treatment I had anticipated, it seems that the basic text has been lifted entirely without change from Volume A.

As a result, I certainly could not expect a novice to take the text away and learn from it by him/herself. Indeed, because no attempt has been made to adapt the text to suit its declared aims, on almost every page peculiar inconsistencies can be found which ensure that it cannot stand alone as a teaching text. It is particularly irritating to encounter so many references to sections that are missing entirely. As typical examples, in the *Guide to the use of the space-group tables*, page 10, the reader is referred to sections 8.3.1 and 9.1 for further details on lattice centring and to section 9.3 for reduced bases. On page 30 the index of a maximal subgroup requires the footnote in section 8.1.5 to be consulted. Again, picking a page at random, I find on page 39 reference to a missing Table 4.3.1, and so on. This occurs so frequently throughout that one might as well use Volume A in the first place.

The main problem with the *Teaching edition* is that it falls between two stools. On the one hand, it is too difficult to act simply as a text for learning about the space-group tables and, on the other, it is not complete enough for the experienced researcher to use as a handbook. In any case, those who already know about space groups and the *International tables* are unlikely to want to consult the introductory texts in this book. I believe that it would have been better either to have rewritten the introductory text to suit the level of reader expected or to have published just the space-group pages, together with the useful key on the inside covers (incidentally, the book could then have been even less expensive!). I wish I could be more positive about the *Teaching edition* but, frankly, I am not sure to whom it can be recommended.

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**The structure of surfaces.** Edited by M. A. VAN HOVE and S. Y. TONG. Pp. xii + 435. **Springer series in surface sciences 2.** Berlin: Springer, 1984. Price DM 138.00, £36.00.

This book is the result of a 1984 conference held in California with the grand title of First International Conference on the Structure of Surfaces. This new series of conferences is planned to relate surface structures with the various physical and chemical properties of surfaces. I find this volume, which is effectively a selection of the conference proceedings, rather disappointing. Indeed, it is as though a direct correlation between properties and structure is being forced on the reader and has been allowed to dictate the layout which I found to be fragmented.

Structural determinations using low-energy electron diffraction (LEED) still form the backbone of the subject and we observe from many contributions that a consolidation stage has been reached with continued refinement of technique and experiment/theory comparison. Some of this refinement is a direct result of the availability of new evidence from some new techniques, such as scanning tunneling microscopy. Generally, new techniques such as this get rather sparse treatment and the reader is left to put them into context. Several contributions on the use of X-rays for surface structure analysis have been dispersed throughout the book rather than collected together, thus reflecting the editors' wish to place less emphasis on 'techniques' and more on the nature of the surface property.

The determination of local order and bonding arrangements in surface structures which do not necessarily display long-range order is clearly one of the biggest contemporary challenges. This is being pursued by variants of X-ray absorption fine structure techniques and by a detailed analysis of the diffuse background in LEED. Another

related active area is the determination of defects and atomic steps on surfaces, and all of these topics have received considerable attention in this volume.

Many of the contributions, there are sixty five in all, are excellent but often represent work already published, albeit in a slightly different form. Few of the contributions are really reviews but many fall into the category of being a statement of the current position. This volume, then, is for the serious surface scientist and it will have a fairly limited 'time of usefulness'.

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**Structure and statistics in crystallography.** Edited by A. J. C. WILSON. Pp. vii+225. New York: Adenine Press, 1985. Price US $65.00.

This book describes the proceedings of the symposium on Crystallographic Statistics held in Hamburg, West Germany in August 1984 in the course of the Thirteenth International Congress of the International Union of Crystallography. It also includes a few papers presented in the main Congress but which were considered as closely linked with the symposium topic.

The first and last contributions in the book stand out on their own, the first by J. Karle on the statistical basis underpinning direct methods and the last on 'expert systems' of data acquisition. The direct-methods contribution does not contain any new material but it is a splendid review of the theoretical developments which led to direct methods having their present pre-eminence and in which Karle and Hauptman played such a leading role. The 'expert systems' paper by H. J. Milledge and her collaborators presents the principles by which the data-acquisition process by a diffractometer may be optimized by analysing the data during collection.

The remainder, the bulk, of the book divides into two roughly equal parts - the first concerned with intensity statistics and the second with refinement processes. A most interesting paper by Weiss *et al.* deals with the representation of probability density functions by Fourier series, which is much better than previous methods using the central-limit theorem or based on the Edgeworth or Gram–Charlier series. There follow three papers dealing respectively with the effects of heavy atoms, non-crystallographic centres of symmetry and non-crystallographic translational symmetry on the normal or cumulative intensity or $|E|$ distributions. Since many crystal structures contain heavy atoms or a great deal of symmetry to do with the chemistry of molecules rather than the requirements of space groups, it is clear that departures from idealized random distributions of almost-equal atoms must be common. The papers presented here show much success in predicting distributions from known structural features; it is not quite so clear that the inverse problem has been solved.

After a paper by Parthasarathy & Elango on the best way of testing for symmetry elements from intensity statistics the section is rounded off by a contribution from Wilson on fluctuations and errors in intensity distributions. He concludes, regretfully, that there is no obvious easy way of representing distributions modified by random or systematic errors.

The second section, on refinement, starts with a paper by Prince commenting on the precision and accuracy which may be obtained in structure refinement by the Rietveld method. He concludes that while the calculated standard deviations may give a general indication of the precision of the parameters found they are not an accurate assessment of the r.m.s. errors. Clearly this paper was controversial; the following paper by Rollett is a discussion of Prince's paper and he comes to a contrary conclusion.

The next two papers are concerned with the application of information theory to refinement. The first, by Collins, is on the very topical subject of parameter estimation by entropy maximization. This is a good paper to read; firstly it confirms that there is a certain arbitrariness in the entropy function which is maximized and secondly it demystifies a topic which for many crystallographers has taken on the characteristics of a deity - all powerful and incomprehensible. The following paper by Wilkins *et al.* is similarly to be commended especially in providing a practical procedure for incorporating prior knowledge into information-theory procedures.

The three papers which follow, on the modification of weights in least-squares analysis, variance of intensities in the Bond method and the use of maximum likelihood and minimax methods, are useful but not exceptional in any way. However, the final paper in this section, by Prince & Nicholson, on the influence of individual reflections on precision in least-squares refinement, links very nicely with the already-mentioned final paper by Milledge *et al.* Here we are shown how one should concentrate time and effort in measuring just that selection of reflections which most influence the determination of parameters rather than measuring everything indiscriminately with equal effort.

The book is well produced, attractively printed and a useful addition to crystallographic literature. There is something here for the theorist and experimentalist alike and, at least, it should be available on the shelf of the local library.

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**Crystal structure analysis: A primer.** 2nd ed. By J. P. GLUSKER and K. N. TRUEBLOOD. Pp. xviii+269. Oxford University Press, 1985. Price hardback £29.00, US $37.50; softback £17.00, US $18.95.

The first edition of this text came out 13 years ago in 1972, and was reviewed then by J. L. Lawrence [*Acta Cryst.* (1972), A**28**, 680], who concluded '... this book can be