Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.

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Crystallographic computing 4: techniques and new technologies. (IUCr Crystallographic Symposia No. 3.) Edited by N. W. ISAACS and M. R. TAYLOR. Pp. xvi+464. Oxford: International Union of Crystallography and Oxford University Press, 1988. Price £35.00.

The last twenty years of crystallography have produced a large number of books on crystallographic methods and crystallographic computing. Some conferences, symposia and summer schools have only 'survived' as good memories and excellent lecture notes, but modern computerized reproduction facilitates the publication of such notes so as to make the development of techniques and technologies available to the entire community of crystallographers.

This new book is the collection of papers presented at the International School of Crystallographic Computing held at the Flinders University of South Australia, Adelaide, 22-29 August 1987, under the auspices of the IUCr Commission on Crystallographic Computing.

One of the objectives of the School was to 'provide instruction on techniques for younger crystallographers...'. This goal may have been achieved for students who followed the practical worksessions or who joined in discussions with the masters. I would not, however, suggest reading this book as an introduction to the field! One exception is the nice chapter on data collection. Another one is the introduction to restraints and constraints in least-squares refinement of small-molecule structures.

The main objective of the school (or so it appears to me) is to provide detailed accounts of modern advances in computerized methods and techniques, and to summarize

the results obtained over the last few years. This goal has certainly been achieved.

Main topics include: (a) methods for single-crystal structure solution (with an emphasis on direct methods) and refinement techniques for 'small-molecule' and macromolecular structures (165 pages), (b) computer graphics and program systems (130 pages), and (c) database techniques (55 pages). Many of these topics were treated by the same authors in earlier books and lecture notes on crystallographic methods, and for the expert it is very exciting to observe the progress that has been made.

Less-common topics are: fibre diffraction, electron diffraction, electrostatic properties from diffraction data, and multivariate analysis of structure data (76 pages). Finally, by and for the computer experts, some lectures on special computing methods: symbolic programming, supercomputers and networking (50 pages).

In addition to the two objectives mentioned above, users of some program systems may be lucky enough to find a good write up or summary of their beloved system, as program manuals usually do not rank among the most readable literature!

This book is a must for all crystallographers who are actively involved in the development of methods as well as of computer programming.

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