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book reviews

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Direct phasing in crystallography. By Carmelo Giacovazzo. **IUCr Monographs on Crystallography** No. 8. Oxford: IUCr/ Oxford Science Publications, 1999. Pp. xxiii + 767. Price US $140.00. ISBN 0-19-850072-6.

Direct methods are one of the great success stories of crystallography. From modest beginnings in the mid 1940's and with the work of such pioneers as Wilson, Sayre, Hauptman, Karle, Woolfson, Main and Sheldrick, we now have a technique for tackling the phase problem that is capable of solving even small protein structures (provided that data to *ca* 1.1 Å are available) as well as structural problems from powder and electron diffraction data. The impact of the methodology on chemistry was acknowledged through the award of a 1985 Nobel Prize to Hauptman and Karle. Among these pioneers, we must also number Carmelo Giacovazzo whose programs *SIR* and *SIRPOW* are used throughout the world, and who is a prolific contributor to Section A of *Acta Crystallographica*. Indeed, this is not his first book on the subject; he is also the author of *Direct methods in crystallography* (Academic Press, 1980), but this is no longer available, and anyway, a great deal has changed in this field in the intervening 20 years, and this alone makes the monograph welcome.

In fact, there are very few books on this subject, which is surprising given its scope and importance; very often it gets relegated to rather incomplete (and sometimes incorrect) coverage in general crystallography texts. The intended audience for Giacovazzo's book is wide, and includes undergraduates, graduate students and professional crystallographers. It is important that books of this sort do address a wide readership, since direct methods are still a very active field. As an indicator of this activity, since this monograph was published there have been major advances in powder diffraction using modelling techniques, the use of direct methods to locate Se atoms from MAD data and the extension of *ab initio* phasing to protein structures with nearly 2000 atoms in the asymmetric unit.

So, what of the book? The first impression is that it represents an immense work of scholarship. With 767 pages and over 1200 references (but with only the first page numbers given), Giacovazzo has constructed an enormous reference volume that scans and surveys the whole of the field of direct methods with authority and useful critical insight. There is very little of the subject that has been missed and not scrutinized. The text is enhanced by descriptions of algorithms, examples of direct methods using real data with the results described in detail, and the use of appendices to keep some of the mathematics under control; given the mathematical nature of direct methods, the proliferation of equations can be a problem for many readers. The contents span Wilson statistics, structure invariants and seminvariants including Giacovazzo's representation theory and their use in tangent type formulae for phase determination. Most of this work is based on probability arguments and the use of Wilson statistics. Extensions to the theory for neutron, electron and powder diffraction data then follow. This is very welcome: it is especially good to see a discussion of electron diffraction, the Cinderella of structural crystallography. All these topics fill over half the book, which then moves on to extending the role of direct methods from a technique of *ab initio* structure solution for small molecules to a phase-refinement and phase-extension method in macromolecular crystallography. To do this, one has to interpret and redefine the term 'direct methods' rather more loosely than many crystallographers would like, but there can be no doubt that this serves a useful function and extends the scope and readership of the book. A footnote on page 468 explains this shift of terminology clearly. In this context, there are discussions of MIR and SIR theory, anomalous dispersion including the MAD method, molecular replacement, and the maximum entropy formalism. The coverage is good, but readers will also need Drenth's book *Principles of protein X-ray crystallography* (Springer, 1999) to put these techniques into a working macromolecular crystallographic context. The monograph concludes with six brief appendices concerned with special mathematical functions and more advanced probability theory – I would have put much more material from the main text here to improve the book's readability.

There are some problems, many of which are inevitable with a book of this size. It is undoubtedly hard to read, and the slightly stilted English does not help. There are some rather unusual expressions, *e.g.* 'home diffractometer'. I must say I don't have one at home, it is safely installed in the lab! The text refuses to flow, and chunks of Giacovazzo's earlier book can be found in a lot of places. Some of the diagrams and figures are poorly presented, and the protein electron-density maps would benefit from the use of colour.

Work is sometimes not referenced properly; *e.g.* the derivation of the maximum entropy equations in a crystallographic environment is almost identical to that derived by Bricogne [*Acta Cryst.* (1984), A**40**, 410–445], but this is not mentioned at this juncture. An excellent book on direct methods by Woolfson & Fan: *Physical and non-physical methods of solving crystal structures* (Cambridge University Press, 1995) is absent from the list of references. In the desire to be complete, some material, *e.g.* origin definition, is given more space that current uses of direct methods would warrant, and a lot of mathematics could be truncated or greatly abbreviated since the full derivations are available elsewhere, and the algebraic details can often obscure the important salient facts. An introductory chapter would also have been very useful; we are thrown directly into Wilson statistics with very little preamble or even a definition of direct methods. As a text for undergraduates, the book is far too demanding; for post-graduates, its appeal will largely be to those working in the field, but as a source book for research workers, however, it is unrivalled.

There is one last very major criticism, however: how can a volume of such a size appear with an index of a mere $2\frac{1}{2}$ pages – only about 250 entries? This is a huge pity since it limits its usefulness as a general reference book; finding what you want is very difficult.

Chris Gilmore

Department of Chemistry
University of Glasgow
Glasgow G12 8QQ
Scotland

E-mail: chris@chem.gla.ac.uk