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Book review

Theory and practice of direct methods in crystallography.

M.F.C. Ladd and R.A. Palmer (Editors), Plenum Press, New York and London, 1980, xiv + 421 pages, \$35.00.

This book comprises a series of articles by workers prominent in the field of direct methods. The introductory chapter by Allegra and the chapter on symbolic addition and multiresolution methods by Ladd and Palmer are suited to the inexperienced chemical crystallographer seeking to know how direct methods can help him in structure determinations and discusses some pitfalls of the methods. One criticism that might be made is that it is couched exclusively in terms of the computer program MULTAN which seems a little unfair to other easily available programs such as for instance those in the SHELX program system of G.M. Sheldrick.

The remaining chapters seem more orientated towards those who already have some experience of direct methods and seek a compilation of current ideas. There is a comprehensive exposition of origin definition and E value calculation by Rogers, and of the probabilistic theory of structure seminvariants by Hauptman. The application of Hauptman's expressions for the cosines of structure invariants in practical phase determination is discussed in a separate multi-author chapter with some real examples given. The use of the phase correlation method is discussed by Beurskens and Van den Hark as also is the application of direct methods to difference structure factors. The remaining three chapters are directed more to the question of phase extension or refinement mainly in large or very large structures. Sayre deals with the use of convolution and related equation systems, whilst Tsoucaris discusses the maximum determinant method. Finally Argos

and Rossman describe the molecular replacement method and how non-crystallographic symmetry can be used in protein structure determination.

This book brings together a wide variety of approaches to the subject and I suspect that it will be more of interest to crystallographers wishing to keep in touch with current ideas rather than to beginners wanting an introduction to the subject.

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