Programming methodology of artificial intelligence; A technique for overlaying common storage.

In addition to the lectures the book includes the work-sessions material of most of the lectures. This book (of about 525 pages) will be most useful to all who are engaged in crystal structure determination. Copies may be obtained from The Editor, Indian Academy of Sciences, Bangalore, 560 080, India. The price of the book is US$17 or 125 Rupees, but individuals may purchase a copy for their personal use at the reduced price of US$8 or 50 Rupees. These prices include postage by surface mail. Copies may be sent by airmail but at extra cost.

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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Theory and practice of direct methods in crystallography. Edited by M. F. C. LADD and R. A. PALMER. Pp. xiv + 421. New York and London: Plenum Press, 1980. Price US $35.00.

Direct methods, in some form, are used routinely in most crystallographic laboratories with so much success that the crystallographer can easily fall into the trap of taking them for granted. This book provides an insight into the workings of these routines that will prove invaluable on those occasions that the structure does not appear at the far end. There are ten chapters, all written by authors, active in the areas covered, who manage to give the reader a working knowledge of their respective subjects within the confines of a single chapter.

The first three chapters cover the basics of the direct-methods routines that are in common use. An excellent and detailed account is given of the rules for origin definition and enantiomorph selection. This is followed by a short section on the calculation of $|E|$'s which, in view of the desirability of starting with the best possible data, could have been more extensive. Symbolic addition and multi-solution methods of phase extension are discussed and the computer program *MULTAN* of G. Germain, P. Main and M. M. Woolfson is described and a number of examples are given. A short section of advice is included for those structures which are not solved at the first attempt.

Chapter 4 develops the theory of structure invariants and semi-invariants. As well as the familiar $\sum_1$ and $\sum_2$ formulae, the use of quartets and quintets is discussed. The 'neighborhood principle' is described whereby the value of a structure invariant is primarily determined by the values of a small number of associated $|E|$'s and is insensitive to the bulk of the data. The next chapter describes methods of calculating values for the cosines of invariants. Although these calculations are not currently very accurate, they do permit the identification of those invariants that have values close to π rather than the predicted 0 and can cause failure in a phase extension routine. An interesting technique of 'strong enantiomorph selection' is described, as is the use of negative quartets as a figure of merit in multi-solution programs.

Chapter 6 presents an update of one of the oldest automated direct methods, that of phase correlation. Essentially a symbolic addition procedure, a quite large set of reflections are represented by symbols and as the procedure progresses relationships between symbols are sought. This routine is enhanced by the calculation of cosine invariants. The following chapter discusses the use of difference structure factors in direct-methods routines when part of the structure is known. This can be a very useful procedure in cases where heavy atoms are at special or pseudo-special positions.

The remainder of the book concerns the use of direct methods for large structures. Although conventional methods are not suitable for solving protein structures a number of applications of direct methods to this problem are described. Phase extension is discussed using convolutional equation systems, one of which is the familiar tangent formula. Karle–Hauptman determinants are examined and the maximum-determinant rule is derived. The relationship between low-order determinants and structure invariants is shown as well as the use of high-order ones in the solution of protein structures.

The final chapter is about molecular-replacement methods, which are not at first sight direct methods, but rather search and match techniques. However, their discussion completes an extensive review of structure-solving methods.

This book is well written and produced and should be of interest to all crystallographers who use direct methods. I already have some ideas for a couple of structures in my 'problem file'.

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