



Computing Methods in Crystallography

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Computing Methods in Crystallography is a collection of lectures given at a two-week Summer School held in Oxford, UK in August 1962. About forty-five crystallographers focused on advances in the use of computing methods in crystallography. The discussions are organized around four themes: algebra, statistics, phase determination, and programming.

This book is comprised of 20 chapters and begins with an introduction to the algebra required for the fundamental operations of transformation of coordinates, interpolation, and approximation of trigonometric and exponential functions, as well as solution of linear equations and derivation of latent roots and vectors. Methods for calculation of structure factors, least-squares adjustment, Fourier series evaluation, and a number of other operations are described. The statistical properties of reciprocal space are also considered, along with probability methods for centrosymmetric crystals. The final chapter looks at some crystallographic programs in FORTRAN.

This monograph will be a valuable resource for crystallographers as well as physics students and researchers interested in the application of computing methods to crystallography.



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