

Computing Methods in Crystallography

Edited by J.S.Rollett
Computing Laboratory,
University of Oxford

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Computing Methods In Crystallography:

Computing Methods in Crystallography J. S. Rollett, 2016-06-06 *Computing Methods in Crystallography* is a collection of lectures delivered at a Summer School held in Oxford in August 1962 The book presents the underlying mathematics and computing methods in crystallography The text covers topics on the algebra required for the fundamental operations of transformation of coordinates interpolation approximation of trigonometric and exponential functions solution of linear equations and derivation of latent roots and vectors methods for calculation of structure factors least squares adjustment and Fourier series evaluation the theory and practice of intensity scaling and symmetry determination and methods of direct phase determination Crystallographers physicists and students in allied fields will find the book very useful [International Tables for Crystallography, Volume B](#) Uri Shmueli, 2008-08-27 *International Tables for Crystallography* are no longer available for purchase from Springer For further information please contact Wiley Inc follow the link on the right hand side of this page Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research After an introductory chapter Part 1 presents the reader with an account of structure factor formalisms an extensive treatment of the theory algorithms and crystallographic applications of Fourier methods and fundamental as well as advanced treatments of symmetry in reciprocal space In Part 2 these general accounts are followed by detailed expositions of crystallographic statistics the theory of direct methods Patterson techniques isomorphous replacement and anomalous scattering and treatments of the role of electron microscopy and diffraction in crystal structure determination including applications of direct methods to electron crystallography Part 3 deals with applications of reciprocal space to molecular geometry and best plane calculations and contains a treatment of the principles of molecular graphics and modelling and their applications A convergence acceleration method of importance in the computation of approximate lattice sums is presented and the part concludes with a discussion of the Ewald method Part 4 contains treatments of various diffuse scattering phenomena arising from crystal dynamics disorder and low dimensionality liquid crystals and an exposition of the underlying theories and or experimental evidence Polymer crystallography and reciprocal space images of aperiodic crystals are also treated Part 5 of the volume contains introductory treatments of the theory of the interaction of radiation with matter dynamical theory as applied to X ray electron and neutron diffraction techniques The simplified trigonometric expressions for the structure factors in the 230 three dimensional space groups which appeared in Volume I of *International Tables for X ray Crystallography* are now given in Appendix 1 4 3 to Chapter 1 4 of this volume Volume B is a vital addition to the library of scientists engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature **COMPUTING METHODS IN CRYSTALLOGRAPHY- MEETING- PAPERS. , Computing Methods in Crystallography. Edited by J.S. Rollett. [By Various Authors.].**

John Sydney ROLLETT,1965 **Computing Methods in Crystallography** Tosio Sakurai,Julio Zukerman Schpector,1979
Mathematics of transformation Algebra of linear transformation Transformation of the crystal lattice Symmetry operations
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factor and least squares Fourier synthesis Molecular model building **Current Methods and Optimization Algorithms
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optical and e ray diffraction techniques for examining single crystals It includes the solution of crystal structures by the
current methods worked examples of crystal structure determination problems and solutions for each chapter

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definitive resource and reference work for crystallography and structural science Volume B presents accounts of the
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on the subject of crystal structure determination one of the standards in the field I did feel daunted by the prospect and
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since the 1912 discoveries of von Laue and the Braggs In the intervening years great advances have been made so that today
it is almost taken for granted that crystal structures can be determined in which hundreds if not thousands of separate
atomic positions can be found with apparent ease In the early years the structures of relatively simple materials such as the
alkali halides were often argued over and even disputed whereas today we routinely see published structures of most
complex molecular crystals including the structures of viruses and proteins **Graphical and Tabular Methods in**

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Holzman,Allen Kent,1977-02-01 This comprehensive reference work provides immediate fingertip access to state of the art

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Techniques of Metals Research: Techniques for the direct observation of structure and imperfections. Editor: R. F. Bunshah. 2 v Rointan Framroze Bunshah, 1969 **Some Statistical Applications in X-ray Crystallography** Ramachandran Srinivasan, S. Parthasarathy, 1976 *Principles of Crystal Structure Determination* Gene B. Carpenter, 1969

University of California Union Catalog of Monographs Cataloged by the Nine Campuses from 1963 Through 1967: Authors & titles University of California (System). Institute of Library Research, University of California, Berkeley, 1972 **World Directory of Crystallographers and of Other Scientists Employing Crystallographic Methods** William Parrish, Donald Wytze Smits, 1986

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