

# Computing Methods in Crystallography

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

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# Computing Methods In Crystallography

**Sydney R. Hall, Tamaichi Ashida**



## **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  
 Fourier transformation Practical procedures in crystallographic computing Basic considerations Data reduction Structure  
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 Crystallography** Marcus Frederick Charles Ladd,Rex A. Palmer,2003-09-30 This book is an account of crystal symmetry and  
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 current methods worked examples of crystal structure determination problems and solutions for each chapter  
     *International Tables for Crystallography, Volume B* U. Shmueli,2008-08-25 *International Tables for Crystallography* is the  
 definitive resource and reference work for crystallography and structural science Volume B presents accounts of the  
 numerous aspects of reciprocal space in crystallographic research This volume is a vital addition to the library of scientists  
 engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic  
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 scattering More information on the series can be found at <http://it.iucr.org>      *Structure Determination by X-ray  
 Crystallography* Mark F.C. Ladd,Rex A. Palmer,2003-09-30 I was highly flattered when I was asked by Mark Ladd and Rex  
 Palmer if I would write the Foreword to this Fourth Edition of their book Ladd Palmer is such a well known and classic book  
 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  
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 atomic positions can be found with apparent ease In the early years the struc tures 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  
 Crystallography** Thomas Vipond Barker,1922      *Encyclopedia of Computer Science and Technology* Jack Belzer,Albert G.  
 Holzman,Allen Kent,1977-02-01 This comprehensive reference work provides immediate fingertip access to state of the art

technology in nearly 700 self contained articles written by over 900 international authorities Each article in the Encyclopedia features current developments and trends in computers software vendors and applications extensive bibliographies of leading figures in the field such as Samuel Alexander John von Neumann and Norbert Wiener and in depth analysis of future directions *International Tables for Crystallography: Reciprocal space*, 1984 **Methods and Applications in**

**Crystallographic Computing** Sydney R. Hall, Tamaichi Ashida, 1984 Thirty five international authorities offer comprehensive review of current computing techniques in crystal structure analysis The volume contains sections on data measurement and processing solution techniques refinement techniques accurate electron density analysis computer software and hardware data base techniques and computer graphics There are also contributions on powder methods and electron diffraction and microscopy **Encyclopedia of Bioinformatics and Computational Biology**, 2018-08-21 Encyclopedia of Bioinformatics and Computational Biology ABC of Bioinformatics Three Volume Set combines elements of computer science information technology mathematics statistics and biotechnology providing the methodology and in silico solutions to mine biological data and processes The book covers Theory Topics and Applications with a special focus on Integrative omics and Systems Biology The theoretical methodological underpinnings of BCB including phylogeny are covered as are more current areas of focus such as translational bioinformatics cheminformatics and environmental informatics Finally Applications provide guidance for commonly asked questions This major reference work spans basic and cutting edge methodologies authored by leaders in the field providing an invaluable resource for students scientists professionals in research institutes and a broad swath of researchers in biotechnology and the biomedical and pharmaceutical industries Brings together information from computer science information technology mathematics statistics and biotechnology Written and reviewed by leading experts in the field providing a unique and authoritative resource Focuses on the main theoretical and methodological concepts before expanding on specific topics and applications Includes interactive images multimedia tools and crosslinking to further resources and databases *Research Awards Index*, 1981

**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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