

**COMPUTING METHODS
AND THE PHASE PROBLEM
IN X-RAY CRYSTAL ANALYSIS**

REPORT OF A CONFERENCE
HELD AT GLASGOW
AUGUST, 1960

EDITED BY
RAY PEPIEK AND J. M. ROBERTSON
AND J. C. SPENCER

PERGAMON PUBLISHING DIVISION
PERGAMON PRESS
NEW YORK - OXFORD - LONDON - PARIS
1961

Computing Methods Phase Problem In Xra

Ray Pepinsky



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Computing Methods and the Phase Problem in X-ray Crystal Analysis Ray Pepinsky, 1952 [Computing Methods and the Phase Problem in X-Ray Crystal Analysis; Report. Edited by Ray Pepinsky, J.M. Robertson and J.C. Speakman ,1961](#)
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 research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature New to this edition A new chapter on modern extensions of the Ewald method for Coulomb interactions in crystals Three new sections on electron diffraction and electron microscopy in structure determination describing point group and space group determination by convergent beam electron diffraction three dimensional reconstruction and single particle reconstruction Substantial revisions to the chapters on space group representations in reciprocal space direct methods Patterson and molecular replacement techniques and disorder diffuse scattering More information on the series can be found at <http://it.iucr.org> **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 **Structure Determination by X-Ray Crystallography** Marcus Frederick Charles Ladd, Rex A. Palmer, 2003-09-30 This book is an account of crystal symmetry and optical and x 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 [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

Advances in Computers, 1964-01-01 The survey articles included in Volume 5 have been selected with two aims in mind to arrive at a balanced sampling of the computer field and to emphasize the subjects of most active current interest Articles cover topics such as the role of computers in delivering election results the state of computer development in the Soviet Union and its neighbors artificial intelligence and applications of computers to the design of optical instruments to nuclear reactor design and to the determination of the structure of crystals or molecules from X ray diffraction patterns

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