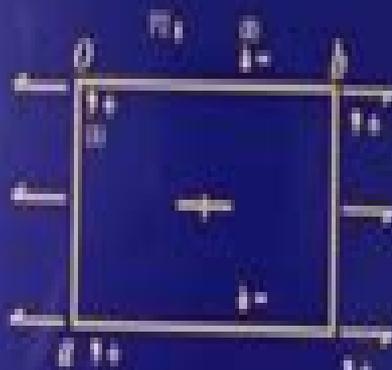


X-RAY STRUCTURE DETERMINATION

A PRACTICAL GUIDE

Second Edition



GEORGE H. STOUT

LYLE H. JENSEN

WILEY

X Ray Structure Determination A Practical Guide

R. Bruce King



X Ray Structure Determination A Practical Guide:

X-Ray Structure Determination George H. Stout, Lyle H. Jensen, 1989-05-08 Closely follows an actual structural determination After some introductory material on the nature of x rays the diffraction process and the internal geometry of crystals the selection and preparation of a crystal are considered Techniques of measuring raw x ray data are covered plus their reduction into a useable form The second part discusses both traditional and novel methods of solving the phase problem the principal difficulty in x ray structure determination The third part considers how to extract the most information from the data and how to evaluate its reliability Finally there is a discussion of sources of error in practice and interpretation

X-ray Structure Determination George Hubert Stout, 1975 Crystal Structure Analysis for Chemists and Biologists Jenny P. Glusker, Mitchell Lewis, Miriam Rossi, 1996-12-17 The fields of structural chemistry and biochemistry have blossomed in the last seventy years since X ray diffraction was discovered in 1912 Dorothy Hodgkin who obtained a Nobel Prize in 1965 for her X ray diffraction work wrote a great advantage of X ray analysis as a method of chemical structure analysis is its power to show some totally unexpected and surprising structure with at the same time complete certainty The results of all X ray diffraction studies are used by chemists and buiochemists but these scientists need to be able to appreciate the significance and extent to which these results may be used A number of books written for practicing crystallographers cover the theory and applications of X ray diffraction but few are of real practical use to non specialists In Crystal Structure Analysis for Biologists and Chemists the general principles of crystal structure are presented in a highly readable way The book of Glusker who is internationally renowned provides good coverage of theory including data and understanding their significance **Current Medicinal Chemistry**, 1996-12 **Structure in Protein Chemistry** Jack Kyte, 2006-11-01 The second edition of Structure in Protein Chemistry showcases the latest developments and innovations in the field of protein structure analysis and prediction The book begins by explaining how proteins are purified and describes methods for elucidating their sequences of amino acids and defining their posttranslational modifications Comprehensive explanations of crystallography and of noncovalent forces ionic interactions hydrogen bonding and the hydrophobic effect act as a prelude to an exhaustive description of the atomic details of the structures of proteins The resulting understanding of protein molecular structure forms the basis for discussions of the evolution of proteins the symmetry of the oligomeric associations that produce them and the chemical mathematical and physical basis of the techniques used to study their structures The latter include image reconstruction nuclear magnetic resonance spectroscopy proton exchange optical spectroscopy electrophoresis covalent cross linking chemical modification immunochemistry hydrodynamics and the scattering of light X radiation and neutrons These procedures are applied to study the folding of polypeptides and the assembly of oligomers Biological membranes and their proteins are also discussed Structure in Protein Chemistry Second Edition bridges the gap between introductory biophysical chemistry courses and research literature It serves as a comprehensive textbook for

advanced undergraduates and graduate students in biochemistry biophysics and structural and molecular biology Professionals engaged in chemical biochemical and molecular biological research will find it a useful reference

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>

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Crystal Structure Determination at the Center for X-ray Crystallography Alexandr Evgenievich Oblezov, 2003 ABSTRACT Initial steps of working with sophisticated equipment and software of single structure X ray determination are not obvious but confusing The main idea of this work is to show to an inexperienced user an operating guideline of Bruker SMART CCD diffractometer and SHELXTL structure solution and refinement software package Detailed description of all operations is provided as well

as examples of step by step structure refinements of various structures *Journal of Rheology*, 1989 The Publishers' Trade List Annual, 1984 **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 **Zeitschrift Für Kristallographie**, 2004 Encapsulation of Metal Sulfide and Oxide Clusters in MoS₂ and WS₂ and Characterization of Restacked MoS₂ and WS₂ Joy Marie Heising, 1999 **Syntheses, Structures and Formation Mechanisms of Metastable Modifications of Metal Dihalides [I] and II, Magnetic and Electrical Properties of Oxidinitrides** Guo Liu, 1990 *A Materials Approach to Improving the Efficiency of Thermoelectric Cooling Devices* Kristin Marie Poduska, 2001 **Structural and Conformational Studies of Purine Nucleoside Analogs** Stephen Robert Sprang, 1977 *Annales Academiae Scientiarum Fennicae*, 1988 **Molecular Structure of D(CGCGTTAACGCG) in the Netropsin-bound and Netropsin-free Orthorhombic Crystal Form** Ganesaratnam K. Balendiran, 1991 **Encyclopedia of Inorganic Chemistry: D-H** R. Bruce King, 2005 *The Location of Hydrogens in a Heavy Atom Structure* Elizabeth Ann

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