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Advanced X-ray Crystallography

JACOBY CONWAY

Crystal Structure Determination Springer-Verlag
X-ray crystallography is the main method used to determine the structure of biological molecules. X-ray crystallography is explained without maths and reading this text allows biologists to assess the quality and accuracy of biological structures.

Mathematical Techniques in Crystallography and Materials Science Springer Science & Business Media
Crystallography and structure theory have recently received increasing interest due to their role in understanding biological structures, high-temperature superconductors, and effects on mineral properties related to changes in temperature and pressure. This book offers a comprehensive account of the wide range of crystallography in many branches of science. The fundamentals, the most frequently used procedures and experimental techniques are all described in a detailed way. A

number of appendices are devoted to more specialist aspects. The book is an updated and fully revised new edition with emphasis on the wide range of topical applications and current areas of research. Ample illustrations help clarify the subject matter. To provide a better understanding of the basics of crystallography, a compact disk has been added to this new edition, offering the facilities of modern graphics to simulate experiments, show complex images, and provide a number of exercises.

Crystal Structure Analysis Oxford University Press, USA

This volume draws on the expertise of leaders in the field of macromolecular crystallography to illuminate the dramatic developments that are accelerating progress in structural biology. Their contributions span the range of techniques from crystallization through data collection, structure solution and analysis. The book shows how modern high-throughput methods are contributing to a deeper understanding of medical problems.

The Rietveld Method Springer Science & Business Media

Crystal Structure Refinement is a mixture of textbook and tutorial. As A Crystallographers Guide to SHELXL it covers advanced aspects of practical crystal structure refinement, which have not been much addressed by textbooks so far. After an introduction to SHELXL in the first chapter, a brief survey of crystal structure refinement is provided. Chapters three and higher address the various aspects of structure refinement, from the treatment of hydrogen atoms to the assignment of atom types, to disorder, to non-crystallographic symmetry and twinning. One chapter is dedicated to the refinement of macromolecular structures and two short chapters deal with structure validation (one for small molecule structures and one for macromolecules). In each of the chapters the book gives refinement examples, based on the program SHELXL, describing every problem in detail. It comes with a CD-ROM with all files necessary to reproduce the refinements.

Crystal Structure Refinement by Least Squares with the IBM 650 Oxford University Press

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.

Applied Crystallography Oxford University Press

This volume summarises recent developments and possible future directions for small molecule X-ray crystallography. It reviews specific areas of crystallography which are rapidly developing and places them in a historical context. The interdisciplinary nature of the technique is emphasised throughout. It introduces and describes the chemical crystallographic and synchrotron facilities which have been at the cutting edge of the subject in recent decades. The introduction of new computer-based algorithms has proved to be very influential and stimulated and accelerated the growth of new areas of science. The challenges which will arise from the acquisition of ever larger databases are considered and the potential impact of artificial intelligence techniques stressed. Recent advances in the

refinement and analysis of X-ray crystal structures are highlighted. In addition the recent developments in time resolved single crystal X-ray crystallography are discussed. Recent years have demonstrated how this technique has provided important mechanistic information on solid-state reactions and complements information from traditional spectroscopic measurements. The volume highlights how the prospect of being able to routinely “watch” chemical processes as they occur provides an exciting possibility for the future. Recent advances in X-ray sources and detectors that have also contributed to the possibility of dynamic single-crystal X-ray diffraction methods are presented. The coupling of crystallography and quantum chemical calculations provides detailed information about electron distributions in crystals and has resulted in a more detailed understanding of chemical bonding. The volume will be of interest to chemists and crystallographers with an interest in the synthesis, characterisation and physical and catalytic properties of solid-state materials. Postgraduate students entering the field will benefit from a historical introduction to the subject and a description of those techniques which are currently used. Since X-ray crystallography is used so widely in modern chemistry it will serve to alert senior chemists to those developments which will become routine in coming decades. It will also be of interest to the broad community of computational chemists who study chemical systems.

Structure Determination by X-ray Crystallography Royal Society of Chemistry

Crystal Structure RefinementOxford University Press

Fundamentals of Crystallography Springer Science & Business Media

By choosing an approach that avoids undue emphasis on the mathematics involved, this book gives practical advice on topics such as growing crystals, solving and refining structures, and understanding and using the results.

Crystal Structure Determination Springer Science & Business Media

Crystals and crystal geometry -- Symmetry operations and point groups -- Lattices -- Space groups -- X-rays and X-ray diffraction -- Solving the structure -- Refinement and molecular geometry -- Computer-assisted studies in X-ray crystallography.

Applied Crystallography Oxford University Press on Demand

This volume contains many examples of how crystallography is important to chemistry and biochemistry. It explains the results of X-ray diffraction analysis, placing it in context with other methods of structural analysis, such as solution studies and molecular modelling.

Symmetriebeziehungen zwischen verwandten Kristallstrukturen Springer Science & Business Media

The book describes phasing techniques in modern crystallography. The main text is dedicated to their simple description, and further mathematical details are contained in the appendices. Practical aspects are described for each specific method, making it a useful tool for the daily work of practising crystallographers.

21st Century Challenges in Chemical Crystallography I Springer Science & Business Media

Despite the tremendous advances in the techniques and equipment for carrying out high-pressure crystallography, the

application or exploration of the high-pressure variable in detailed structural studies remains rare. The chapters in this book provide a set of lecture notes and supplementary material for a course on high pressure crystallography. The material comprises state-of-the-art reviews of high-pressure experiments using X-ray and neutron diffraction techniques at synchrotron and neutron facilities and in the laboratory, as well as complementary experimental high-pressure techniques and theoretical methods for investigating matter at elevated pressures. The materials studies range from elemental solids and liquids to inorganic compounds, minerals, organic compounds, clathrates and pharmaceutical compounds, to large biological molecules such as proteins and viruses. The book provides a reference for workers in high-pressure science wishing to learn more about crystallography and for established crystallographers potentially interested in high pressure as a variable, as well as an introductory guide to new researchers in the field.

Evolving Methods for Macromolecular Crystallography Springer Science & Business Media

An excellent book for professional crystallographers! In 2012 the crystallographic community celebrated 100 years of X-ray diffraction in honour of the pioneering experiment in 1912 by Max von Laue, Friedrich and Knipping. Experimental developments e.g. brilliant X-ray sources, area detection, and developments in computer hardware and software have led to increasing applications in X-ray analysis. This completely revised edition is a guide for practical work in X-ray analysis. An introduction to basic crystallography moves quickly to a practical and experimental treatment of structure analysis. Emphasis is placed on understanding results and avoiding pitfalls. Essential reading for researchers from the student to the professional level interested in understanding the structure of molecules.

High-Pressure Crystallography John Wiley & Sons

A powerful and relatively new method for extracting detailed crystal structural information from X-ray and neutron powder diffraction data, the Rietveld method attracts a great deal of interest from researchers in physics, chemistry, materials science, and crystallography. Now available inpaperback, this book comprises chapters from international researchers on all aspects of this important technique. It will be of great interest to all researchers in the fields, as well as graduate students seeking a solid introduction and comprehensive survey.

Electron Crystallography OUP Oxford

Während der letzten 20 Jahre hat sich dank der zunehmenden Verbreitung von Vierkreis-Diffraktometern und der enormen Steigerung der Computerlei stung die Methode der Kristallstrukturbestimmung mittels Röntgenbeugung lawinenartig ausgebreitet. Wegen ihrer hohen Aussagekraft und Genauigkeit ist sie zu einem der wichtigsten Werkzeuge in der chemischen Grundlagenfor schung geworden, in der anorganischen wie der organischen Chemie. Obwohl die Kristallographie in der Ausbildung der Chemiestudenten noch immer eine sehr untergeordnete Rolle spielt, sind viele davon gehalten, während ihrer Diplom-oder Doktorarbeit diese Methode selbst einzusetzen oder zumindest ihre Ergebnisse kompetent zu verwerten. Die vielen und komplizierten Stufen einer Röntgenstrukturanalyse sind dank immer raffinierterer Programmsy steme tatsächlich zunehmend auch von kristallographisch weniger Geübten zu

meistern. Eine solche Anwendung als "black box"-Methode birgt jedoch dann erhebliche Fehlerrisiken. Das vorliegende Buch richtet sich deshalb vorwiegend an fortgeschrittene Studenten der Chemie oder benachbarter Fächer, die einen Blick in den schwarzen Kasten tun wollen, bevor sie selbst auf diesem Gebiet tätig werden, oder die sich über Grundlagen, Leistungsfähigkeit und Risiken der Methode informieren wollen. Da erfahrungsgemäß die Bereitschaft, ein Buch wirklich zu lesen, umgekehrt proportional zur Seitenzahl ist, wurde versucht, die Behand lung der methodischen Grundlagen möglichst kurz und anschaulich zu halten. Es erscheint wichtiger, daß ein Chemiker bei einer Rechnung das Grundprin zip und die Voraussetzungen für ihre sinnvolle Anwendung verstanden hat, als daß er in der Lage ist, den ohnehin von Programmen erledigten mathe matischen Formalismus nachzuvollziehen.

Structure Determination from Powder Diffraction Data World Scientific

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.

The Essence of Crystallography World Scientific

The purpose of this book is to explain why molecular structure can be determined by single-crystal diffraction of X rays. It is not an account of the practical procedural details, but rather an account of the underlying physical principles, and the kinds of experiments and methods of handling the experimental data that are used.

Incommensurate Crystallography Vieweg+Teubner Verlag

'To summarise, Professor Ladd has written a highly engaging text designed to provide the underlying principles of crystal structure determination through X-ray diffraction data. This text would be most appropriate for an early stage postgraduate or researcher interested in learning both the underlying principles of crystallography and gaining some practice with structure-solving software.'Contemporary PhysicsDesigned for those who wish to understand and engage with the principles behind the process of crystal structure determination by X-ray diffraction, this title contains a comprehensive series of chapters, each of which concludes with a set of problems, for which solutions are provided. An ideal resource for senior undergraduates and early-stage postgraduates, The Essence of Crystallography has an accompanying website with programs written for the text, including an interactive simulation of crystal structure determination using prepared intensity data sets.

Crystals, X-rays and Proteins Books on Demand

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 wondered if I could do justice to it. The determination of crystal structures by X-ray crystallography has come a long way 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 sepa rate 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.

Phasing in Crystallography Walter de Gruyter

This textbook gives a concise introduction to modern crystal structure determination, emphasising both its theoretical background and the way it actually occurs. The theoretical and experimental sections are supported by many illustrations, and lay emphasis on a good understanding rather than rigorous mathematics. The actual data collection techniques, and the methods of data reduction, structure solution and refinement are discussed from a practical point of view. Many tips and insigths help readers to recognise and avoid possible errors and traps, and to judge the quality of results. In the third English edition, based on the German eighth edition (Springer 2015), treatment of film methods, now extinct, and of the nearly extinct four-circle diffractometers has been omitted. Instead, the methods of obtaining and interpreting area detector data have been expanded, and e.g. actual alternative direct methods and time-resolved crystallography are included.

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