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KEY=POWDER - HIGGINS HOOD

Structure Determination from Powder Diffraction Data

OUP Oxford The art of solving a structure from powder diffraction data has developed rapidly over the last ten years to the point where numerous crystal structures, both organic and inorganic, have been solved directly from powder data. However, it is still an art and, in contrast to its single crystal equivalent, is far from routine. The art lies not only in the correct application of a specific experimental technique or computer program, but also in the selection of the optimal path for the problem at hand. Written and edited by experts active in the field, and covering both the fundamental and applied aspects of structure solution from powder diffraction data, this book guides both novices and experienced practitioners alike through the maze of possibilities.

Novel Methods of Structure Determination from X-ray Powder Diffraction Data

Fundamentals of Powder Diffraction and Structural Characterization of Materials, Second Edition

Springer Science & Business Media A little over ?ve years have passed since the ?rst edition of this book appeared in print. Seems like an instant but also eternity, especially considering numerous developments in the hardware and software that have made it from the laboratory test beds into the real world of powder diffraction. This prompted a revision, which had to be beyond cosmetic limits. The book was, and remains focused on standard laboratory powder diffractometry. It is still meant to be used as a text for teaching students about the capabilities and limitations of the powder diffraction method. We also hope that it goes beyond a simple text, and therefore, is useful as a reference to practitioners of the technique. The original book had seven long chapters that may have made its use as a text - convenient. So the second edition is broken down into 25 shorter chapters. The ?rst ?fteen are concerned with the fundamentals of powder diffraction, which makes it much more logical, considering a typical 16-week long semester. The last ten ch- ters are concerned with practical examples of structure solution and re?nement, which were preserved from the ?rst edition and expanded by another example – R solving the crystal structure of Tylenol .

Using Texture to Facilitate Structure Determination from Powder Diffraction Data

Structure Determination by X-ray Crystallography

Analysis by X-rays and Neutrons

Springer Science & Business Media The advances in and applications of x-ray and neutron crystallography form the essence of this new edition of this classic textbook, while maintaining the overall plan of the book that has been well received in the academic community since the first edition in 1977. X-ray crystallography is a universal tool for studying molecular structure, and the complementary nature of neutron diffraction crystallography permits the location of atomic species in crystals which are not easily revealed by X-ray techniques alone, such as hydrogen atoms or other light atoms in the presence of heavier atoms. Thus, a chapter discussing the practice of neutron diffraction techniques, with examples, broadens the scope of the text in a highly desirable way. As with previous editions, the book contains problems to illustrate the work of each chapter, and detailed solutions are provided. Mathematical procedures related to the material of the main body of the book are not discussed in detail, but are quoted where needed with references to standard mathematical texts. To address the computational aspect of crystallography, the suite of computer programs from the fourth edition has been revised and expanded. The programs enable the reader to participate fully in many of the aspects of x-ray crystallography discussed in the book. In particular, the program system XRAY* is interactive, and enables the reader to follow through, at the monitor screen, the computational techniques involved in single-crystal structure determination, albeit in two dimensions, with the data sets provided. Exercises for students can be found in the book, and solutions are available to instructors.

Fundamentals of Powder Diffraction and Structural Characterization of Materials

Springer Science & Business Media Requires no prior knowledge of the subject, but is comprehensive and detailed making it useful for both the novice and experienced user of the powder diffraction method. Useful for any scientific or engineering background, where precise structural information is required. Comprehensively describes the state-of-the-

art in structure determination from powder diffraction data both theoretically and practically using multiple examples of varying complexity. Pays particular attention to the utilization of Internet resources, especially the well-tested and freely available computer codes designed for processing of powder diffraction data.

Structure Determination and Refinement from Powder Diffraction Data

Crystal Structure Determination from Powder Diffraction

Amer Crystallographic Assn

Powder Diffraction

The Rietveld Method and the Two Stage Method to Determine and Refine Crystal Structures from Powder Diffraction Data

Springer Science & Business Media Crystal structure analysis from powder diffraction data has attracted considerable and ever growing interest in the last decades. X-ray powder diffraction is best known for phase analysis (Hanawalt files) dating back to the 30s. In the late 60s the inherent potential of powder diffraction for crystallographic problems was realized and scientists developed methods for using powder diffraction data at first only for the refinement of crystal structures. With the development of ever growing computer power profile fitting and pattern decomposition allowed to extract individual intensities from overlapping diffraction peaks opening the way to many other applications, especially to ab initio structure determination. Powder diffraction today is used in X-ray and neutron

diffraction, where it is a powerful method in neutron diffraction for the determination of magnetic structures. In the last decade the interest has dramatically improved. There is hardly any field of crystallography where the Rietveld, or full pattern method has not been tried with quantitative phase analysis the most important recent application.

Structure Determination by X-Ray Crystallography

Springer Science & Business Media Crystallography may be described as the science of the structure of materi als, using this word in its widest sense, and its ramifications are apparent over a broad front of current scientific endeavor. It is not surprising, therefore, to find that most universities offer some aspects of crystallography in their undergraduate courses in the physical sciences. It is the principal aim of this book to present an introduction to structure determination by X-ray crystal lography that is appropriate mainly to both final-year undergraduate studies in crystallography, chemistry, and chemical physics, and introductory post graduate work in this area of crystallography. We believe that the book will be of interest in other disciplines, such as physics, metallurgy, biochemistry, and geology, where crystallography has an important part to play. In the space of one book, it is not possible either to cover all aspects of crystallography or to treat all the subject matter completely rigorously. In particular, certain mathematical results are assumed in order that their applications may be discussed. At the end of each chapter, a short bibliog raphy is given, which may be used to extend the scope of the treatment given here. In addition, reference is made in the text to specific sources of information. We have chosen not to discuss experimental methods extensively, as we consider that this aspect of crystallography is best learned through practical experience, but an attempt has been made to simulate the interpretive side of experimental crystallography in both examples and exercises.

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determination from powder diffraction data both theoretically and practically using multiple examples of varying complexity. Pays particular attention to the utilization of Internet resources, especially the well-tested and freely available computer codes designed for processing of powder diffraction data.

Powder Diffraction

DIANE Publishing

VII. Workshop Powder Diffraction

Structure Determination and Refinement from Powder Diffraction Data

The Determination Af Accurate Intensities from Powder Diffraction Data and Their Use in Direct Methods

Structure Determination

Structure Envelopes and Their Application in Structure

Determination from Powder Diffraction Data

Enhanced Structure Determination from Powder Diffraction Data Via Algorithm Optimisation and the Use of Conformational Information

Pushing the Limits of Structure Determination from Powder Diffraction Data Using Global Optimisation and DFT-D

The Determination of Accurate Intensities from Powder Diffraction Data and Their Use in Direct Methods Structure Determination

Enhancing and Accelerating Computational Methods of Crystal Structure Determination from Powder Diffraction Data

Was kosten Planungsleistungen?

Kalkulieren - aber richtig!

Ab Initio Structure Determination from X-ray Powder Diffraction Data

Structure Determination of Fe(II) Spin-crossover Complexes from Powder Diffraction Data with Direct-space Methods

Structure Determination of Melamine Phosphates from Powder Diffraction Data with a New Direct-space Approach

X-Ray Diffraction Crystallography

Introduction, Examples and Solved Problems

Springer Science & Business Media X-ray diffraction crystallography for powder samples is a well-established and widely used method. It is applied to materials characterization to reveal the atomic scale structure of various substances in a variety of states. The book deals with fundamental properties of X-rays, geometry analysis of crystals, X-ray scattering and diffraction in polycrystalline samples and its application to the determination of the crystal structure. The reciprocal lattice and integrated diffraction intensity from crystals and symmetry analysis of crystals are explained. To learn the method of X-ray diffraction crystallography well and to be able to cope with the given subject, a certain number of exercises is presented in the book to calculate specific values for typical examples. This is particularly important for beginners in X-ray diffraction crystallography. One aim of this book is to offer guidance to solving the problems of 90 typical substances. For further convenience, 100 supplementary exercises are also provided with solutions. Some essential points with basic equations are summarized in each chapter, together with some relevant physical constants and the atomic scattering factors of the elements.

Fundamental Studies and Applications of Structure

Determination of Organic Materials from Powder X-ray Diffraction Data

Development of Novel Evolutionary Algorithms for Crystal Structure Determination from Powder Diffraction Data

Determination of Molecular Crystal Structures from Powder Diffraction Data

Crystal Structure Analysis

Principles and Practice

Oxford University Press 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.

Uniting Electron Crystallography and Powder Diffraction

Springer The polycrystalline and nanocrystalline states play an increasingly important role in exploiting the properties of materials, encompassing applications as diverse as pharmaceuticals, catalysts, solar cells and energy storage. A knowledge of the three-dimensional atomic and molecular structure of materials is essential for understanding and controlling their properties, yet traditional single-crystal X-ray diffraction methods lose their power when only polycrystalline and nanocrystalline samples are available. It is here that powder diffraction and single-crystal electron diffraction techniques take over, substantially extending the range of applicability of the crystallographic principles of structure determination. This volume, a collection of teaching contributions presented at the Crystallographic Course in Erice in 2011, clearly describes the fundamentals and the state-of-the-art of powder diffraction and electron diffraction methods in materials characterisation, encompassing a diverse range of disciplines and materials stretching from archeometry to zeolites. As such, it is a comprehensive and valuable resource for those wishing to gain an understanding of the broad applicability of these two rapidly developing fields.

The Complementary Use of Theoretical Structure Prediction and X-ray Powder Diffraction Data in Crystal Structure Determination

The successful prediction of the crystal structure and symmetry of a material can give valuable insight into many of its properties, as well as the feasibility of thermodynamically stable poly-morphs to exist. It is not uncommon, however, for numerous theoretical structures to be found within a narrow energy range, making absolute characterisation of the crystal structure impossi-ble. The aim of this project was to investigate a number of structures from this scenario, high-lighting the key differences between three potential methods for the automated comparison of predicted and experimental crystal structures. This work was carried out by comparing the simulated powder diffraction patterns of theoretical predicted crystal structures of small organic materials with their experimental powder diffraction patterns,

so that the experimentally identified structure could be automatically singled out from the many calculated. The use of traditional agreement factors (eg. Rwp) was compared with more sophisticated approaches namely PolySNAP, which uses principal-component analysis, and Compare.x, an algorithm based on weighted cross-correlation. Five structures were analysed, two of which had not been previously characterised. As the structure prediction calculations are carried out at 0K, and experimental data were collected over a range of temperatures (10K-293K), the effect of the resulting variations in lattice parameters on the automated processes is discussed. In all cases, Rwp has proven to be a poor and unreliable discriminator in the comparison of pre-dicted and experimental structures. The more contemporary methods based on PolySNAP and Compare.x both gave encouraging results when used to study the three known structures imida-zole, chlorothalonil and 5-azauracil, and they have consequently been used in the successful so-lution of the two previously unknown structures adenine and guanine. A difference in sensitivity in the matching of data collected at different te.

The Complementary Use of Theoretical Structure Prediction and X-ray Powder Diffraction Data in Crystal Structure Determination

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Crystal Structure Determination

Springer Science & Business Media A concise introduction to modern crystal structure determination, emphasizing both the crystallographic background and the successive practical steps. In the theoretical sections, more importance is attached to a good understanding, than to a rigorous mathematical treatment. The most important measuring techniques, including the use of modern area detectors, and the methods of data reduction, structure solution and refinement are discussed from a practical point of view. Special emphasis is put on the ability to recognize and avoid possible errors and traps, and to judge the quality of results.

The Determination of Accurate Intensities from Powder Diffraction Data and Their Use in Direct Methods

Structure Determination

Collection of Simulated XRD Powder Patterns for Zeolites

Fifth (5th) Revised Edition

Elsevier This 5th edition of the Zeolite Powder Pattern Collection contains calculated patterns of 218 zeolite materials representing 174 framework topologies. The almost exponential growth of new zeolite topologies reflects the continued success of zeolite synthesis researchers in producing novel materials. Collection of Simulated XRD Powder Patterns for Zeolites includes materials of interest to zeolite scientists following the policies established at recent IZA conferences. The materials included have corner-sharing tetrahedral frameworks with no restrictions on chemical composition. Covers an increase of 41 new topologies since the 4th edition in 2001 Data collected from diverse literature sources Represents an extensive compilation of data

Organic Molecular Solids

Properties and Applications

CRC Press Interest in organic molecular solids extends to a range of fields including chemistry, physics, electrical engineering, and materials science. In chemistry, it applies to such topics as solid state reactivity, crystal engineering, theoretical approaches to crystal structure determination, and morphology control. In physics, electrical engineering, and materials science, the possibility of producing organic-based materials (such as crystals, polymers, thin films, or liquid crystals) with potential electronic, opto-electronic, and magnetic uses is a major area of current research interest throughout the world. Organic Molecular Solids examines the uses of organic-based materials over a wide range of applications and interests. Each chapter surveys a relevant topic, providing appropriate introductory background information and modern developments.

Advanced X-ray Crystallography

Springer Science & Business Media Computational Studies of Crystal Structure and Bonding, by Angelo Gavezzotti Cryo-Crystallography: Diffraction at Low Temperature and More, by Piero Macchi High-Pressure Crystallography, by Malcolm I. McMahon Chemical X-Ray Photodiffraction: Principles, Examples, and Perspectives, by Panče Naumov

Powder Diffraction Crystallography of Molecular Solids, by Kenneth D. M. Harris

Bond Valences

Springer The series Structure and Bonding publishes critical reviews on topics of research concerned with chemical structure and bonding. The scope of the series spans the entire Periodic Table and addresses structure and bonding issues associated with all of the elements. It also focuses attention on new and developing areas of modern structural and theoretical chemistry such as nanostructures, molecular electronics, designed molecular solids, surfaces, metal clusters and supramolecular structures. Physical and spectroscopic techniques used to determine, examine and model structures fall within the purview of Structure and Bonding to the extent that the focus is on the scientific results obtained and not on specialist information concerning the techniques themselves. Issues associated with the development of bonding models and generalizations that illuminate the reactivity pathways and rates of chemical processes are also relevant. The individual volumes in the series are thematic. The goal of each volume is to give the reader, whether at a university or in industry, a comprehensive overview of an area where new insights are emerging that are of interest to a larger scientific audience. Thus each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years should be presented using selected examples to illustrate the principles discussed. A description of the physical basis of the experimental techniques that have been used to provide the primary data may also be appropriate, if it has not been covered in detail elsewhere. The coverage need not be exhaustive in data, but should rather be conceptual, concentrating on the new principles being developed that will allow the reader, who is not a specialist in the area covered, to understand the data presented. Discussion of possible future research directions in the area is welcomed. Review articles for the individual volumes are invited by the volume editors.

NMR Crystallography

John Wiley & Sons The content of this volume has been added toeMagRes (formerly Encyclopedia of MagneticResonance) - the ahref="http://onlinelibrary.wiley.com/book/10.1002/9780470034590/homepage/rf_coils_virtual_issue.htm?cm=on-chem&cs=chem-analytic&cu=sitename-ln&cd=sitename-ln-MRIgroup-VI" target="_blank"ultimate online resource for NMR

and MRI/a. The term "NMR Crystallography" has only recently come intocommon usage, and even now causes raised eyebrows within some partsof the diffraction community. The power of solid-state NMR to givecrystallographic information has considerably increased since theCPMAS suite of techniques was introduced in 1976. In the firstyears of the 21st century, the ability of NMR to provideinformation to support and facilitate the analysis ofsingle-crystal and powder diffraction patterns has become widelyaccepted. Indeed, NMR can now be used to refine diffraction resultsand, in favorable cases, to solve crystal structures with minimal(or even no) diffraction data. The increasing ability to relatechemical shifts (including the tensor components) to thecrystallographic location of relevant atoms in the unit cell viacomputational methods has added significantly to the practice ofNMR crystallography. Diffraction experts will increasingly welcomeNMR as an allied technique in their structural analyses. Indeed, itmay be that in the future crystal structures will be determined bysimultaneously fitting diffraction patterns and NMR spectra. This Handbook is organised into six sections. The first containsan overview and some articles on fundamental NMR topics, followedby a section concentrating on chemical shifts, and one on couplinginteractions. The fourth section contains articles describing howNMR results relate to fundamental crystallography concepts and todiffraction methods. The fifth section concerns specific aspects ofstructure, such as hydrogen bonding. Finally, four articles in thesixth section give applications of NMR crystallography tostructural biology, organic & pharmaceutical chemistry,inorganic & materials chemistry, and geochemistry. About EMR Handbooks / eMagResHandbooks The Encyclopedia of Magnetic Resonance (up to 2012) andeMagRes (from 2013 onward) publish a wide range of onlinearticles on all aspects of magnetic resonance in physics,chemistry, biology and medicine. The existence of this large numberof articles, written by experts in various fields, is enabling thepublication of a series of EMR Handbooks / eMagResHandbooks on specific areas of NMR and MRI. Thechapters of each of these handbooks will comprise a carefullychosen selection of articles from eMagRes. In consultationwith the eMagRes Editorial Board, the EMRHandbooks / eMagRes Handbooks are coherentlyplanned in advance by specially-selected Editors, and new articlesare written (together with updates of some already existingarticles) to give appropriate complete coverage. The handbooks areintended to be of value and interest to research students,postdoctoral fellows and other researchers learning about thescientific area in question and undertaking relevant experiments,whether in academia or industry. Have the content of this Handbook and the complete content ofeMagRes at your fingertips! Visit:
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