



Crystallographically Determined Structure

Uri Shmueli



Crystallographically Determined Structure:

Structure Determination by X-ray Crystallography Mark Ladd, Rex Palmer, 2014-07-08 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

Electron Crystallography Xiaodong Zou, Sven Hovmöller, Peter Oleynikov, 2011-08-18 In the modern world of ever smaller devices and nanotechnology electron crystallography emerges as the most important method capable of determining the structure of minute objects down to the size of individual atoms Crystals of only a few millionths of a millimetre are studied This is the first textbook explaining how this is done Great attention is given to symmetry in crystals and how it manifests itself in electron microscopy and electron diffraction and how this symmetry can be determined and taken advantage of in achieving improved electron microscopy images and solving crystal structures from electron diffraction patterns Theory and practice are combined experimental images diffraction patterns formulae and numerical data are discussed in parallel giving the reader a complete understanding of what goes on inside the black boxes of computer programs This up to date textbook contains the newest techniques in electron crystallography including detailed descriptions and explanations of the recent remarkable successes in determining the very complex structures of zeolites and intermetallics The controversial issue of whether there is phase information present in electron microscopy images or not is also resolved once and for all The extensive appendices include computer labs which have been used at various courses at Stockholm University and international schools in electron crystallography with applications to the textbook Students can download image processing programs and follow these lab instructions to get a hands on experience of electron crystallography

Comprehensive Coordination Chemistry II J. A. McCleverty, T.J. Meyer, 2003-12-03 Comprehensive

Coordination Chemistry II CCC II is the sequel to what has become a classic in the field Comprehensive Coordination Chemistry published in 1987 CCC II builds on the first and surveys new developments authoritatively in over 200 newly commissioned chapters with an emphasis on current trends in biology materials science and other areas of contemporary scientific interest

Data Mining in Crystallography D. W. M. Hofmann, Liudmila N. Kuleshova, 2009-11-26 Humans have been manually extracting patterns from data for centuries but the increasing volume of data in modern times has called for more automatic approaches Early methods of identifying patterns in data include Bayes theorem 1700s and Regression analysis 1800s The proliferation ubiquity and increasing power of computer technology has increased data collection and storage As data sets have grown in size and complexity direct hands on data analysis has increasingly been augmented with indirect automatic data processing Data mining has been developed as the tool for extracting hidden patterns from data by using computing power and applying new techniques and methodologies for knowledge discovery This has been aided by other discoveries in computer science such as Neural networks Clustering Genetic algorithms 1950s Decision trees 1960s and Support vector machines 1980s Data mining commonly involves four classes of tasks Classification Arranges the data into predefined groups For example an e mail program might attempt to classify an e mail as legitimate or spam Common algorithms include Nearest neighbor Naive Bayes classifier and Neural network Clustering Is like classification but the groups are not predefined so the algorithm will try to group similar items together Regression Attempts to find a function which models the data with the least error A common method is to use Genetic Programming Association rule learning Searches for relationships between variables For example a supermarket might gather data of what each customer buys

The Crystalline State: The determination of crystal structures, by H. Lipson and W. Cochran Sir William Lawrence Bragg, 1876 A Survey of Existing Crystal Structures Data Ralph Walter Graystone Wyckoff, 1923 Theories and Techniques of Crystal Structure Determination Uri Shmueli, 2007-06-07 This concise book is for chemists material scientists and physicists who deal with description of crystalline matter and the determination of its structure and would like to gain more understanding of the principles involved The main purpose of the book is to introduce the reader to principles of crystallographic symmetry to discuss some traditional as well as modern experimental techniques to formulate the phase problem of crystallography and present in some detail the methods for its indirect and direct solution which are indispensable for further work The book also contains discussions of structure factor statistics of value for resolving space group ambiguities and atomic displacement parameters which form an inseparable part of the structure A discussion of the refinement of structural parameters conventional constrained and restrained concludes the book Derivations are as far as possible self contained and wherever mathematical detail might disrupt the line of reasoning the reader is referred to one of four appendices present in the book The book is of course valuable for students of crystallography at a graduate and upper undergraduate level No previous course on crystallography is a prerequisite for graduates in the above fields

Contemporary Boron Chemistry Matthew Davidson, 2000 The continued and evolving significance of boron chemistry to the wider chemical community is demonstrated by the international and interdisciplinary nature of the research reported in this book Contemporary Boron Chemistry encompasses inorganic and organic compounds as well as polymers solid state materials medicinal aspects and theoretical studies Covering many areas of chemistry with boron at its centre topics include applications to polyolefin catalysis medicine materials and polymers boron cluster chemistry including carboranes and metal containing clusters organic and inorganic chemistry of species containing only 1 or 2 boron atoms and theoretical studies of boron containing compounds New materials with novel optical and electronic properties are also discussed Comprehensive and up to date graduates and researchers in a wide range of fields particularly those in organometallic and organic chemistry and materials science will welcome this book

International Tables for Crystallography, Volume H Christopher J. Gilmore, James A. Kaduk, Henk Schenk, 2019-09-16 Die Pulverdiffraktion ist in der Kristallographie die am weitesten verbreitete Methode Die Anwendungen umfassen sämtliche Bereiche der Strukturwissenschaften Dieser neue Band aus der Reihe International Tables deckt alle Aspekte des Verfahrens in über 50 Kapiteln ab Autoren sind Experten des Fachgebiets Dieser Band umfasst sieben Teile mit folgenden Inhalten Überblick über die Prinzipien der Pulverdiffraktion Erläuterung der bei der Pulverdiffraktion eingesetzten Strahlungsquellen Instrumente und Ausrüstung Einsatz unterschiedlicher Probenumgebungen und Methoden der Probenvorbereitung Information zu Methoden einschließlich Datenverarbeitung Indexierung und Reduktion Whole Pattern Modellierung und quantitative Analyse sowie Überblick über die relevanten Datenbanken der Kristallographie Fokus auf Strukturbestimmung einschließlich Methoden im realen und reziproken Raum sowie Methode der maximalen Entropie Strukturverfeinerung und Strukturvalidierung Erläuterung von Defekten Textur Mikrostruktur und Fasern einschließlich Belastung und Beanspruchung Domänen und Dünnschicht Untersuchung der für die Pulverdiffraktion verfügbaren Software Beschreibung der Anwendungsmöglichkeiten in vielen wichtigen Bereichen Industrie und Wissenschaften einschließlich Makromoleküle Mineralien Keramik Zement Polymere Forensik Archäologie und Pharmazeutika sowie Erklärung von Theorie und Anwendungen Band H ist das wichtigste Referenzwerk für alle die im Bereich Pulverdiffraktion tätig sind ob Anfänger und erfahrener Praktiker wurde für die Praxis entwickelt ohne Sorgfalt und Genauigkeit zu vernachlässigen Die Methode der Pulverdiffraktion wird anhand vieler Beispiele ausführlich behandelt Die Beispieldaten stehen teilweise als Download zur Verfügung

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