

WORLD SCIENTIFIC Crystal Structure Analysis 426

# Crystal Structure Analysis

## Principles and Practice

W. CLEGG, A. J. BEANE  
R. D. GOWLEN, B. MANN

Edited by W. CLEGG



WILEY

# Crystal Structure Analysis

**AW Chickering**



## Crystal Structure Analysis:

*Crystal Structure Analysis* Alexander J Blake, Jacqueline M Cole, John S O Evans, Peter Main, Simon Parsons, David J Watkin, 2009-06-18 This text focuses on the practical aspects of crystal structure analysis and provides the necessary conceptual framework for understanding and applying the technique By choosing an approach that does not put too much emphasis on the mathematics involved the book gives practical advice on topics such as growing crystals solving and refining structures and understanding and using the results The technique described is a core experimental method in modern structural chemistry and plays an ever more important role in the careers of graduate students postdoctoral and academic staff in chemistry and final year undergraduates Much of the material of the first edition has been significantly updated and expanded and some new topics have been added The approach to several of the topics has changed reflecting the book's new authorship and recent developments in the subject

*Crystal Structure Analysis* Jenny Pickworth Glusker, Kenneth N. Trueblood, 2010-05-27 This book aims to explain how and why the detailed three dimensional architecture of molecules can be determined by an analysis of the diffraction patterns obtained when X rays or neutrons are scattered by the atoms in single crystals Part 1 deals with the nature of the crystalline state diffraction generally and diffraction by crystals in particular and briefly the experimental procedures that are used Part II examines the problem of converting the experimentally obtained data into a model of the atomic arrangement that scattered these beams Part III is concerned with the techniques for refining the approximate structure to the degree warranted by the experimental data It also describes the many types of information that can be learned by modern crystal structure analysis There is a glossary of terms used and several appendixes to which most of the mathematical details have been relegated

*Crystal-structure Analysis* Martin Julian Buerger, 1980

*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 biochemists 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

**Crystal Structure Analysis** William Clegg, 2009 This text focuses on the practical aspects of crystal structure analysis and provides the necessary conceptual framework for understanding and applying the technique By choosing an approach that does not put

too much emphasis on the mathematics involved the book gives practical advice on topics such as growing crystals solving and refining structures and understanding and using the results The technique described is a core experimental method in modern structural chemistry and plays an ever more important role in the careers of graduate students postdoctoral and academic staff in chemistry and final year undergraduates Much of the material of the first edition has been significantly updated and expanded and some new topics have been added The approach to several of the topics has changed reflecting the book's new authorship and recent developments in the subject

Crystal Structure Analysis Using the "superposition"- and "complementary"-structures Ernst Höhne, Leo Kutschabsky, 1981

X-ray Analysis and the Structure of Organic Molecules Jack D. Dunitz, 1995 This book is the second corrected reprint of *2X Ray Analysis 2* published in 1979 and consists of two parts Part one is about Crystal Structure Analysis part two deals with Molecular Structure All the information in this volume is of considerable value especially to those engaged in or about to embark upon X ray crystal structure analysis

Crystal-structure analysis, 1980 *Crystal Structure Analysis for Chemists and Biologists* Jenny Pickworth Glusker, Mitchell Lewis, Miriam Rossi, 1994

**The Theory of Crystal Structure Analysis** A. Kitaigorodskii, 2012-12-06

Structure analysis is based on the phenomena of the diffraction of radiation by materials In the first ten to twenty years after Laue's discovery a very complete theory was developed for the diffraction of x rays and later of electrons This theory led to equations by means of which it was possible to compute the intensity pattern for a given structure The theory of structure analysis came to mean that of the diffraction of radiation In 1935 Patterson pointed out a way leading to the solution of the inverse problem the finding of the structure from a given intensity distribution pattern At first the conservatism of researchers and then the war hampered the development and broad application of the ideas set forth in this work It was only during the last ten years that all the rich possibilities of the Patterson method the method of the analysis of the convolution of the electron density were brought to light and applied in practice

**Theory of Crystal Structure Analysis** Aleksandr Isaakovich Kitaigorodskii, 1961-03

**The Roots of Crystal Structure Analysis** Talal Atif Debs, 1993

Modern X-Ray Analysis on Single Crystals Peter Luger, 2014-04-01 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

*Theætheorie of Crystal Structure Analysis* Aleksandr Isaakovic Kitajgorodskii, 1961

The theory crystal structure analysis Aleksandr I. Kitajgorodskij, 1966

**Crystal Structure Analysis** Jenny Pickworth Glusker, Kenneth N.

Trueblood,2010-05-27 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 *A Semi-expert System for Crystal Structure Analysis* Cooper Richard Ian,2000 **Crystal Structure Analysis Using the Superposition and Complementary Structures** , The International Union of Crystallography presents the teaching pamphlet Crystal Structure Analysis Using the Superposition and Complementary Structures by Ernst Hohne and Leo Kutschabsky The pamphlet is sponsored by the Commission on Crystallographic Teaching and published by University College Cardiff Press The pamphlet covers special methods linear structure factor equations the application of direct methods to centrosymmetric structures containing heavy atoms and the steps of structure determination *Numerical Methods in Crystal Structure Analysis* L. I. Hodgson,1963 *The Essence Of Crystallography* Mark Ladd,2019-11-19 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 Physics Designed 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

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