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Fundamentals and Applications

Carmelo Giacovazzo

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Direct Phasing In Crystallography Fundamentals And Applications

Uri Shmueli, Professor of Chemistry Uri Shmueli



Direct Phasing In Crystallography Fundamentals And Applications:

Direct Phasing in Crystallography Carmelo Giacovazzo, 1998 Direct methods are at present applied to a large variety of cases X ray neutron or electron data single crystal and powder data small molecules and macromolecules While direct methods solved in practice the phase problem for small molecules their application to macromolecules is recent and still undergoing strong development The fundamentals of the methods are described in particular it is shown how the methods can be optimized for powder neutron or electron data and how they can be integrated with isomorphous replacement molecular replacement and anomalous dispersion techniques Maximum Entropy methods are also described and discussed Sets of test structures are used to verify throughout the various chapters the mathematical techniques there described and to provide practical examples of applications This book will appeal to a wide variety of readers offering both a comprehensive description of direct methods in crystallography and an invaluable reference tool The first three chapters can be considered as an introduction to the field with sufficient material to constitute a university course and for allowing the expert use of most direct methods programs Subsequent chapters are aimed at graduate students and working crystallographers Basic results are described and discussed in the main body of the text while the appendices complement these with in depth mathematical details The quoted literature is extremely wide and the interested reader can find suggestions for future work and further reading throughout the book *Electron Crystallography* Thomas E. Weirich, Xiaodong Zou, 2006 **Theories and Techniques of Crystal Structure Determination** Uri Shmueli, Professor of Chemistry Uri Shmueli, 2007-06-07 The book is a detailed but concise exposition of crystal structure determination at a graduate level Discussions range from geometrical principles of crystallography through relevant experimental methods to techniques of reliable and accurate determination of crystal structures **Surface Structure Determination by LEED and X-rays** Wolfgang Moritz, Michel A. Van Hove, 2022-08-25 This timely text covers the theory and practice of surface and nanostructure determination by low energy electron diffraction LEED and surface X ray diffraction SXRD it is the first book on such quantitative structure analysis in over 30 years It provides a detailed description of the theory including cutting edge developments and tested experimental methods The focus is on quantitative techniques while the qualitative interpretation of the LEED pattern without quantitative I V analysis is also included Topics covered include the future study of nanoparticles quasicrystals thermal parameters disorder and modulations of surfaces with LEED with introductory sections enabling the non specialist to follow all the concepts and applications discussed With numerous colour figures throughout this text is ideal for undergraduate and graduate students and researchers whether experimentalists or theorists in the fields of surface science nanoscience and related technologies It can serve as a textbook for graduate level courses of one or two semesters *Protected Metal Clusters: From Fundamentals to Applications*, 2015-09-06 Protected Metal Clusters From Fundamentals to Applications surveys the fundamental concepts and potential applications of atomically precise metal clusters protected by

organic ligands As this class of materials is now emerging as a result of breakthroughs in synthesis and characterization that have taken place over the last few years the book provides the first reference with a focus on these exciting novel nanomaterials explaining their formation and how and why they play an important role in the future of molecular electronics catalysis sensing biological imaging and medical diagnosis and therapy Surveys the fundamental concepts and potential applications of atomically precise metal clusters protected by organic ligands Provides well organized tutorial style chapters that are ideal for teaching and self study In depth descriptions by top scientists in the field Presents the state of the art of protected metal clusters and their future prospects

Metal Organic Frameworks as Heterogeneous Catalysts

Francesc X. Llabrés i Xamena, Jorge Gascon (Profesor), 2013-07-01 This book examines the latest research and discovery in the use of MOFs in catalysis highlighting the extent to which these materials have been embraced by the community

The Weak Hydrogen Bond Gautam R. Desiraju, Thomas Steiner, 2001 The weak or non conventional hydrogen bond has been subject of intense scrutiny over recent years in several fields in particular in structural chemistry structural biology and also in the pharmaceutical sciences There is today a large body of experimental and theoretical evidence confirming that hydrogen bonds like C H O N H π C H π and even bonds like O H metal play distinctive roles in molecular recognition guiding molecular association and in determining molecular and supramolecular architectures The relevant compound classes include organometallic complexes organic and bio organic systems and also DNA and proteins The book provides a comprehensive assessment of this interaction type and is of interest to all those interested in structural and supramolecular science including fields as crystal engineering and drug design

Comprehensive Supramolecular Chemistry II

George W. Gokel, Len Barbour, 2017-06-22 Comprehensive Supramolecular Chemistry II Second Edition Nine Volume Set is a one stop shop that covers supramolecular chemistry a field that originated from the work of researchers in organic inorganic and physical chemistry with some biological influence The original edition was structured to reflect in part the origin of the field However in the past two decades the field has changed a great deal as reflected in this new work that covers the general principles of supramolecular chemistry and molecular recognition experimental and computational methods in supramolecular chemistry supramolecular receptors dynamic supramolecular chemistry supramolecular engineering crystallographic engineered assemblies sensors imaging agents devices and the latest in nanotechnology Each section begins with an introduction by an expert in the field who offers an initial perspective on the development of the field Each article begins with outlining basic concepts before moving on to more advanced material Contains content that begins with the basics before moving on to more complex concepts making it suitable for advanced undergraduates as well as academic researchers Focuses on application of the theory in practice with particular focus on areas that have gained increasing importance in the 21st century including nanomedicine nanotechnology and medicinal chemistry Fully rewritten to make a completely up to date reference work that covers all the major advances that have taken place since the First Edition

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 through relevant examples and without relying on complex mathematics that the basic ideas behind crystallography and
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