

# Reactivity of Molecular Solids

Edited by  
**Elena Boldyreva** and  
**Vladimir Boldyrev**



THE MOLECULAR SOLID STATE

# Reactivity Of Molecular Solids

**Kari Rissanen**



## Reactivity Of Molecular Solids:

Reactivity of Molecular Solids Elena Boldyreva, Vladimir Boldyrev, 1999-10-18 Reporting on advances in the field of molecular solid state chemistry each volume focuses on selected areas and highlights methods and results in syntheses properties and applications The volumes in this series provide a forum for the discussion of chemical physical biological and crystallographic aspects of the molecular solid state Eight chapters focus on the theoretical aspects of the reactivity of solids and the applications that are of practical importance In a collection of reviews that highlight hot topics in the field of molecular solids the authors of this volume emphasise the problems facing them Contents Interplay between Intra and Intermolecular Interactions in Solid State Reactions Cooperative Effects in Solid State Reactions Some Aspects of Bimolecular Photoreactions in Crystals Kinetics and Spatial Propagation of Intramolecular Reactions in Solids Kinetic Descriptions of the Simplest Bimolecular Reactions in Organic Solids Radical Solid State Reactions at High Pressure Polymorphs and Solvates of Molecular Solids in the Pharmaceutical Industry Mechanochemical Synthesis and Mechanical Activation of Drugs Reactivity of Molecular Solids will be of interest to all chemists working in the pharmaceutical fine chemicals and food industries and also in molecular electronics and materials science **Organic Molecular Solids**

William Jones, 2019-09-17 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

*Reactivity in Molecular Crystals* Yuji Ohashi, 2008-09-26 Do you need to design syntheses that are highly selective fast enantioselective with quantitative enantiomeric yield This book describes in detail how best to exploit the enormous synthetic potential of solid state reactions Written by leading experts it provides in depth information on the theoretical and physico chemical approach to solid state reactions solid to solid organic reactions stereoselective solid state photoreactions reactivity and crystal structure An ideal companion to Dunitz and Brgi's Structure Correlation this book will be highly useful to synthetic organic chemists stereochemists crystallographers and solid state chemists *Organic Solid-State Reactions* Fumio Toda, 2013-03-14 Most organic reactions have long been carried out in organic solvents without concern for their real necessity reaction efficiency and pollution problems Very recently we have found that most organic reactions can be carried out in the absence of a solvent namely in the solid state In many cases the solid state reaction proceeds more easily and efficiently and even more selectively than solution reaction This shows that molecules move easily and selectively in the solid

state This finding changed the classical idea which suggests molecules do not move and reactions do not occur in the solid state and opened up a new research field for the study molecular dynamics in the solid state The organic solid state reactions have many possibilities to be developed For example enantioselective reactions can easily be accomplished by carrying out the reaction in an inclusion complex crystal with an optically active host compound Catalytic reactions also proceed in the solid state Moreover the solid state reactions are more economical and ecologically sound In the future pollution free synthetic procedures in the solid state will become increasingly important not only in chemical industries but also in university laboratories

**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 published in 1996

**Controlling Reactivity in Molecular Solids Using Linear Templates** Dushyant Brajendra Varshney, 2005 *New Directions in Solid State Chemistry* C. N. R. Rao, J. Gopalakrishnan, 1997-02-28 In the new edition of this widely praised textbook all the chapters have been revised and the authors have brought the work completely up to date by the addition of new material on numerous topics In recent years solid state chemistry has emerged as a very important element of mainstream chemistry and materials science Students teachers and researchers need to understand the chemistry of solids because of the crucial role this plays in determining the properties of materials An understanding of solid state chemistry is also essential in materials design and many fascinating relationships between the structure and properties of solids have been discovered by chemists This text requires only an understanding of basic physics chemistry and crystallography and is enhanced with the most recent examples case studies and references It will be of value to advanced students and researchers studying solid state chemistry and materials science as a text and reference work

**Hot Topics in Crystal Engineering** Kari Rissanen, 2021-08-24 Hot

Topics in Crystal Engineering covers the design and synthesis of single crystalline solid state materials their properties and applications focusing on the understanding and use of intermolecular interactions that constitute single crystalline materials Many of the most modern materials such as metal organic frameworks MOFs capable of gas storage and separation and selective entrapment of harmful substances are the result of the rational use of crystal engineering Topics covered in this work highlight breakthroughs in this rapidly developing field This work offers a carefully chosen cross section of the latest developments some in their early infancy and some covered for the first time Provides comprehensive and authoritative articles giving readers access to a wealth of information to fully support their research and activities Covers the latest developments in crystal engineering including topics which are in their early infancy Written by leading international experts

Chemical Reactivity Savaş Kaya,Laszlo von Szentpaly,Goncagul Serdaroglu,Lei Guo,2023-05-15 The growth of technology for chemical assessment has led to great developments in the investigation of chemical reactivity in recent years but key information is often dispersed across many different research fields Exploring both traditional and advanced methods Chemical Reactivity Volume 2 Approaches and Applications present the latest approaches and strategies for the computational assessment of chemical reactivity Following an insightful introduction the book begins with an overview of conformer searching techniques before progressing to explore numerous different techniques and methods including confined environments quantum similarity descriptors volume based thermodynamics and polarizability A unified approach to the rules of aromaticity is followed by methods for assessing interaction energies and the role of electron density for varied different analyses Algorithms for conformer searching partitioning and a whole range of quantum chemical methods are also discussed Consolidating the knowledge of a global team of experts in the field Chemical Reactivity Volume 2 Approaches and Applications is a useful resource for both students and researchers interested in applying and refining their use of the latest approaches for assessing chemical reactivity in their own work Compiles a broad range of contemporary methods and approaches for reactivity and structure prediction Highlights the application of chemical reactivity strategies for the investigation of such areas as aromaticity halogen bonds and electronic materials Includes discussion of computational tools for exploring molecular spaces from different angles including interaction energies quantum similarity and electron density

**High-Pressure Crystallography** Elena Boldyreva,Przemyslaw Dera,2010-08-20 This unique book is devoted to the theme of crystallographic studies at high pressure It places emphasis on the phenomena characteristic to the compressed state of matter as well as experimental and theoretical techniques used to study these phenomena Chemistry James N. Spencer,George M. Bodner,Lyman H. Rickard,2010-12-28 CHEMISTRY Encyclopedia of Supramolecular Chemistry J. L. Atwood,Jonathan W. Steed,2004 Covers the fundamentals of supramolecular chemistry supramolecular advancements and methods in the areas of chemistry biochemistry biology environmental and materials science and engineering physics computer science and applied mathematics Grants and Awards for the Fiscal Year Ended ... National Science Foundation

(U.S.),1980      The Future of Dynamic Structural Science Judith A.K. Howard,Hazel A. Sparkes,Paul R. Raithby,Andrei V. Churakov,2014-07-08 This work focuses on complementary crystallographic and spectroscopic areas of dynamic structural science from papers presented at the 46th NATO sponsored course in Erice Sicily 2013 These papers cover a range of material from background concepts to more advanced material and represent a fully inter disciplinary collection of the latest ideas and results within the field They will appeal to practising or novice crystallographers both chemical and biological who wish to learn more about modern spectroscopic methods and convergent advances and hence vice versa for experimental and computational spectroscopists The chapters refer to the latest techniques software and results and each chapter is fully referenced The volume provides an excellent starting point for new comers in the emerging multi disciplinary area of time resolved science

**Crystal Engineering: A Textbook** Gautam R Desiraju,Jagadese J Vittal,Arunachalam Ramanan,2011-06-20 This book is important because it is the first textbook in an area that has become very popular in recent times There are around 250 research groups in crystal engineering worldwide today The subject has been researched for around 40 years but there is still no textbook at the level of senior undergraduates and beginning PhD students This book is expected to fill this gap The writing style is simple with an adequate number of exercises and problems and the diagrams are easy to understand This book consists major areas of the subject including organic crystals and co ordination polymers and can easily form the basis of a 30 to 40 lecture course for senior undergraduates

*Strength from Weakness: Structural Consequences of Weak Interactions in Molecules, Supramolecules, and Crystals* Aldo Domenicano,Istvan Hargittai,2002-06-30 Proceedings of the NATO Advanced Research Workshop on Physical Chemical Properties from Weak Interactions held in Erice Italy from 23 to 29 May 2001

EPR of Free Radicals in Solids II Anders Lund,Masaru Shiotani,2012-12-09 EPR of Free Radicals in Solids Trends in Methods and Applications 2nd ed presents a critical two volume review of the methods and applications of EPR ESR for the study of free radical processes in solids Emphasis is on the progress made in the developments in EPR technology in the application of sophisticated matrix isolation techniques and in the advancement in quantitative EPR that have occurred since the 1st edition was published Improvements have been made also at theoretical level with the development of methods based on first principles and their application to the calculation of magnetic properties as well as in spectral simulations EPR of Free Radicals in Solids II focuses on the trends in applications of experimental and theoretical methods to extract structural and dynamical properties of radicals and spin probes in solid matrices by continuous wave CW and pulsed techniques in nine chapters written by experts in the field It examines the studies involving radiation and photo induced inorganic and organic radicals in inert matrices the high spin molecules and metal based molecular clusters as well as the radical pro cesses in photosynthesis Recent advancements in environmental applications in cluding measurements by myon resonance of radicals on surfaces and by quantitative EPR in dosimetry are outlined and the applications of optical detection in material research with much increased sensitivity reviewed The potential

use of EPR in quantum computing is considered in a newly written chapter This new edition is aimed to experimentalists and theoreticians in research involving free radicals as well as for students of advanced courses in physical chemistry chemical physics materials science biophysics biochemistry and related fields *Frontiers in Crystal Engineering* Edward R. T. Tiekink, Jagadeś Vittal, 2006-05-01 Crystal engineering where the myriad of intermolecular forces operating in the solid state are employed to design new nano and functional materials is a key new technology with implications for catalysis pharmaceuticals synthesis and materials science *Frontiers in Crystal Engineering* gathers personal perspectives from international specialists working in molecular aspects of crystal engineering on the practical and theoretical challenges of the discipline and future prospects These demonstrate the approaches that are being used to tackle the problems associated with the complexity design and functionality of crystalline molecular solids Topics include how intermolecular forces direct and sustain crystal structures functional engineering and design elements coordination polymers and network structures applications in green and pharmaceutical chemistry *Frontiers in Crystal Engineering* is a useful guide to this exciting new discipline for both entrants to the field as well as established practitioners and for those working in crystallography medicinal and pharmaceutical sciences solid state chemistry and materials and nanotechnology *Thermal Decomposition of Solids and Melts* Boris V. L'vov, 2007-08-24 The appearance of this English edition of my book first published in Russian in mid 2006 is related to the help and support of two prominent scientists Professor Michael Brown Rhodes University Grahamstown South Africa and Dr Judit Simon Budapest University of Technology and Economics Hungary The story is as follows In the winter of 2006 in the process of exchange of views by email with Michael on some problems of decomposition kinetics I asked him about the possibility of publishing my book in English He suggested that I should contact Judit the Series Editor of *Hot Topics in Thermal Analysis and Calorimetry* My application was kindly accepted considered and approved As a result Judit strongly recommended this book to Springer for publication and Michael kindly agreed to help me with linguistic improvements of my hurriedly translated book In the process of editing he made some critical comments and questions which stimulated me to improve and clarify the text but we did have to agree to put our differences of scientific opinions aside so as not to delay the process Without this invaluable help this book would not be as readable as I hope it is now The author uses this opportunity to express his sincere thanks to Michael and Judit for their significant help and support Although only about a year has gone after the preparation of the original edition of the book in Russian this English version of the manuscript has undergone considerable revision These changes refer to Sections 2.2.2 *Radical and Radical Ion Reactivity in Nucleic Acid Chemistry* Michael D. Greenberg, 2009-10-05 Comprehensive coverage of radical reactive intermediates in nucleic acid chemistry and biochemistry The Wiley Series on Reactive Intermediates in Chemistry and Biology investigates reactive intermediates from the broadest possible range of disciplines The contributions in each volume offer readers fresh insights into the latest findings emerging applications and ongoing research in the field from a diverse perspective The chemistry and

biochemistry of reactive intermediates is central to organic chemistry and biochemistry and underlies a significant portion of modern synthetic chemistry Radical and Radical Ion Reactivity in Nucleic Acid Chemistry provides the only comprehensive review of the chemistry and biochemistry of nucleic acid radical intermediates With contributions by world leaders in the field the text covers a broad range of topics including A discussion of the relevant theory Ionization of DNA Nucleic acid sugar radicals Halopyrimidines Oxidative reductive and low energy electron transfer Electron affinity sensitizers Photochemical generative of reactive oxygen species Reactive nitrogen species Ene-yne rearrangements Phenoxy radicals A unique compilation on the cutting edge of our understanding Radical and Radical Ion Reactivity in Nucleic Acid Chemistry provides an unparalleled resource to student and professional researchers in such fields as organic chemistry biochemistry molecular biology and physical chemistry as well as the industries associated with these disciplines



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