

CHEMICAL TOPOLOGY

INTRODUCTION AND FUNDAMENTALS

D. BONCHEV and
D.H. ROUVRAY

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Chemical Topology Introduction And Fundamentals

Danail D. Bonchev, O.G. Mekenyan



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Chemical Topology D Bonchev,D.H Rouvray,1999-04-23 Topology is becoming increasingly important in chemistry because of its rapidly growing number of applications Here its many uses are reviewed and the authors anticipate what future developments might bring This work shows how significant new insights can be gained by representing molecular species as topological structures known as topographs The text explores carbon structures establishing how the stability of fullerene species can be accounted for and also predicting which fullerenes will be most stable It is pointed out that molecular topology rather than molecular geometry characterizes molecular shape and various tools for shape characterization are described Several of the fascinating ideas that arise from regarding topology as a unifying principle in chemical bonding theory are discussed and in particular the novel concept of the molecular topoid is shown to have numerous uses The topological description of polymers is examined and the reader is gently guided through the realms of branched and tangled polymers Overall this work outlines the fact that topology is not only a theoretical discipline but also one that has practical applications and high relevance to the whole domain of chemistry

Chemical Topology Danail Bonchev,Dennis H Rouvray,2000-07-06 Topology has been extensively applied in the study of chemically linked and knotted structures and also in the study of many biologically significant molecules such as proteins and DNA These are the themes that are addressed in this volume of the Mathematical Chemistry series The topological chirality of knotted and linked molecular species and the invariants that may characterize them are explored in detail

PHYSICAL CHEMISTRY 2016 Željko Čupić,Slobodan Anić,2016-09-26 **Advances in Molecular Similarity** R. Carbó-Dorca,P.G. Mezey,1999-02-18 This volume highlights some of the advances in molecular similarity Molecular similarity research is a dynamic field where the rapid transfer of ideas and methodologies from the theoretical quantum chemical and mathematical chemistry disciplines to efficient algorithms and computer programs used in industrially important applications is especially evident These applications often serve as motivating factors toward new advances in the fundamental and theoretical fields and the combination of intellectual challenge and practical utility provides mutual advantages to theoreticians and experimentalists The aim of this volume is to present an overview of the current methodologies of molecular similarity studies and to point out new challenges unsolved problems and areas where important new advances can be expected

Electron Localization-Delocalization Matrices Chérif F. Matta,Paul W. Ayers,Ronald Cook,2024-05-02 This book builds bridges between two yet separated branches of theoretical and mathematical chemistry Chemical Graph Theory and Electronic Structure Calculations Although either of the fields have developed their own techniques problems methods and favorite benchmark cases independent from each other the authors have managed to bring them together by using the localization delocalization matrix LDM The LDM is a novel molecular descriptor that fingerprints a molecule by condensing the complicated electronic information in one mathematically manageable object In this book the authors introduce the readers

to modeling techniques based on LDMs Their technique offers a high accuracy as well as robust predictive power often dramatically surpassing the potential of either of the constituting methods on their own In addition to the comprehensive and accessible introduction to this new field of theoretical chemistry the authors offer their self developed software free to download so that readers can try running their own simulations The described methods are very general and can easily be implemented for calculating various properties and parameters such as mosquito repelling activity ionic liquid properties local aromaticity of ring molecules log P s pKa s LD50 corrosion inhibition activities and Lewis acidities and basicities to only name a few The free downloadable software helps readers automate the analysis of the matrices described in this book and hence facilitates application of the described methodology The Development of Chemical Principles Cooper Harold Langford,Ralph Alonzo Beebe,1995-01-01 Undergraduate level text focuses on three lines of the development of contemporary chemical structural theory the classical theory of bonding in molecules the ionic interpretation of electrolyte solutions and the physical theory of atomic structure 186 illustrations 1969 edition **Conference Proceedings** Society of Plastics Engineers. Technical Conference,1983 *Progress in Quantum Chemistry Research* Erik O. Hoffman,2007 This book presents new and important research from around the world in quantum chemistry which is a branch of theoretical chemistry Quantum chemistry applies quantum mechanics and quantum field theory to address issues and problems in chemistry The description of the electronic behaviour of atoms and molecules as pertaining to their reactivity is one of the applications of quantum chemistry Quantum chemistry lies on the border between chemistry and physics and significant contributions have been made by scientists from both fields It has a strong and active overlap with the field of atomic physics and molecular physics as well as physical chemistry *Intermolecular Interactions in Crystals* Juan J Novoa,2017-10-25 The field of crystal engineering concerns the design and synthesis of molecular crystals with desired properties This requires an in depth understanding of the intermolecular interactions within crystal structures This new book brings together the latest information and theories about intermolecular bonding providing an introductory text for graduates The book is divided into three parts The first part covers the nature physical meaning and methods for identification and analysis of intermolecular bonds The second part explains the different types of bond known to occur in molecular crystals with each chapter written by a specialist in that specific bond type The final part discusses the cooperativity effects of different bond types present in one solid This comprehensive textbook will provide a valuable resource for all students and researchers in the field of crystallography materials science and supramolecular chemistry **Molecular Descriptors for Chemoinformatics** Roberto Todeschini,2009 The number one reference on the topic now contains a wealth of new data The entire relevant literature over the past six years has been painstakingly surveyed resulting in hundreds of new descriptors being added to the list and some 3 000 new references in the bibliography section Volume 1 contains an alphabetical listing of more than 3300 descriptors and related terms for chemoinformatic analysis of chemical compound properties while the second volume

lists over 6 000 references selected from 450 journals To make the data even more accessible the introductory section has been completel

30th European Symposium on Computer Aided Chemical Engineering Sauro Pierucci, Flavio Manenti, Giulia Luisa Bozzano, Davide Manca, 2020-10-23 30th European Symposium on Computer Aided Chemical Engineering Volume 47 contains the papers presented at the 30th European Symposium of Computer Aided Process Engineering ESCAPE event held in Milan Italy May 24 27 2020 It is a valuable resource for chemical engineers chemical process engineers researchers in industry and academia students and consultants for chemical industries Presents findings and discussions from the 30th European Symposium of Computer Aided Process Engineering ESCAPE event Offers a valuable resource for chemical engineers chemical process engineers researchers in industry and academia students and consultants for chemical industries

Potential Energy Hypersurfaces Paul G. Mezey, 1987 The importance of the potential surface model has led naturally to a large number of studies on the subject where the emphasis has usually been placed on lower dimensional problems such as the reaction dynamics of diatomic to four atom systems or conformational problems restricted to few internal rotations The purposes and methods of this book are however somewhat different from those of most studies on potential surface problems The emphasis here is placed on those fundamental properties of potential energy hypersurfaces that are general for higher dimensions that is for larger molecules The study of these properties requires some of the tools of global analysis that are not among the routine mathematical techniques of quantum chemists topology homotopy and homology This book provides the reader with an introduction to the fundamentals and to some of the more recent developments in the theory of potential energy hypersurfaces The text is fairly self contained It requires no previous mathematical knowledge from the reader beyond that needed in an undergraduate quantum chemistry course

Molecules in Physics, Chemistry and Biology J. Maruani, 1988-10-31 The book merits a place in any Science Library and I recommend it to anyone who shares the obvious fascination of the writers with molecules and accepts that molecular properties are often best described with the aid of mathematical expressions M Godfrey Journal of Electroanalytical Chemistry 269 1989 provide a panoramic view of the status and potential of molecular sciences at the end of the nineteen eighties This four volume set represents a great value for any scientific library or private collections creating a broad based and rich mini series on molecular sciences Structural Chemistry 1 5

Annual Catalogue Massachusetts Institute of Technology, 1964

Match, 2000

Graph Theoretical Approaches to Chemical Reactivity Danail D. Bonchev, O.G. Mekenyan, 1994-06-30 The progress in computer technology during the last 10 15 years has enabled the performance of ever more precise quantum mechanical calculations related to structure and interactions of chemical compounds However the qualitative models relating electronic structure to molecular geometry have not progressed at the same pace There is a continuing need in chemistry for simple concepts and qualitatively clear pictures that are also quantitatively comparable to ab initio quantum chemical calculations Topological methods and more specifically graph theory as a fixed point topology provide in principle a chance to

fill this gap With its more than 100 years of applications to chemistry graph theory has proven to be of vital importance as the most natural language of chemistry The explosive development of chemical graph theory during the last 20 years has increasingly overlapped with quantum chemistry Besides contributing to the solution of various problems in theoretical chemistry this development indicates that topology is an underlying principle that explains the success of quantum mechanics and goes beyond it thus promising to bear more fruit in the future *Subject Guide to Books in Print* ,1997

British Books in Print ,1986 Indian Journal of Chemistry ,2003 *The Cumulative Book Index* ,1994 A world list of books in the English language

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