



# Shape in Chemistry: An Introduction to Molecular Shape and Topology.

Mezey, Paul

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# Shape In Chemistry An Introduction To Molecular Shape And Topology

**Danail D. Bonchev, O.G. Mekenyan**



## **Shape In Chemistry An Introduction To Molecular Shape And Topology:**

**Shape in Chemistry** Paul G. Mezey, 1993      **Progress in Biological Chirality** Gyula Palyi, Claudia Zucchi, Luciano Caglioti, 2004-12-13 Following on from Advances in BioChirality Progress in Biological Chirality provides a unique summary and review of the most recent developments in the field of biochirality Living organisms use only one enantiomer of chiral molecules in the majority of biologically important processes The exact origin and mechanisms for this surprising selectivity are not yet known This book discusses current research aimed at identifying the scientific reasons that may contribute to this phenomenon Progress in Biological Chirality takes an interdisciplinary approach to this exciting field covering a wide range of topics such as theory palaeontology and food technology to name but a few This book presents findings via a broad spectrum of scientific approaches making it an excellent overview of Biological Chirality suitable for postgraduate students practitioners and researchers in the field of chemistry biochemistry biology palaeontology and food science with an interest in Chirality This book contains 32 chapters written by Authors who are leading authorities in the field Presents the most recent research taking place in this highly challenging field Contains both reference material for the specialist and provides an overview for those who are interested in the fundamental problems of biology and chemistry      **Fundamentals of Molecular Similarity** Ramon Carbó-Dorca, Paul G. Mezey, 2013-04-17 In recent years the fundamental concepts and applied methodologies of molecular similarity analysis have experienced a revolutionary development Motivated by the increased degree of understanding of elementary molecular properties on the levels ranging from fundamental quantum chemistry to the complex interactions of biomolecules and aided by the spectacular progress in computer technology and access to computer power the area has opened up to many new ideas and new approaches This book covers topics in quantum similarity approaches electron density shape analysis methods and it provides better theoretical understanding of molecular similarity Additionally quantitative shape analysis especially activity relations QShAR and the prediction of the pharmacological or toxicological effects of molecules in the related context of quantum QSAR QQSAR This volume written by the experts in the various subfields of molecular similarity provides a collection of the most recent ideas advances and methodologies It is the hope of the Editors that by representing these topics within a single volume the readers will find a balanced overview of the status of the field We also hope that the book will serve as a tool for selecting and assessing the best approach for various new types of problems of molecular similarity that may arise and it will provide a set of easy references for further studies and applications      **Handbook of Molecular Descriptors** Roberto Todeschini, Viviana Consonni, 2008-07-11 Quantitative studies on structure activity and structure property relationships are powerful tools in directed drug research In recent years various strategies have been developed to characterize and classify structural patterns by means of molecular descriptors It has become possible not only to assess diversities or similarities of structure databases but molecular descriptors also facilitate the identification of potential bioactive molecules from the rapidly

increasing number of compound libraries They even allow for a controlled de novo design of new lead structures This is the most comprehensive collection of molecular descriptors and presents a detailed review from the origins of this research field up to present day This practically oriented reference book gives a thorough overview of the different molecular descriptors representations and their corresponding molecular descriptors All descriptors are listed with their definition symbols and labels formulas some numerical examples data and molecular graphs while numerous figures and tables aid comprehension of the definitions Cross references throughout a list of acronyms and notations allow easy access to the information needed to solve a specific research problem Examples of descriptor calculations along with tables of descriptor values for a set of selected reference compounds and an up to date reference list add to the practical value of the book making it an invaluable guide for all those dealing with bioactive molecules as well as for researchers

### **Molecular Descriptors for**

**Chemoinformatics** Roberto Todeschini, Viviana Consonni, 2009-10-30 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 completely re written and now contains several walk through reading lists of selected keywords for novice users

**Computational Medicinal Chemistry for Drug Discovery** Patrick Bultinck, Hans De Winter, Wilfried Langenaeker, Jan P. Tollenare, 2003-12-17 Observing computational chemistry's proven value to the introduction of new medicines this reference offers the techniques most frequently utilized by industry and academia for ligand design Featuring contributions from more than fifty pre eminent scientists Computational Medicinal Chemistry for Drug Discovery surveys molecular structure computation intermolecular behavior ligand receptor interaction and modeling responding to market demands in its selection and authoritative treatment of topics The book examines molecular mechanics semi empirical methods wave function based quantum chemistry density functional theory 3 D structure generation and hybrid methods

**Shape in Chemistry** Paul G. Mezey, 1993 **From Chemical Topology to Three-Dimensional Geometry** Alexandru T. Balaban, 2006-04-11 Even high speed supercomputers cannot easily convert traditional two dimensional databases from chemical topology into the three dimensional ones demanded by today's chemists particularly those working in drug design This fascinating volume resolves this problem by positing mathematical and topological models which greatly expand the capabilities of chemical graph theory The authors examine QSAR and molecular similarity studies the relationship between the sequence of amino acids and the less familiar secondary and tertiary protein structures and new topological methods

**Electron, Spin and Momentum Densities and Chemical Reactivity** Paul G. Mezey, Beverly E. Robertson, 2006-04-11 The electron density of a non degenerate ground state system determines essentially all physical

properties of the system This statement of the Hohenberg Kohn theorem of Density Functional Theory plays an exceptionally important role among all the fundamental relations of Molecular Physics In particular the electron density distribution and the dynamic properties of this density determine both the local and global reactivities of molecules High resolution experimental electron densities are increasingly becoming available for more and more molecules including macromolecules such as proteins Furthermore many of the early difficulties with the determination of electron densities in the vicinity of light nuclei have been overcome These electron densities provide detailed information that gives important insight into the fundamentals of molecular structure and a better understanding of chemical reactions The results of electron density analysis are used in a variety of applied fields such as pharmaceutical drug discovery and biotechnology If the functional form of a molecular electron density is known then various molecular properties affecting reactivity can be determined by quantum chemical computational techniques or alternative approximate methods

**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

*Applications of Topological Methods in Molecular Chemistry* Remi Chauvin,Christine Lepetit,Bernard Silvi,Esmail Alikhani,2016-04-19 This is the first edited volume that features two important frameworks Hckel and quantum chemical topological analyses The contributors which include an array of academics of international distinction describe recent applications of such topological methods to various fields and topics that provide the reader with the current state of the art and give a flavour of the wide range of their potentialities

**International Tables for Crystallography, Volume C** E. Prince,2004-01-16 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Each of the volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials Emphasis is given to symmetry diffraction methods and techniques of crystal structure determination and the physical and chemical properties of crystals The data are accompanied by discussions of theory

practical explanations and examples all of which are useful for teaching Volume C provides the mathematical physical and chemical information needed for experimental studies in structural crystallography This volume covers all aspects of experimental techniques using all three principal radiation types X ray electron and neutron from the selection and mounting of crystals and production of radiation through data collection and analysis to interpretation of results Each chapter is supported by a substantial collection of references and the volume ends with a section on precautions against radiation injury Eleven chapters have been revised corrected or updated for the third edition of Volume C More information on the series can be found at <http://it.iucr.org>

**Theoretical and Quantum Chemistry at the Dawn of the 21st Century** Tanmoy Chakraborty, Ramon Carbo-Dorca, 2018-06-19 This volume edited by a well known specialist in the field of theoretical chemistry gathers together a selection of papers on theoretical chemistry within the themes of mathematical computational and quantum chemistry The authors present a rich assembly of some of the most important current research in the field of quantum chemistry in modern times In Quantum Chemistry at the Dawn of the 21st Century the editors aim to replicate the tradition of the fruitful Girona Workshops and Seminars held at the University of Girona Italy annually for many years which offered important scientific gatherings focusing on quantum chemistry This volume like the workshops showcases a large variety of quantum chemical contributions from different points of view from some of the leading scientists in the field today This unique volume does not pretend to provide a complete overview of quantum chemistry but it does provide a broad set of contributions by some of the leading scientists on the field under the expert editorship of two leaders in the field

**Hydrogen Bonding - New Insights** Slawomir Grabowski, 2006-10-07 Hydrogen Bonding New Insights is an extensive text which takes numerous examples from experimental studies and uses these to illustrate theoretical investigations to allow a greater understanding of hydrogen bonding phenomenon The most important topics in recent studies are considered including Intra molecular H bonds Differences between H bond and van der Waals interactions from one side and covalent bonds from the other Bader theory to analyze H bonding Influence of weak H bonds upon structure and function of biological molecules H bonds in crystal structures With contributions from some of the foremost experts in this field this volume provides an invaluable resource for all members of the academic community looking for a comprehensive text on hydrogen bonding It will be of particular interest to physical and theoretical chemists spectroscopists crystallographers and those involved with chemical physics

**Second Conference on Current Trends in Computational Chemistry**, 1993 **New Theoretical Concepts for Understanding Organic Reactions** Juan Bertrán, Imre G. Csizmadia, 2012-12-06 People who attended the NATO Advanced Study Institute ASI entitled NEW THEORETICAL CONCEPTS FOR UNDERSTANDING ORGANIC REACTIONS held at Sant Feliu de Guixols on the Costa Brava of Spain had a unique experience They have seen the evolution of the field from qualitative arguments through the generation of Potential Energy Surfaces PES to the use of PES in molecular dynamics The excellent lectures that were dedicated to the various aspects of Potential Energy Surfaces

clearly revealed a colossal amount of material that represents our current understanding of the overall problem. It is our hope that the present volume will recreate the excitement in the readers that we all experienced during the meeting in Spain. One can say without too much exaggeration that chemistry has become an exercise on potential energy surfaces (PES). Structural position of the energy minima, spectroscopic vicinity around the minima and reactivity reaction path along the surface properties may be determined from the analysis of PES. New theoretical tools together with recent developments in computer technology and programming have allowed to obtain a better knowledge of these surfaces and to extract further chemical information from them so new horizons have been added to Theoretical Organic Chemistry. **Graph Theoretical**

**Approaches to Chemical Reactivity** Danail D. Bonchev, O.G. Mekenyan, 2012-12-06. 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. **Advances in Molecular Structure Research** M. Hargittai, I.

Hargittai, 1998-08-02. This volume is the fourth in the series and offers both quality and breadth. As a whole, it reflects two increasingly discernible trends in modern structural chemistry. One trend is that parallel to the ever increasing specialization of techniques, there is a strong interaction between the techniques. This interaction crosses the boundaries between various experiments, between the experiments and computations, experiments and theory, and organic and inorganic chemistry. The other trend is the ever increasing penetration of the most modern aspects of structural chemistry into the rest of chemistry, making the demarcation of structural chemistry increasingly fuzzy, which is the most welcome development from a structural chemist's point of view. **Computational Chemistry** Jerzy Leszczynski, 1996. This book presents an overview of recent

progress in computational techniques as well as examples of the application of existing computational methods in different areas of chemistry, physics and biochemistry. Introductory chapters cover a broad range of fundamental topics including state of the art basis set expansion methods for computing atomic and molecular electronic structures based on the use of relativistic quantum mechanics, the most recent developments in Hartree-Fock methods, particularly in techniques suited for very large systems, the current analysis of the solute-solvent free energy of interaction and the physical bases used to

evaluate the electrostatic cavitation and dispersion terms an introduction to the additive fuzzy electron density fragmentation scheme within various ab initio Hartree Fock quantum chemical computational schemes which has provided the means for generating representative molecular fragment densities characteristic to their local environment within a molecule This book also features a review of recent ab initio calculations on the structure and interactions of DNA bases a chapter on computational approaches to the design of safer drugs and their molecular properties and a systematic conceptual study on a route which allows one to stuff fullerenes

**Modeling Complex Data for Creating Information** Jacques-Emile Dubois, Nahum Gershon, 2012-12-06 J E DUBOIS and N GERSHON As with Volume 1 in this series this book was inspired by the Symposium on Communications and Computer Aided Systems held at the 14th International CODATA Conference in September 1994 in Chambéry France This book was conceived and influenced by the discussions at the Symposium and most of the contributions were written following the Conference Whereas the first volume dealt with the numerous challenges facing the information revolution especially its communication aspects this one provides an insight into the recent tools provided by computer science for handling the complex aspects of scientific and technological data This volume Modeling Complex Data for Creating Information is concerned with real and virtual objects often involved with data handling processes encountered frequently in modeling physical phenomena and systems behavior Topics concerning modeling complex data for creating information include Object oriented approach for structuring data and knowledge Imprecision and uncertainty in information systems Fractal modeling and shape and surface processing Symmetry applications for molecular data The choice of these topics reflects recent developments in information systems technologies One example is object oriented technology Recently research development and applications have been using object oriented modeling for computer handling of data and data management Object oriented technology offers increasingly easy to use software applications and operating systems As a result science and technology research and applications can now provide more flexible and effective services



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