



# Polyhedral Boranes

**Harry R. Allcock**



## Polyhedral Boranes:

*Polyhedral Boranes* Earl L. Muetterties, Walter Henry Knoth, 1968      *Symmetry through the Eyes of a Chemist* Magdolna Hargittai, Istvan Hargittai, 2009-02-28 It is gratifying to launch the third edition of our book Its coming to life testifies about the task it has fulfilled in the service of the community of chemical research and learning As we noted in the Prefaces to the first and second editions our book surveys chemistry from the point of view of symmetry We present many examples from chemistry as well as from other fields to emphasize the unifying nature of the symmetry concept Our aim has been to provide aesthetic pleasure in addition to learning experience In our first Preface we paid tribute to two books in particular from which we learned a great deal they have influenced significantly our approach to the subject matter of our book They are Weyl's classic *Symmetry* and Shubnikov and Koptsik's *Symmetry in Science and Art* The structure of our book has not changed Following the Introduction Chapter 1 Chapter 2 presents the simplest symmetries using chemical and non chemical examples Molecular geometry is discussed in Chapter 3 The next four chapters present theoretical methods Chapter 4 and based on them discussions of molecular vibrations Chapter 5 electronic structures Chapter 6 and chemical reactions Chapter 7 For the last two chapters we return to a qualitative treatment and introduce space group symmetries Chapter 8 concluding with crystal structures Chapter 9 For the third edition we have further revised and streamlined our text and renewed the illustrative material      **50th Anniversary of Electron Counting Paradigms for Polyhedral Molecules** D. Michael P.

Mingos, 2022-01-01 The 50 Year Anniversary of the development of electron counting paradigms for polyhedral molecules is celebrated in two volumes of *Structure and Bonding* Volume 1 covers the historical development theoretical models and applications to boranes and metalloboranes      *Boranes and Beyond* M. Frederick Hawthorne, 2023-04-11 Tracing the life of a giant in inorganic chemistry and key trends in his science *Boranes and Beyond* follows Hawthorne from his mid American origins to the halls of Harvard and UCLA and back again It naturally details the accomplishments in his lab This book is a fascinating mixture of science and autobiography Prof Hawthorne won the Priestley Medal the highest award of the American Chemical Society for his pioneering work in elucidating the chemistry of boron He has chronicled in this book the developments in his lab which ultimately led to this achievement Not content to rest on his laurels after retiring from UCLA Prof Hawthorne explored the use of boron in biomedicine and directed the International Institute of Nano Molecular Medicine at the University of Missouri Columbia      *Handbook Of Boron Science: With Applications In Organometallics, Catalysis, Materials And Medicine (In 4 Volumes)* Narayan S Hosmane, Robert D Eagling, 2018-08-07 Boron science features in numerous fields including organic chemistry organometallic chemistry and medicine Boron is unique in all aspects of science and engineering and has made a significant impact in our daily lives through its use in fertilizers germicides fungicides soaps detergents cancer drugs as well as many household glassware utensils ceramics and cell phone windows These volumes bring together an array of internationally renowned scientists to discuss the very latest developments in the

application of boron in a broad range of disciplines This multi reference work describes the topic by appointing leading researchers to write on current developments in boron science showcasing its importance to the four separate areas described in each volume Organometallic Chemistry Catalysis Materials Chemistry and Medicine Written to cover the full range of applications and innovations in boron science this all encompassing work offers us a one stop reference compiled by world leading researchers and practitioners of the subject making it perfect for undergraduate and graduate students of chemistry and researchers and practitioners interested in their professional development

**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

**Advances in Organometallic Chemistry**, 1983-01-26 Advances in Organometallic Chemistry

Computational Inorganic and Bioinorganic Chemistry Edward I. Solomon, Robert A. Scott, R. Bruce King, 2013-02-19 Over the past several decades there have been major advances in our ability to computationally evaluate the electronic structure of inorganic molecules particularly transition metal systems This advancement is due to the Moore's Law increase in computing power as well as the impact of density functional theory DFT and its implementation in commercial and freeware programs for quantum chemical calculations Improved pure and hybrid density functionals are allowing DFT calculations with accuracy comparable to high level Hartree Fock treatments and the results of these calculations can now be evaluated by experiment When calculations are correlated to and supported by experimental data they can provide fundamental insight into electronic structure and its contributions to physical properties and chemical reactivity This interplay continues to expand and contributes to both improved value of experimental results and improved accuracy of computational predictions The purpose of this EIC Book is to provide state of the art presentations of quantum mechanical and related methods and their applications written by many of the leaders in the field Part 1 of this volume focuses on methods their background and implementation and their use in describing bonding properties energies transition states and spectroscopic features Part 2 focuses on applications in bioinorganic chemistry and Part 3 discusses inorganic chemistry where electronic structure calculations have already had a major impact This addition to the EIC Book series is of significant value to both experimentalists and theoreticians and we anticipate that it will stimulate both further development of the methodology and its applications in the many interdisciplinary fields that comprise modern inorganic and bioinorganic chemistry This volume is also available as part of Encyclopedia of Inorganic Chemistry 5 Volume Set This set combines all volumes published as EIC Books from 2007 to 2010 representing areas of key developments in the field of inorganic

chemistry published in the Encyclopedia of Inorganic Chemistry Find out more at <http://eu.wiley.com/WileyCDA/WileyTitle/productCd/1119994284.html> *Introduction to Materials Chemistry* Harry R. Allcock, 2011-09-20 Introduction to Materials Chemistry will appeal to advanced undergraduates and graduate students in chemistry materials science and chemical engineering by leading them stepwise from the elementary chemistry on which materials science depends through a discussion of the different classes of materials and ending with a description of how materials are used in devices and general technology *Boron* Drahomír Hnyk, Michael McKee, 2015-12-17 This multi author edited volume reviews the recent developments in boron chemistry with a particular emphasis on the contribution of computational chemistry The contributors come from Europe the USA and Asia About 60% of the book concentrates on theoretical and computational themes whilst 40% is on topics of interest to experimental chemists Specific themes covered include structure topology modelling and prediction the role of boron clusters in synthetic chemistry and catalysis as medical agents when acting as inhibitors of HIV protease and carbonic anhydrases *Inorganic Chemistry* J. E. House, 2012-10-30 This textbook provides essential information for students of inorganic chemistry or for chemists pursuing self study The presentation of topics is made with an effort to be clear and concise so that the book is portable and user friendly Inorganic Chemistry 2E is divided into five major themes structure condensed phases solution chemistry main group and coordination compounds with several chapters in each There is a logical progression from atomic structure to molecular structure to properties of substances based on molecular structures to behavior of solids etc The author emphasizes fundamental principles including molecular structure acid base chemistry coordination chemistry ligand field theory and solid state chemistry and presents topics in a clear concise manner There is a reinforcement of basic principles throughout the book For example the hard soft interaction principle is used to explain hydrogen bond strengths strengths of acids and bases stability of coordination compounds etc The book contains a balance of topics in theoretical and descriptive chemistry New to this Edition New and improved illustrations including symmetry and 3D molecular orbital representations Expanded coverage of spectroscopy instrumental techniques organometallic and bio inorganic chemistry More in text worked out examples to encourage active learning and to prepare students for their exams Concise coverage maximizes student understanding and minimizes the inclusion of details students are unlikely to use Discussion of elements begins with survey chapters focused on the main groups while later chapters cover the elements in greater detail Each chapter opens with narrative introductions and includes figures tables and end of chapter problem sets **Carboranes** Russell N. Grimes, 2016-08-09 Carboranes Third Edition by Russell Grimes is the definitive resource on the subject Completely updated with a wealth of research and review articles published in this active field since the previous volume was released in 2011 the book provides a readable and concise introduction to the basic principles underlying the synthesis structures and reactions of carboranes heterocarboranes and metallocarboranes Following the valuable foundational information the book explores the advances in practical applications for the many areas

in which experts have discovered that carboranes afford new possibilities for solving problems and advancing the science These disciplines include polymer science catalysis biomedicine nanomaterials and others Winner of a 2017 Textbook Excellence Award Texty from the Textbook and Academic Authors Association Includes over 2 000 molecular structure drawings throughout the text Features expanded coverage on applications of carboranes particularly in biomedicine and nanomaterials given the growth of research in these areas Presents extended and updated tables listing thousands of compounds with key literature references provided online via the book s website Explores the advances in practical applications for the many areas in which experts have discovered that carboranes afford new possibilities for solving problems and advancing the science

**Inorganic Chemistry** Rory Reid,2018-01-11 Inorganic chemistry deals with the synthesis and behavior of inorganic and organometallic compounds This field covers all chemical compounds except the myriad organic compounds which are the subjects of organic chemistry The distinction between the two disciplines is far from absolute as there is much overlap in the subdiscipline of organometallic chemistry Today our understanding of chemical bonding molecular reactivities and various other fundamental chemical problems rests heavily on our knowledge of the detailed behaviour of electrons in atoms and molecules This book describes in detail some of the basic principles methods and results of quantum chemistry that lead to our understanding of electron behaviour The basic aspects of inorganic chemistry are presented significantly in this book Many applications and practical problems are described The order of the techniques included is conventional and would be liked by students The chapters have been arranged in a conventional way as it may be easy for students to pass from one to another chapter with continuity

**Aromaticity** Israel Fernandez,2021-05-16 Evaluating the aromaticity of a molecular system and the influence of this concept on its properties is a crucial step in the development of novel aromatic systems Modern computational methods can provide researchers with a high level of insight into such aromaticity but identifying the most appropriate method for assessing a specific system can prove difficult Aromaticity Modern Computational Methods and Applications reviews the latest state of the art computational methods in this field and discusses their applicability for evaluating the aromaticity of a system In addition to covering aromaticity for typical organic molecules this volume also explores systems possessing transition metals in their structures macrocycles and even transition structures The influence of the aromaticity on the properties of these species including the structure magnetic properties and reactivity is highlighted along with potential applications in fields including materials science and medicinal chemistry Finally the controversial and fuzzy nature of aromaticity as a concept is discussed providing the basis for an updated and more comprehensive definition of this concept Drawing on the knowledge of an international team of experts Aromaticity Modern Computational Methods and Applications is a unique guide for anyone researching studying or applying principles of aromaticity in their work from computational and organic chemists to pharmaceutical and materials scientists Reviews a range of computational methods to assess the aromatic nature of different compounds helping

readers select the most useful tool for the system they are studying Presents a complete guide to the key concepts and fundamental principles of aromaticity Provides guidance on identifying which variables should be modified to tune the properties of an aromatic system for different potential applications

**Boron-Based Compounds** Evamarie Hey-Hawkins, Clara Viñas Teixidor, 2018-04-03 Noted experts review the current status of boron containing drugs and materials for molecular medical diagnostics Boron Based Compounds offers a summary of the present status and promotes the further development of new boron containing drugs and advanced materials mostly boron clusters for molecular medical diagnostics The knowledge accumulated during the past decades on the chemistry and biology of bioorganic and organometallic boron compounds laid the foundation for the emergence of a new area of study and application of boron compounds as lipophilic pharmacophores and modulators of biologically active molecules This important text brings together in one comprehensive volume contributions from renowned experts in the field of medicinal chemistry of boron compounds The authors cover a range of the most relevant topics including boron compounds as modulators of the bioactivity of biomolecules boron clusters as pharmacophores or for drug delivery boron compounds for boron neutron capture therapy BNCT and for diagnostics as well as in silico molecular modeling of boron and carborane containing compounds in drug design Authoritative and accessible Boron Based Compounds Contains contributions from a panel of internationally renowned experts in the field Offers a concise summary of the current status of boron containing drugs and materials used for molecular diagnostics Highlights the range and capacity of boron based compounds in medical applications Includes information on boron neutron capture therapy and diagnostics Designed for academic and industrial scientists this important resource offers the cutting edge information needed to understand the current state of boron containing drugs and materials for molecular medical diagnostics

**Symmetry through the Eyes of a Chemist** Istvan Hargittai, Magdolna Hargittai, 2007-08-29 We have been gratified by the warm reception of our book by reviewers colleagues and students alike Our interest in the subject matter of this book has not decreased since its first appearance on the contrary The first and second editions envelop eight other symmetry related books in the creation of which we have participated I Hargittai ed Symmetry Unifying Human Understanding Pergamon Press New York 1986 I Hargittai and B K Vainshtein eds Crystal Symmetries Shubnikov Centennial Papers Pergamon Press Oxford 1988 M Hargittai and I Hargittai Fedezsiikf6l a szimmetri6t Discover Sym try in Hungarian Tank6nyvkiad6 Budapest 1989 I Hargittai ed Symmetry 2 Unifying Human Understanding Pergamon Press Oxford 1989 I Hargittai ed Quasicrystals Networks and Molecules of Fivefold Sym try VCH New York 1990 I Hargittai ed Fivefold Symmetry World Scientific Singapore 1992 I Hargittai and C A Pickover eds Spiral Symmetry World Scientific Singapore 1992 I Hargittai and M Hargittai Symmetry A Unifying Concept Shelter Publications Bolinas California 1994 We have also pursued our molecular structure research and some books have appeared related to these activities vi Preface to the Second Edition I Hargittai and M Hargittai eds Stereochemical Applications of Gas Phase

Electron Diffraction Parts A and B VCH New York 1988 R Gillespie and I Hargittai VSEPR Model of Molecular Geometry Allyn and Bacon Boston 1991 A Domenicano and I Hargittai eds Accurate Molecular Structures Oxford University Press Oxford 1992

**Selected Topics in Inorganic Chemistry - Part II** Dr. A. AHMED RAZA & Dr. SEENU RAVI, 2024-09-05

This book is for the postgraduate students of chemistry aspiring to crack competitive examinations such as CSIR NET GATE SLET SET and PhD entrance examinations Presently admission to PhD programs in premier institutions like IITs NITs CSIR laboratories central universities and state universities is based on either NET GATE certificate or PhD entrance examinations Further the minimum eligibility criteria laid by UGC for the direct recruitment of Assistant Professors in the higher educational institutions is a postgraduate degree with NET SLET SET certificate Thus the students are bound to pass these examinations to pursue a bright career either in research or in academic teaching The cut off for qualifying these exams is 40 to 50% However the qualifying percentage of the candidates appearing for these examinations is around 5% only Therefore an attempt has been made by authors to develop study material pertaining to the syllabus of these exams along with the solved problems from the previous year question papers which will guide the students to qualify easily

*Molecular Clusters of the Main Group Elements* Matthias Driess, Heinrich Nöth, 2008-11-21 With more than 20 contributions from leading research groups this book provides essential information for chemists and materials scientists working with molecular clusters It treats both homonuclear and heteronuclear clusters including the theory and concepts in main group cluster chemistry novel boranes and heteroboranes silicon germanium tin clusters alkali metal suboxides clusters in alloys with mercury chalcogen clusters and numerous other compound classes The whole is illustrated by examples of the great potential for technical applications such as electron storage cancer therapy and in optoelectronic devices Its systematic coverage of all relevant main group elements makes this the prime reference source in the field

Applications of Graph Theory and Topology in Inorganic Cluster and Coordination Chemistry R. Bruce King, 1992-12-01 Applications of Graph Theory and Topology in Inorganic Cluster and Coordination Chemistry is a text reference that provides inorganic chemists with a rudimentary knowledge of topology graph theory and related mathematical disciplines The book emphasizes the application of these topics to metal clusters and coordination compounds The book's initial chapters present background information in topology graph theory and group theory explaining how these topics relate to the properties of atomic orbitals and are applied to coordination polyhedra Subsequent chapters apply these ideas to the structure and chemical bonding in diverse types of inorganic compounds including boron cages metal clusters solid state materials metal oxide derivatives superconductors icosahedral phases and carbon cages fullerenes The book's final chapter introduces the application of topology and graph theory for studying the dynamics of rearrangements in coordination and cluster polyhedra

**Fundamentals and Applications of Boron Chemistry** Yinghuai Zhu, 2022-03-17 Fundamentals and Applications of Boron Chemistry highlights its impressive potential for current and future developments across a range of fields providing



foundational information on boron chemistry and systematically summarizing applications of boron in energy medicinal chemistry and materials chemistry Beginning with an introduction to boron chemistry which outlines the boron element and its physical and chemical properties this book goes on to discuss advances in boron coordination chemistry before delving deeper into key fields of application The latest developments in boron based catalysts in organic reactions are reviewed followed by novel emerging boron containing materials and their potential applications in areas such as hydrogen storage and boron materials with special optical activity Finally advance boron based drugs and therapies are explored This book fills the current market gap systematically summarizing developments and applications of boron in energy medicinal chemistry and materials chemistry in a single accessible volume It is a valuable reference for chemists students and researchers in relative areas Outlines the foundational principles and properties of boron chemistry Highlights developments in the application of boron chemistry across key areas including catalysis sustainable energy material development and pharmaceuticals Using active words to start them off Inspires researchers in developing future applications based on boron s chemical characteristics and activity

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