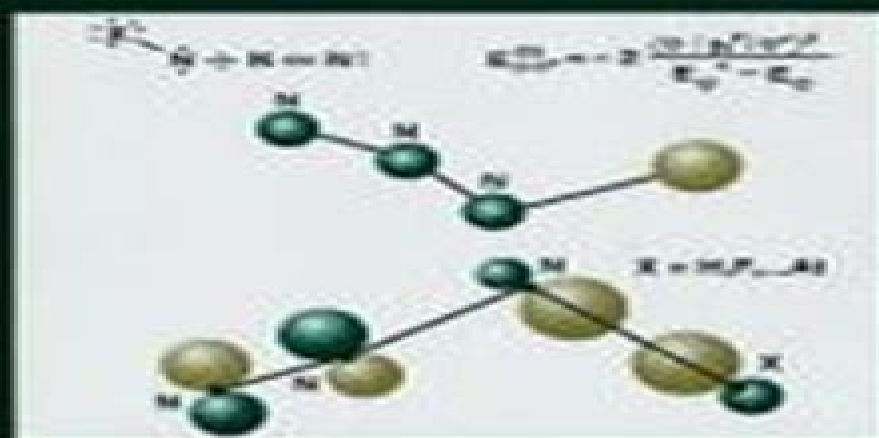


QUANTUM CHEMICAL METHODS IN MAIN-GROUP CHEMISTRY



Thomas M. Klapötke and Axel Schulz

With an invited chapter by
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Quantum Chemical Methods In Main Group Chemistry

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Quantum Chemical Methods In Main Group Chemistry Thomas M Klap tke Axel Schulz University of Munich Germany With an invited chapter by Richard D Harcourt University of Melbourne Australia Computational quantum chemistry has emerged in recent years as a key tool for the elucidation of molecular structure and molecular properties However it is still sometimes regarded as a highly theoretical subject of limited practical value In this book the authors emphasize the strong link between quantum chemical calculations and experiment The book is a fascinating blend of theory and experiment and deals with topical and interesting molecules using state of the art techniques and accompanied by full explanations In Part 1 of Quantum Chemical Methods in Main Group Chemistry modern quantum mechanical procedures are described in a concise and systematic manner Sufficient theory is provided to enable the reader to come to terms with the primary features of the methodology In Part II numerous applications of these procedures are described These applications provide extensive consideration of highly topical and interesting modern chemistry and also illustrate aspects of the methodology Part III which is new in the English edition is written by Professor Richard D Harcourt To provide a fully balanced approach to the subject this part provides valence bond descriptions and considerable attention is given to the use of Pauling three electron bonds and increased valence structures Relevant valence bond concepts are reviewed briefly in the first chapters of Part III Quantum Mechanical Methods in Main Group Chemistry provides an invaluable link between computational quantum chemical techniques and practical modern chemistry As such it is an important resource for both the advanced undergraduate and postgraduate student and also for the more experienced researcher

Problems in Structural Inorganic Chemistry Wai-Kee Li, Yu-San Cheung, Kendrew Kin Wah Mak, Thomas Chung Wai Mak, 2012-10-11 This book consists of over 300 problems and their solutions in structural inorganic chemistry at the senior undergraduate and beginning graduate level The topics covered comprise Atomic and Molecular Electronic States Atomic Orbitals Hybrid Orbitals Molecular Symmetry Molecular Geometry and Bonding Crystal Field Theory Molecular Orbital Theory Vibrational Spectroscopy and Crystal Structure The central theme running through these topics is symmetry molecular or crystalline The problems collected in this volume originate in examination papers and take home assignments that have been part of the teaching of the book s two senior authors at The Chinese University of Hong Kong over the past four decades The authors courses include Chemical Bonding Elementary Quantum Chemistry Advanced Inorganic Chemistry X Ray Crystallography etc The problems have been tested by generations of students taking these courses

Advanced Structural Inorganic Chemistry Wai-Kee Li, Gong-Du Zhou, Thomas C. W. Mak, 2008-03-27 A revised and updated English edition of a textbook based on teaching at the final year undergraduate and graduate level It presents structure and bonding generalizations of structural trends crystallographic data as well as highlights from the recent literature

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>

Relativistic Theory of Atoms and Molecules III Pekka Pyykkö, 2013-06-29 Relativistic effects are of major importance for understanding the properties of heavier atoms and molecules Volumes I-III of Relativistic Theory of Atoms and Molecules constitute the only available bibliography on related calculations In Volume III 3792 new references covering 1993-1999 are added to the database The material is characterized by an analysis of the respective papers The volume gives the user a comprehensive bibliography on relativistic atomic and molecular calculations including studies on the Dirac equation and related solid state work

Bonding in Electron-Rich Molecules Richard D. Harcourt, 2015-10-30 This second edition was updated to include some of the recent developments such as increased valence structures for 3 electron 3 centre bonding benzene electron conduction and reaction mechanisms spiral chain O₄ polymers and recoupled pair bonding The author provides qualitative molecular orbital and valence bond descriptions of the electronic structures for primarily electron rich molecules with strong emphasis given to the valence bond approach that uses increased valence structures He describes how long bond Lewis structures as well as standard Lewis structures are incorporated into increased valence structures for electron rich

molecules Increased valence structures involve more electrons in bonding than do their component Lewis structures and are used to provide interpretations for molecular electronic structure bond properties and reactivities Attention is also given to Pauling 3 electron bonds which are usually diatomic components of increased valence structures for electron rich molecules

Exploring Chemical Concepts Through Theory and Computation Shubin Liu, 2024-12-23 Deep theoretical resource on the essence of chemistry explaining a variety of important concepts including redox states and bond types Exploring Chemical Concepts Through Theory and Computation provides a comprehensive account of how the three widely used theoretical frameworks of valence bond theory molecular orbital theory and density functional theory along with a variety of important chemical concepts can between them describe and efficiently and reliably predict key chemical parameters and phenomena By comparing the three main theoretical frameworks readers will become competent in choosing the right modeling approach for their task The authors go beyond a simple comparison of existing algorithms to show how data driven theories can explain why chemical compounds behave the way they do thus promoting a deeper understanding of the essence of chemistry The text is contributed to by top theoretical and computational chemists who have turned computational chemistry into today's data driven and application oriented science Exploring Chemical Concepts Through Theory and Computation discusses topics including Orbital based approaches density based approaches chemical bonding partial charges atoms in molecules oxidation states aromaticity and antiaromaticity and acidity and basicity Electronegativity hardness softness HSAB sigma hole interactions charge transport and energy transfer and homogeneous and heterogeneous catalysis Electrophilicity nucleophilicity cooperativity frustration homochirality and energy decomposition Chemical concepts in solids excited states spectroscopy and machine learning and catalysis and machine learning as well as key connections between related concepts Aimed at both novice and experienced computational theoretical and physical chemists Exploring Chemical Concepts Through Theory and Computation is an essential reference to gain a deeper more advanced holistic understanding of the field of chemistry as a whole *Understanding Organometallic Reaction Mechanisms and Catalysis* Valentin P.

Ananikov, 2014-08-29 Exploring and highlighting the new horizons in the studies of reaction mechanisms that open joint application of experimental studies and theoretical calculations is the goal of this book The latest insights and developments in the mechanistic studies of organometallic reactions and catalytic processes are presented and reviewed The book adopts a unique approach exemplifying how to use experiments spectroscopy measurements and computational methods to reveal reaction pathways and molecular structures of catalysts rather than concentrating solely on one discipline The result is a deeper understanding of the underlying reaction mechanism and correlation between molecular structure and reactivity The contributions represent a wealth of first hand information from renowned experts working in these disciplines covering such topics as activation of small molecules C C and C Heteroatom bonds formation cross coupling reactions carbon dioxide conversion homogeneous and heterogeneous transition metal catalysis and metal graphene systems With the knowledge

gained the reader will be able to improve existing reaction protocols and rationally design more efficient catalysts or selective reactions An indispensable source of information for synthetic analytical and theoretical chemists in academia and industry

Computational Quantum Chemistry Masoud Soroush, 2018-10-16 Computational Quantum Chemistry Insights into Polymerization Reactions consolidates extensive research results couples them with computational quantum chemistry CQC methods applicable to polymerization reactions and presents those results systematically CQC has advanced polymer reaction engineering considerably for the past two decades The book puts these advances into perspective It also allows you to access the most up to date research and CQC methods applicable to polymerization reactions in a single volume The content is rigorous yet accessible to graduate students as well as researchers who need a reference of state of the art CQC methods with polymerization applications Consolidates more than 10 years of theoretical polymerization reaction research currently scattered across journal articles Accessibly presents CQC methods applicable to polymerization reactions Provides researchers with a one stop source of the latest theoretical developments in polymer reaction engineering

Reviews in Computational Chemistry, Volume 17 Kenny B. Lipkowitz, Donald B. Boyd, 2003-04-24 Computational chemistry is increasingly used in most areas of molecular science including organic inorganic medicinal biological physical and analytical chemistry Researchers in these fields who do molecular modelling need to understand and stay current with recent developments This volume like those prior to it features chapters by experts in various fields of computational chemistry Two chapters focus on molecular docking one of which relates to drug discovery and cheminformatics and the other to proteomics In addition this volume contains tutorials on spin orbit coupling and cellular automata modeling as well as an extensive bibliography of computational chemistry books FROM REVIEWS OF THE SERIES Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry JOURNAL OF MOLECULAR GRAPHICS AND MODELLING One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry The basic philosophy of the editors seems to be to help the authors produce chapters that are complete accurate clear and accessible to experimentalists in particular and other nonspecialists in general JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Theory and Applications of the Empirical Valence Bond Approach Fernanda Duarte, Shina Caroline Lynn Kamerlin, 2017-04-17 A comprehensive overview of current empirical valence bond EVB theory and applications one of the most powerful tools for studying chemical processes in the condensed phase and in enzymes Discusses the application of EVB models to a broad range of molecular systems of chemical and biological interest including reaction dynamics design of artificial catalysts and the study of complex biological problems Edited by a rising star in the field of computational enzymology Foreword by Nobel laureate Arie Warshel who first developed the EVB approach

New Developments in Medicinal Chemistry: Volume 1 Carlton Anthony Taft, Carlos Henrique Tomich de Paula Da Silva, 2010-12-31 This book is recommended for readers who are interested in or work with current theoretical and

experimental research in medicinal chemistry with an emphasis on computer aided drug design and organic synthesis for therapeutic purposes This book encompasses **Spin Chemical Physics of Graphene** Elena Sheka, 2017-11-23 Graphene's nickname miracle material normally means the material's superior properties However all these characteristics are only the outward manifestation of the wonderful nature of graphene The real miracle of graphene is that the species is a union of two entities a physical and a chemical one each of which is unique in its own way The book concerns a very close interrelationship between graphene physics and chemistry as expressed via typical spin effects of a chemical physics origin Based on quantum chemical computations the book is nevertheless addressed to the reflection of physical reality and it is aimed at an understanding of what constitutes graphene as an object of material science sci graphene on the one hand and as a working material high tech graphene for a variety of attractive applications largely discussed and debated in the press on the other The book is written by a user of quantum chemistry sufficiently experienced in material science and the chemical physics of graphene is presented as the user view based on results of extended computational experiments in tight connection with their relevance to physical and chemical realities The experiments have been carried out at the same theoretical platform which allows considering different sides of the graphene life at the same level in light of its chemical peculiarity Advances in Inorganic Chemistry: Recent Highlights II Rudi van Eldik, 2022-03-15 Advances in Inorganic Chemistry Volume 79 the latest release in an esteemed series that highlights new advances in the field of inorganic chemistry presents new and interesting topics authored by an international field of experts Provides the authority and expertise of leading contributors from an international board of authors Presents the latest release in the Advances in Inorganic Chemistry series *Main Group Strategies towards Functional Hybrid Materials* Thomas Baumgartner, Frieder Jaekle, 2018-03-12 Showcases the highly beneficial features arising from the presence of main group elements in organic materials for the development of more sophisticated yet simple advanced functional materials Functional organic materials are already a huge area of academic and industrial interest for a host of electronic applications such as Organic Light Emitting Diodes OLEDs Organic Photovoltaics OPVs Organic Field Effect Transistors OFETs and more recently Organic Batteries They are also relevant to a plethora of functional sensory applications This book provides an in depth overview of the expanding field of functional hybrid materials highlighting the incredibly positive aspects of main group centers and strategies that are furthering the creation of better functional materials Main Group Strategies towards Functional Hybrid Materials features contributions from top specialists in the field discussing the molecular supramolecular and polymeric materials and applications of boron silicon phosphorus sulfur and their higher homologues Hypervalent materials based on the heavier main group elements are also covered The structure of the book allows the reader to compare differences and similarities between related strategies for several groups of elements and to draw crosslinks between different sections The incorporation of main group elements into functional organic materials has emerged as an efficient strategy for tuning

materials properties for a wide range of practical applications Covers molecular supramolecular and polymeric materials featuring boron silicon phosphorus sulfur and their higher homologues Edited by internationally leading researchers in the field with contributions from top specialists Main Group Strategies towards Functional Hybrid Materials is an essential reference for organo main group chemists pursuing new advanced functional materials and for researchers and graduate students working in the fields of organic materials hybrid materials main group chemistry and polymer chemistry

Reviews in Computational Chemistry Kenny B. Lipkowitz, Donald B. Boyd, 2009-09-22 Not only a major reference work for sale to the library market this series is now receiving an increase in purchases by individuals This increase is due to the explosive growth in the use of computational chemistry throughout many scientific disciplines As each volume does not follow a singular theme the table of contents is a vital tool in the defining the areas examined by a volume The series contains updated and comprehensive compendiums of molecular modeling software that list hundreds of programs services suppliers and other information that every chemist will find useful Detailed author and subject indices on each volume help the reader to quickly discover particular topics Uniting the most respected authors in their fields the series is designed to help the reader stay abreast of the many new developments in computational techniques The chapters are approached in a tutorial manner and written in a non mathematical style allowing students and researchers to access computational methods outside their immediate area of expertise *Issues in Specialized Chemical and Chemistry Topics: 2011 Edition*, 2012-01-09 *Issues in Specialized Chemical and Chemistry Topics 2011 Edition* is a ScholarlyEditions eBook that delivers timely authoritative and comprehensive information about Specialized Chemical and Chemistry Topics The editors have built *Issues in Specialized Chemical and Chemistry Topics 2011 Edition* on the vast information databases of ScholarlyNews You can expect the information about Specialized Chemical and Chemistry Topics in this eBook to be deeper than what you can access anywhere else as well as consistently reliable authoritative informed and relevant The content of *Issues in Specialized Chemical and Chemistry Topics 2011 Edition* has been produced by the world's leading scientists engineers analysts research institutions and companies All of the content is from peer reviewed sources and all of it is written assembled and edited by the editors at ScholarlyEditions and available exclusively from us You now have a source you can cite with authority confidence and credibility More information is available at <http://www.ScholarlyEditions.com> **Coal Spontaneous**

Combustion Theory with Chain Self-promoted Oxidizing Induced by Active Group Jun Deng, Yaqing Li, Saeid Zeinali Heris, Chi-Min Shu, 2025-07-23 This book provides a scientific basis for development of targeted inhibitors and directional inhibitors of preventing spontaneous combustion of coal This book applied solvent extraction assisted by ultrasonic into the study of coal spontaneous combustion and hence broken through the technical bottlenecks of existing studies for mechanisms of coal spontaneous combustion Further the theories of particles physics were firstly combined with theories of coal chemistry and finally explained some previous conjectures scientifically in this book Thus the theory of spontaneous

combustion of coal has been greatly broadened and deepened Moreover a new theory named Chain self promoted oxidizing coal spontaneous combustion theory induced by active group was proposed in this book This theory elucidates the correlation mechanism between coal active groups and indicator gases explaining the mechanism of indicator gas generation in coal spontaneous combustion and providing a theoretical basis for establishing an early warning indicator system for coal spontaneous combustion This is very easy to be understood by audience with working in the field of mining or coal chemistry Besides principles of theories used in this book were explained in detail in this book That is to say there are almost no challenges or pain points for the audiences to overcome *Modern Aspects of Main Group Chemistry* Michael Lattman, Richard Alan Kemp, 2006 The last twenty years has seen a resurgence in main group chemistry from the fundamental breakthroughs involving multiple bonding in silicon phosphorus and other heavier elements to the present day applications in materials and nanotechnology Main group compounds are used in the synthesis of nano and mesoporous materials via sol gel methods particularly in silicate chemistry and in the preparation of materials such as boron nitrides and chemically modified single walled nanotubes Ceramics and dense materials are almost all made using oxides carbides nitrides or borides Inorganic polymers such as polyphosphazenes semiconductor group 13 15 14 16 compounds coatings catalysts all are important aspects of main group chemistry The contents of this book cover a broad range of main group chemistry from the fundamental to the applied *Comprehensive Inorganic Chemistry II*, 2013-07-23 Comprehensive Inorganic Chemistry II Nine Volume Set reviews and examines topics of relevance to today's inorganic chemists Covering more interdisciplinary and high impact areas Comprehensive Inorganic Chemistry II includes biological inorganic chemistry solid state chemistry materials chemistry and nanoscience The work is designed to follow on with a different viewpoint and format from our 1973 work Comprehensive Inorganic Chemistry edited by Bailar Emel us Nyholm and Trotman Dickenson which has received over 2 000 citations The new work will also complement other recent Elsevier works in this area Comprehensive Coordination Chemistry and Comprehensive Organometallic Chemistry to form a trio of works covering the whole of modern inorganic chemistry Chapters are designed to provide a valuable long standing scientific resource for both advanced students new to an area and researchers who need further background or answers to a particular problem on the elements their compounds or applications Chapters are written by teams of leading experts under the guidance of the Volume Editors and the Editors in Chief The articles are written at a level that allows undergraduate students to understand the material while providing active researchers with a ready reference resource for information in the field The chapters will not provide basic data on the elements which is available from many sources and the original work but instead concentrate on applications of the elements and their compounds Provides a comprehensive review which serves to put many advances in perspective and allows the reader to make connections to related fields such as biological inorganic chemistry materials chemistry solid state chemistry and nanoscience Inorganic chemistry is rapidly developing which brings about the need for a

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