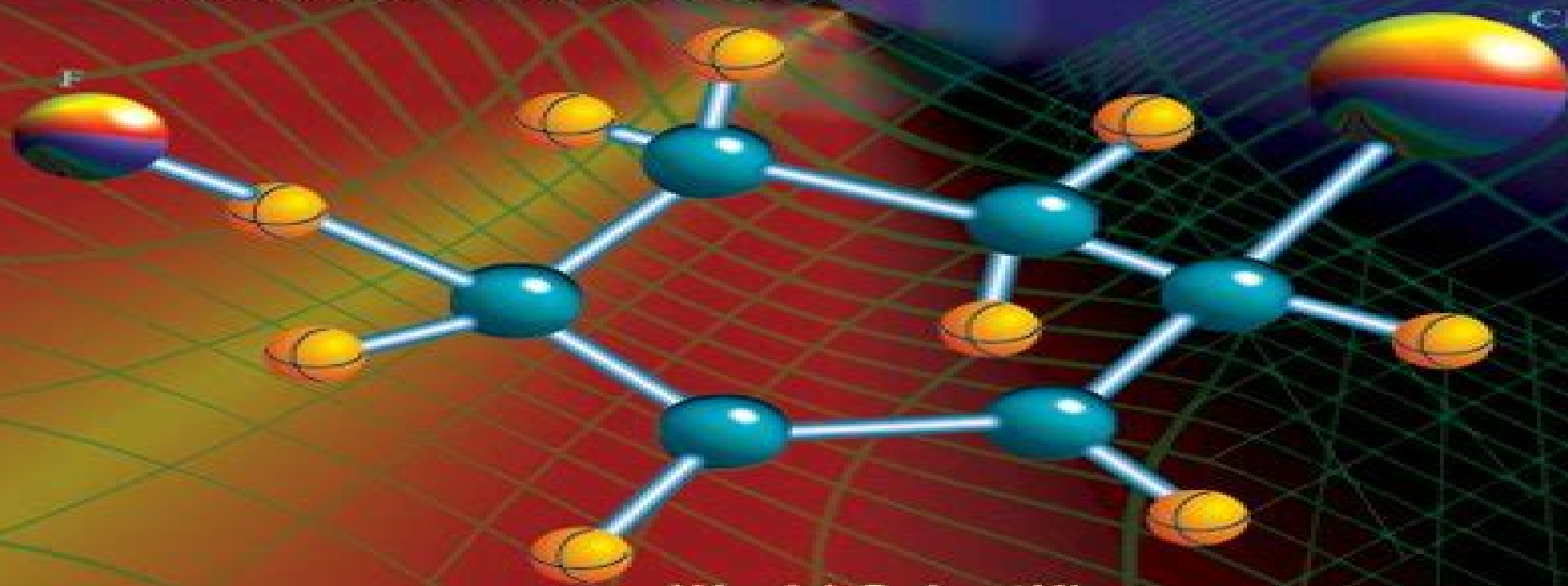


MODERN ELECTRONIC STRUCTURE THEORY AND APPLICATIONS IN ORGANIC CHEMISTRY

Editor
Ernest R Davidson



World Scientific

Modern Electronic Structure Theory And Applications In Organic Chemistry

Ernest R. Davidson



Modern Electronic Structure Theory And Applications In Organic Chemistry:

Modern Electronic Structure Theory and Applications in Organic Chemistry Ernest R. Davidson, 1997 This volume focuses on the use of quantum theory to understand and explain experiments in organic chemistry High level ab initio calculations when properly performed are useful in making quantitative distinctions between various possible interpretations of structures reactions and spectra Chemical reasoning based on simpler quantum models is however essential to enumerating the likely possibilities The simpler models also often suggest the type of wave function likely to be involved in ground and excited states at various points along reaction paths This preliminary understanding is needed in order to select the appropriate higher level approach since most higher level models are designed to describe improvements to some reasonable zeroth order wave function Consequently most of the chapters in this volume begin with experimental facts and model functions and then progress to higher level theory only when quantitative results are required In the first chapter Zimmerman discusses a wide variety of thermal and photochemical reactions of organic molecules Gronert discusses the use of ab initio calculations and experimental facts in deciphering the mechanism of elimination reactions in the gas phase Bettinger et al focus on carbene structures and reactions with comparison of the triplet and singlet states Next Hrovat and Borden discuss more general molecules with competitive triplet and singlet contenders for the ground state structure Cave explains the difficulties and considerations involved with many of the methods and illustrates the difficulties by comparing with the UV spectra of short polyenes Jordan et al discuss long range electron transfer using model compounds and model Hamiltonians Finally Hiberty discusses the breathing orbital valence bond model as a different approach to introducing the crucial correlation that is known to be important in organic reactions

Perspectives in Electronic Structure Theory

Roman F. Nalewajski, 2012-03-26 The understanding in science implies insights from several different points of view Alternative modern outlooks on electronic structure of atoms and molecules all rooted in quantum mechanics are presented in a single text Together these complementary perspectives provide a deeper understanding of the localization of electrons and bonds the origins of chemical interaction and reactivity behavior the interaction between the geometric and electronic structure of molecules etc In the opening two parts the basic principles and techniques of the contemporary computational and conceptual quantum chemistry are presented within both the wave function and electron density theories This background material is followed by a discussion of chemical concepts including stages of the bond formation processes chemical valence and bond multiplicity indices the hardness softness descriptors of molecules and reactants and general chemical reactivity stability principles The insights from Information Theory the basic elements of which are briefly introduced including the entropic origins and Orbital Communication Theory of the chemical bond are the subject of Part IV The importance of the non additive interference information tools in exploring patterns of chemical bonds and their covalent and ionic components will be emphasized

Modern Physical Organic Chemistry Eric V. Anslyn, Dennis A.

Dougherty, 2006 Making explicit the connections between physical organic chemistry and critical fields such as organometallic chemistry materials chemistry bioorganic chemistry and biochemistry this book escorts the reader into an area that has been thoroughly updated in recent times **Reviews in Computational Chemistry, Volume 20** Kenny B. Lipkowitz, Raima Larter, Thomas R. Cundari, Donald B. Boyd, 2004-08-02 THIS VOLUME LIKE THOSE PRIOR TO IT FEATURES CHAPTERS BY EXPERTS IN VARIOUS FIELDS OF COMPUTATIONAL CHEMISTRY TOPICS COVERED IN VOLUME 20 INCLUDE VALENCE THEORY ITS HISTORY FUNDAMENTALS AND APPLICATIONS MODELING OF SPIN FORBIDDEN REACTIONS CALCULATION OF THE ELECTRONIC SPECTRA OF LARGE MOLECULES SIMULATING CHEMICAL WAVES AND PATTERNS FUZZY SOFT COMPUTING METHODS AND THEIR APPLICATIONS IN CHEMISTRY AND DEVELOPMENT OF COMPUTATIONAL MODELS FOR ENZYMES TRANSPORTERS CHANNELS AND RECEPTORS RELEVANT TO ADME TOX 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 MODELING 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 **A Chemist's Guide to Valence Bond Theory** Sason S. Shaik, Philippe C. Hiberty, 2007-12-04 This reference on current VB theory and applications presents a practical system that can be applied to a variety of chemical problems in a uniform manner After explaining basic VB theory it discusses VB applications to bonding problems aromaticity and antiaromaticity the dioxygen molecule polyradicals excited states organic reactions inorganic organometallic reactions photochemical reactions and catalytic reactions With a guide for performing VB calculations exercises and answers and numerous solved problems this is the premier reference for practitioners and upper level students

Modern Electronic Structure Theory David Yarkony, 1995 Modern Electronic Structure Theory provides a didactically oriented description of the latest computational techniques in electronic structure theory and their impact in several areas of chemistry The book is aimed at first year graduate students or college seniors considering graduate study in computational chemistry or researchers who wish to acquire a wider knowledge of this field **A Chemist's Guide to Density Functional Theory** Wolfram Koch, Max C. Holthausen, 2015-11-18 Chemists familiar with conventional quantum mechanics will applaud and benefit greatly from this particularly instructive thorough and clearly written exposition of density functional theory its basis concepts terms implementation and performance in diverse applications Users of DFT for structure energy and molecular property computations as well as reaction mechanism studies are guided to the optimum choices of the most effective methods Well done Paul von Rague Schleyer A conspicuous hole in the computational chemist's library is nicely filled by this book which provides a wide ranging and pragmatic view of the subject It should justifiably become the favorite

text on the subject for practioneers who aim to use DFT to solve chemical problems J F Stanton J Am Chem Soc The authors aim is to guide the chemist through basic theoretical and related technical aspects of DFT at an easy to understand theoretical level They succeed admirably P C H Mitchell Appl Organomet Chem The authors have done an excellent service to the chemical community A Chemist s Guide to Density Functional Theory is exactly what the title suggests It should be an invaluable source of insight and knowledge for many chemists using DFT approaches to solve chemical problems M Kaupp Angew Chem

Advances in Carbene Chemistry, Volume 3 U.H. Brinker,2001-10-24 Our understanding of carbene chemistry has advanced dramatically especially in the last decade and new developments continue to emerge Some of the recent exciting findings have been collected in the first and second volumes of Advances in Carbene Chemistry With the third volume the series continues to provide a periodic coverage of carbene chemistry in its broadest sense Beginning as chemical curiosities carbenes are now solidly established as reactive intermediates with fascinating and productive research areas of their own Five decades of divalent carbon chemistry have provided us with a vast repertoire of new unusual and surprising reactions Some of those reactions once classified as exotic have become standard methods in organic synthesis These highly reactive carbene species have been harnessed and put to work to achieve difficult synthetic tasks other reactive intermediates cannot easily perform The fruitful relationship between experiment and theory has pushed carbene chemistry further toward the direction of reaction control that is regio and stereoselectivity in intra and intermolecular addition and insertion reactions The interplay between experiment and modern spectroscopy has led to the characterization of many carbenes that are crucial to both an understanding and further development of this field

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

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Modern Electronic Structure Theory (In 2 Parts) - Part 1 David R Yarkony,1995-09-28 Modern Electronic Structure Theory provides a didactically oriented description of the latest

computational techniques in electronic structure theory and their impact in several areas of chemistry The book is aimed at first year graduate students or college seniors considering graduate study in computational chemistry or researchers who wish to acquire a wider knowledge of this field

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