

## A Chemists Guide To Valence Bond Theory

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A Chemist's Guide to Valence Bond Theory by Sason S. Shaik and Philippe C. Hiberty offers a wealth of information on valence bond theory (VBT) that is on the cutting edge of molecular bond computational theory (MBCT). Since their conception, molecular orbital theory (MOT) and valence bond theory have been hotly debated topics in chemistry regarding whether and which theory describes the empirical and computational behavior of the molecular bond.

**Review of A Chemist's Guide to Valence Bond Theory ...**

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 ...

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**A Chemist's Guide to Valence Bond Theory: Shaik, Sason ...**

After an introduction, A Chemist's Guide to Valence Bond Theory pre-sents a practical system that can be applied to a variety of chemical problems in a uniform manner. Concise yet comprehensive, it includes: A tour of some VB outputs and terminology. An explanation of basic VB theory

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a chemists guide to valence bond theory is for upper level undergraduate students graduate level students or researchers interested in the vbt approach to molecular bond computations a thorough understanding of quantum theory and a familiarity with molecular bond calculations is a must when reading this book chapters 2 9 and 10 are devoted to the understanding and workings of vbt

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chemists guide to get this from a library a chemists guide to valence bond theory sason s shaik philippe c hiberty intended for chemists who are not necessarily experts on theory but have some background in quantum chemistry the chemists guide to valence bond theory is designed to teach chemists how to use vb chemists guide to valence

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.

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Along with the doctrine of atomism, the electron theory of valance ranks as one of the most fundamental developments in the history of modern chemistry. Yet, because the problems this theory solved were difficult ones, the modern understanding of electron bonding came only slowly and only after the minor contributions of many scientists and the major contributions of a few. Following the discovery of the electron by J. J. Thomson at Cambridge in 1897, scientists quickly concluded that the bonds holding atoms in a molecule were electrostatic or polar and resulted from complete electron transfer. Soon, though, other chemists pointed out that the behavior of many organic molecules was inconsistent with the polar theory. Despite the work of many scientists, it was not until 1916 that one---G. N. Lewis---succeeded in putting forward the currently accepted electronic mechanism for the non polar bond---the shared electron pair. In this lucidly written and carefully documented study, the author traces the gradual transition from a purely polar theory to one requiring two kinds of bonds, polar and nonpolar, and demonstrates that Lewis, with his far-reaching idea of the shared electron pair bond, was the central figure in this scientific drama. The focus on Lewis and other major researchers and the detailed attention to more minor actors illustrate both how individual contributions to the solution of perplexing problems fit within general trends and how one individual mind can rise above an era's state of knowledge to advance science. The coherent story told here helps meet a great need for the historical study of recent periods in the development of the sciences and should appeal not only to chemists but to all interested in the history of science and the history of thought.

The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research. The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology, medicine and materials science. The goal of each thematic volume is to give the non-specialist reader, whether in academia or industry, a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience. Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years are presented using selected examples to illustrate the principles discussed. The coverage is not intended to be an exhaustive summary of the field or include large quantities of data, but should rather be conceptual, concentrating on the methodological thinking that will allow the non-specialist reader to understand the information presented. Contributions also offer an outlook on potential future developments in the field. Review articles for the individual volumes are invited by the volume editors. Readership: research chemists at universities or in industry, graduate students

This book explains key concepts in theoretical chemistry and explores practical applications in structural chemistry. For experimentalists, it highlights concepts that explain the underlying mechanisms of observed phenomena, and at the same time provides theoreticians with explanations of the principles and techniques that are important in property design. Themes covered include conceptual and applied wave functions and density functional theory (DFT) methods, electronegativity and hard and soft (Lewis) acid and base (HSAB) concepts, hybridization and aromaticity, molecular magnetism, spin transition and thermochromism. Offering insights into designing new properties in advanced functional materials, it is a valuable resource for undergraduates of physical chemistry, cluster chemistry and structure/reactivity courses as well as graduates and researchers in the fields of physical chemistry, chemical modeling and functional materials.

Winner of 2018 PROSE Award for MULTIVOLUME REFERENCE/SCIENCE This encyclopedia offers a comprehensive and easy reference to physical organic chemistry (POC) methodology and techniques. It puts POC, a classical and fundamental discipline of chemistry, into the context of modern and dynamic fields like biochemical processes, materials science, and molecular electronics. Covers basic terms and theories into organic reactions and mechanisms, molecular designs and syntheses, tools and experimental techniques, and applications and future directions Includes coverage of green chemistry and polymerization reactions Reviews different strategies for molecular design and synthesis of functional molecules Discusses computational methods, software packages, and more than 34 kinds of spectroscopies and techniques for studying structures and mechanisms Explores applications in areas from biology to materials science The Encyclopedia of Physical Organic Chemistry has won the 2018 PROSE Award for MULTIVOLUME REFERENCE/SCIENCE. The PROSE Awards recognize the best books, journals and digital content produced by professional and scholarly publishers. Submissions are reviewed by a panel of 18 judges that includes editors, academics, publishers and research librarians who evaluate each work for its contribution to professional and scholarly publishing. You can find out more at: proseawards.com Also available as an online edition for your library, for more details visit Wiley Online Library

A novel proposal for teaching organic chemistry based on a broader and simplified use of quantum chemistry theories and notions of some statistical thermodynamic concepts aiming to enrich the learning process of the organic molecular properties and organic reactions. A detailed physical chemistry approach to teach organic chemistry for undergraduate students is the main aim of this book. A secondary objective is to familiarize undergraduate students with computational chemistry since most of illustrations of optimized geometries (plus some topological graphs) and information is from quantum chemistry outputs which will also enable students to obtain a deeper understanding of organic chemistry.

Divided into five major parts, the two volumes of this ready reference cover the tailoring of theoretical methods for biochemical computations, as well as the many kinds of biomolecules, reaction and transition state elucidation, conformational flexibility determination, and drug design. Throughout, the chapters gradually build up from introductory level to comprehensive reviews of the latest research, and include all important compound classes, such as DNA, RNA, enzymes, vitamins, and heterocyclic compounds. The result is in-depth and vital knowledge for both readers already working in the field as well as those entering it. Includes contributions by Prof. Ada Yonath (Nobel Prize in Chemistry 2009) and Prof. Jerome Karle (Nobel Prize in Chemistry 1985).

"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 Ragué 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 [...] should justifiably become the favorite text on the subject for practitioners 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.

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