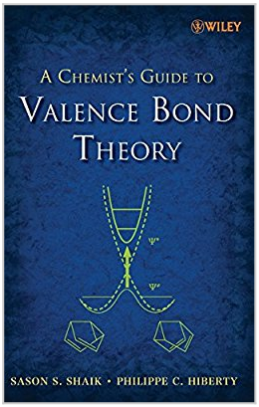

A Chemist's Guide to Valence Bond Theory

By Sason S. Shaik, Philippe C. Hiberty

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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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Editorial Review

Review
"The textbook provides a qualitative overview of the possibilities within the VB approach. As such, we strongly recommend it, both to interested chemists and to university libraries." (*Angewandte Chemie International Edition*, December 8, 2008)

From the Back Cover

Modern valence bond theory and state-of-the-art methodologies

Since the 1980s, valence bond (VB) theory has enjoyed a renaissance characterized both in the qualitative application of the theory and in the development of new methods for its computer implementation. Written by leading authorities, this is the premier reference on current VB theory and applications in a pedagogical context, perhaps the first such attempt since Pauling's The Nature of the Chemical Bond. 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
- A discussion of various applications of the VB method to chemical problems, encompassing bonding problems, aromaticity and antiaromaticity, the dioxygen molecule, polyradicals, excited states, organic reactions, inorganic/organometallic reactions, photochemical reactions, and catalytic reactions
- Samples of inputs/outputs and instructions for interpreting results
- A short programmable outline for converting molecular orbital wave functions to VB structures
- A guide for performing VB calculations

Complete with exercises and answers at the end of chapters, numerous solved problems, and a glossary of terms and symbols, this is the authoritative guide for computational chemists, chemical physicists, and research chemists in organic and organometallic/inorganic chemistry concerned with reactivity and molecular structure. It is also an excellent text for advanced undergraduate and graduate students.

About the Author
Sason S. Shaik, PhD, is a Professor and the Director of the Lise Meitner-Minerva Center for Computational Quantum Chemistry in the Hebrew University in Jerusalem. He has been a Fulbright Fellow (1974-1979) and became a Fellow of the AAAS in 2005. Among his awards are the Israel Chemical Society Medal for the Outstanding Young Chemist (1987), the Alexander von Humboldt Senior Award in 1996-1999, the 2001 Kolthoff Award, the 2001 Israel Chemical Society Prize, and the 2007 Schrödinger Medal of WATOC. His research interests are in the use of quantum chemistry to develop paradigms that can pattern data and lead to the generation and solution of new problems. From 1981-1992, the main focus of his research was on valence bond theory and its relationship to MO theory, and during that time, he developed a general model of reactivity based on a blend of VB and MO elements. In 1994, he entered the field of oxidation and bond activation by metal oxo catalysts and enzymes, an area where he has contributed several seminal ideas (e.g., two-state reactivity) that led to resolution of major controversies and new predictions.

Philippe C. Hiberty is Director of Research at the Centre National de la Recherche Scientifique (CNRS)

and a member of the Theoretical Chemistry Group in the Laboratoire de Chimie Physique at the?University of Paris-Sud. He taught quantum chemistry for years at the Ecole Polytechique in Palaiseau. He received the Grand Prix Philippe A. Guye from the French Academy of Sciences in 2002. Under the supervision of Professor Lionel Salem, he devoted his PhD to building a bridge between MO and VB theories by devising a method for mapping MO wave functions to VB ones. In collaboration with Professor Sason Shaik, he applied VB theory to fundamental concepts of organic chemistry such as aromaticity, hypervalence, odd-electron bonds, prediction of reaction barriers from properties of reactants and products, and so on. He is the originator of the Breathing-Orbital Valence Bond method, which is aimed at combining the lucidity of compact VB wave functions with a good accuracy of the energetics.

Users Review

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Mike Hendrix:

As people who live in typically the modest era should be revise about what going on or info even knowledge to make them keep up with the era which is always change and advance. Some of you maybe will update themselves by reading through books. It is a good choice in your case but the problems coming to you actually is you don't know what one you should start with. This A Chemist's Guide to Valence Bond Theory is our recommendation to cause you to keep up with the world. Why, because this book serves what you want and need in this era.

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