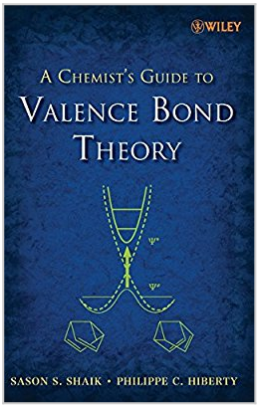

A Chemist's Guide to Valence Bond Theory

By Sason S. Shaik, Philippe C. Hiberty

A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty

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.

A Chemist's Guide to Valence Bond Theory

By Sason S. Shaik, Philippe C. Hiberty

A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty

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.

A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty Bibliography

- Sales Rank: #3910621 in Books
- Published on: 2007-12-04
- Original language: English
- Number of items: 1
- Dimensions: 9.50" h x .80" w x 6.40" l, 1.35 pounds
- Binding: Hardcover
- 332 pages

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

From reader reviews:

James Reed:

This A Chemist's Guide to Valence Bond Theory book is absolutely not ordinary book, you have it then the world is in your hands. The benefit you obtain by reading this book is usually information inside this e-book incredible fresh, you will get details which is getting deeper you actually read a lot of information you will get. This specific A Chemist's Guide to Valence Bond Theory without we realize teach the one who studying it become critical in considering and analyzing. Don't be worry A Chemist's Guide to Valence Bond Theory can bring any time you are and not make your handbag space or bookshelves' turn out to be full because you can have it in your lovely laptop even telephone. This A Chemist's Guide to Valence Bond Theory having excellent arrangement in word and layout, so you will not really feel uninterested in reading.

Mildred Miller:

The particular book A Chemist's Guide to Valence Bond Theory will bring one to the new experience of reading any book. The author style to describe the idea is very unique. In the event you try to find new book to see, this book very suited to you. The book A Chemist's Guide to Valence Bond Theory is much recommended to you to read. You can also get the e-book from the official web site, so you can easier to read the book.

Rose Ibarra:

Is it you actually who having spare time after that spend it whole day by watching television programs or just laying on the bed? Do you need something new? This A Chemist's Guide to Valence Bond Theory can be the answer, oh how comes? A fresh book you know. You are and so out of date, spending your extra time by reading in this brand new era is common not a geek activity. So what these guides have than the others?

Bruno Reed:

In this particular era which is the greater man or woman or who has ability to do something more are more special than other. Do you want to become among it? It is just simple approach to have that. What you are related is just spending your time very little but quite enough to possess a look at some books. One of the

books in the top collection in your reading list is definitely A Chemist's Guide to Valence Bond Theory. This book which is qualified as The Hungry Hills can get you closer in turning into precious person. By looking right up and review this reserve you can get many advantages.

Read A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty for online ebook

A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty Free PDF d0wnl0ad, audio books, books to read, good books to read, cheap books, good books, online books, books online, book reviews epub, read books online, books to read online, online library, greatbooks to read, PDF best books to read, top books to read A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty books to read online.

Online A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty ebook PDF download

A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty Doc

A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty Mobipocket

A Chemist's Guide to Valence Bond Theory By Sason S. Shaik, Philippe C. Hiberty EPub