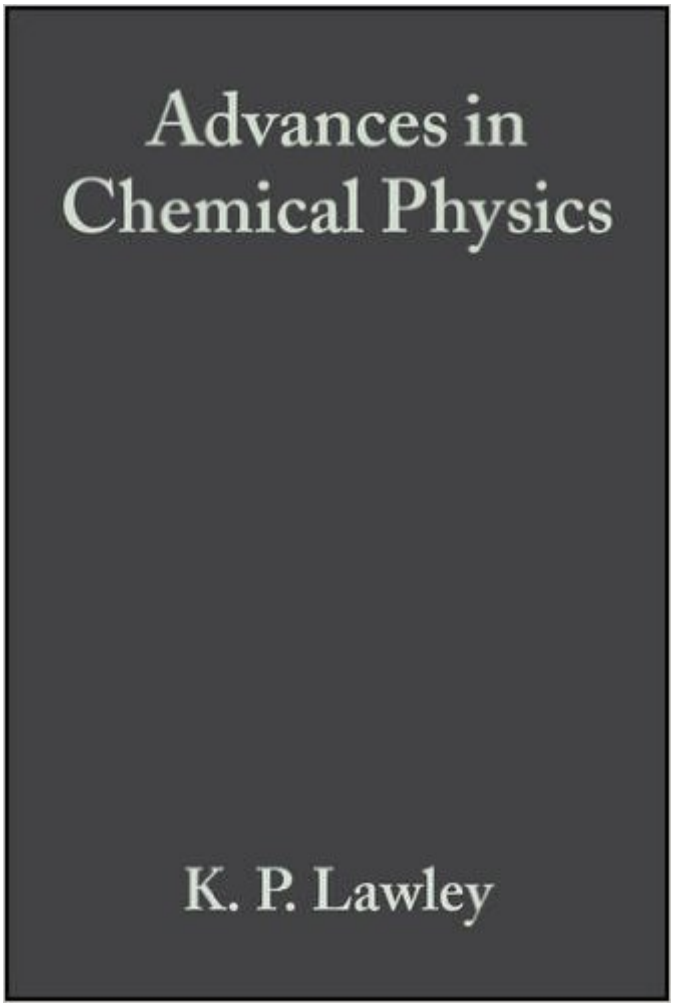
# AB INITIO Methods In Quantum Chemistry 2 (Advances In Chemical Physics) (Vol 67)



## Synopsis

The Advances in Chemical Physics series provides the chemical physics and physical chemistry fields with a forum for critical, authoritative evaluations of advances in every area of the discipline. Filled with cutting-edge research reported in a cohesive manner not found elsewhere in the literature, each volume of the Advances in Chemical Physics series serves as the perfect supplement to any advanced graduate class devoted to the study of chemical physics.

## Book Information

Series: Advances in Chemical Physics (Book 69)

Hardcover: 598 pages

Publisher: Wiley-Interscience; 1 edition (May 20, 1987)

Language: English

ISBN-10: 0471909017

ISBN-13: 978-0471909019

Product Dimensions: 6.3 x 1.4 x 9.3 inches

Shipping Weight: 2.2 pounds

Average Customer Review: 4.0 out of 5 starsÂ Â See all reviewsÂ (2 customer reviews)

Best Sellers Rank: #4,894,770 in Books (See Top 100 in Books) #70 inÂ Books > Science & Math > Chemistry > Chemical Physics #332 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #10862 inÂ Books > Science & Math > Chemistry > General & Reference

## Customer Reviews

There have been a few good books covering the basic molecular orbital theory but they offer very little information on how one should deal with structures beyond ground state closed-shell systems. Such problems are commonly known as closed-shell HF-type problems and are only a small fraction of the issues in the electronic strucuture theory. It is impossible to go through graduate school let alone publish papers and win grants with just the HF-type capabilities and one’s minimal knowledge today should really include a good grasp on the multiconfigurational thoeries. It is a vast and deep field like others and a compact yet efficient review is very rare indeed. This review should serve as an effective guide to elevate oneself above the closed-shell HF theory, provided that he has acquired sufficient knowledge on the textbook molecular orbital theory and basic linear algebra. Experimental chemists will probably find the material a little indigestable. Recommended for more physics-oriented readers who are prepared to spend time on other references quoted therein, as it

is not a self-contained introduction on the multiconfigurational SCF theory.

This book is essentially a textbook on MCSCF theory, and a very good one at that. Werner, Shephard and Roos all write about their particular area of MCSCF theory: Werner on direct CI methods, Shepard a 198 page summary of everything one might need to know, from theory to optimal Fortran loops, and Roos on CASSCF. The section by Pulay on analytic derivatives is excellent as well, while the rest of the book is quite dated (Xa DFT, "modern VB theory", and the two applications chapters are not worth reading. Finally, the chapter on propagators by Oddershede is not bad at all; unfortunately those methods have gone out of favor in the general community, although good work using these methods still comes out of the Gainesville-Uppsala school. More recent articles can be found in the "Advances in Quantum Chemistry" series, particularly the recent on in honor of Ohrn and Lindenberg.Because of the absence of an authoritative book on MCSCF theory, this is one of the few books in this series worth actually buying, since more than half of the book is worth photocopying.I disagree with the other reviewer’s characterization that this is for the physics-minded. This is a book for serious quantum chemists who own or internalized Helgaker-Olsen-Jorgensen’s masterpiece, "Molecular Electronic Structure Theory". If you’re not fluent at that level, do not bother with this book. This series is meant for experts (see the first few pages).

Advances in Chemical Physics: Modern Nonlinear Optics, Volume 119, Part 1, 2nd Edition AB INITIO Molecular Orbital Theory Physical Chemistry Vol 2: Quantum Chemistry The Physics and Philosophy of the Bible: How Relativity, Quantum Physics, Plato, and History Meld with Biblical Theology to Show That God Exists and That ... Live Forever (The Inevitable Truth Book 1) Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond (Dover Books on Physics) The Chemical Physics of Ice (Cambridge Monographs on Physics) Fundamental Aspects of Plasma Chemical Physics: Transport (Springer Series on Atomic, Optical, and Plasma Physics) Introduction to Chemical Physics (International Series In Pure And Applied Physics)