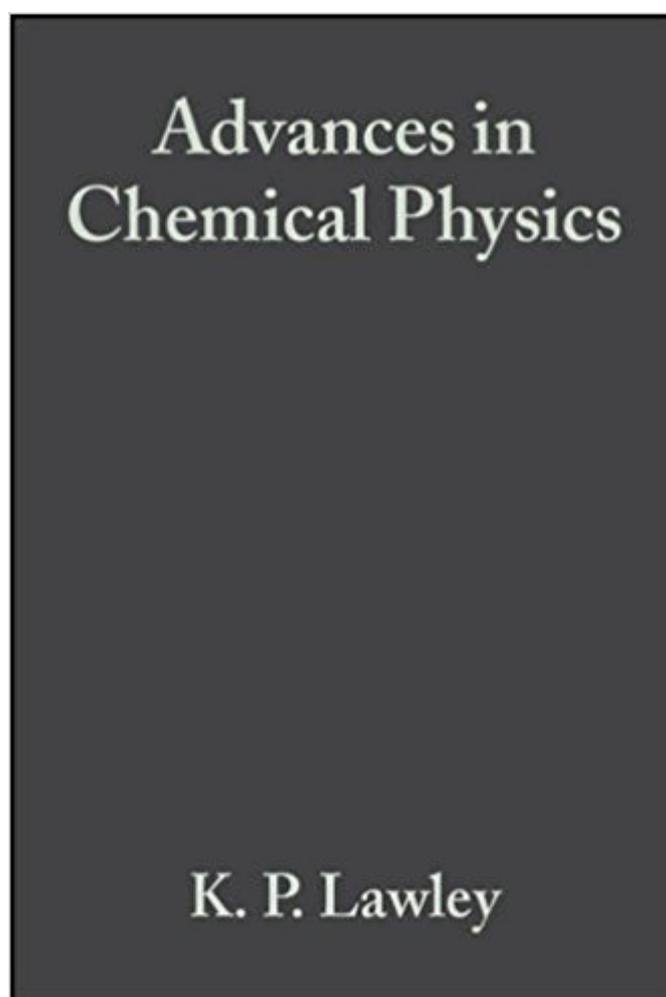


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# AB INITIO Methods In Quantum Chemistry 2 (Advances In Chemical Physics) (Vol 67)



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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 structure 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 theories. 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 indigestible. 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 one 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).

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