# BOOK REVIEWS

Selection of books for review is based on the editor's opinions regarding possible reader interest and on the availability of the book to the editor. Occasional selections may include books on topics somewhat peripheral to the subject matter ordinarily considered acceptable.

## The Hartree-Fock Method for Atoms

*Author* Charlotte Froese Fischer

*Publisher* John Wiley and Sons, Inc., New York (1977)

*Pages* 308

*Price* $22.95

*Reviewer* Jack Simons

This research-level reference book by Charlotte Froese Fischer represents a major contribution to the numerical calculation of Hartree-Fock (HF) wave functions for atomic systems. Froese Fischer's own research efforts have established her as a leading expert in this area of quantum theory. In fact, many of the computational and numerical analysis tools discussed in this book have resulted from her own scientific investigations. It is my opinion that Froese Fischer's experience and knowledge make her an eminently qualified scientist to undertake the task of presenting an up-to-date overview of numerical HF theory.

The first two chapters of this book are devoted to a review of the HF method as well as various further approximations that are currently very widely used (e.g., UHF, RHF, EHF). The derivation of the HF equations, including a clear treatment of the Lagrange multipliers, is combined with good illustrative numerical results and a discussion of the shapes of the radial wave functions.

Chapters 3 and 4 contain a discussion of several techniques for treating electron correlation in atomic systems. Little attempt is made to cover a wide variety of modern approaches to the correlation problem. Instead, the author emphasizes the perturbation theory approach and the multiconfigurational HF (MCHF) method. The MCHF variational equations are derived, and the results of applying this method to several states of small atoms are clearly discussed. In Chap. 5, Froese Fischer analyzes how one computes atomic expectation values and transition properties at both the HF and correlated levels. As in her earlier treatment of correlation contributions to atomic state energies, the author does not attempt to cover more recent approaches to these problems (e.g., many-body techniques, equations-of-motion theory, or Green's function theory).

In Chaps. 6 and 7, Froese Fischer presents what, in her opinion, represents the optimal numerical methods for use in HF and MCHF calculations. As in the earlier chapters, the author employs results that have been taken from the literature to illustrate the accuracy and/or limitations of these numerical techniques. Largely through the research efforts of Froese Fischer, the solution procedures for the HF equations outlined in Chap. 6 have become well accepted and widely used within the theoretical chemistry community. Because the MCHF approach to electronic structure investigation is more modern, its numerical methods are not yet as widely known. Hence, it is likely that most researchers in atomic structure theory will derive much benefit from Chap. 7.

In summary, I feel that this book contains an excellent research-level discussion of the numerical approach to HF and MCHF calculations. I believe that scientists whose research is in atomic and molecular physics, theoretical chemistry, or nuclear structure theory should read this book.

*Jack Simons (BS, chemistry, Case Institute of Technology, 1967; PhD, chemistry, University of Wisconsin, 1970) has been on the chemistry faculty at the University of Utah since 1971. He is a recognized leader in the application and development of quantum chemical methods to the electronic structure of atoms and molecules. He is especially well known for his pioneering research into the electronic structure of negative molecular ions.*

## Traité de Neutronique—Physique et Calcul des Réacteurs Nucléaires

*Authors* J. Bussac and P. Reuss

*Publisher* Hermann, Éditeurs des Sciences et des Arts

*Pages* 662

*Price* 190 francs

*Reviewer* H. J. M. Bowen

This volume is, I believe, the first detailed monograph in French describing theories of neutron behavior and their application to nuclear reactors. It is aimed at post-graduate