

of establishing the forms of relativistic wave functions and the specific relativistic effects as defined by the Breit–Pauli approximation.

The fourth chapter begins with the presentation of the relativistic Hamiltonian operator appropriate for use in calculations on molecular systems. The second section presents relativistic effective core potentials (RECPs) and their use in representing the core electrons and core- and valence-electron interactions. The author then shows in Section 3 how the RECPs provide the point of departure for the computational electronic structure methods that he and others have developed over the past 20 years. Clearly, the author has chosen to present the methods he has used in his extensive list of published studies on molecules and clusters. Alternative methods developed by other groups using RECPs, model potentials, and all-electron procedures are largely neglected, although some are referenced at the end of the chapter. Readers especially interested in all-electron relativistic methods will not find this volume useful as a resource in gaining an in-depth understanding of these approaches. The works alluded to above will address these areas and should be available soon. It is this reviewer's opinion that the basic philosophy behind the research directions of Balasubramanian and his colleagues has been one belonging to a chemist and molecular spectroscopist; viz., core electrons do not play a role in chemical bonding and spectra and, consequently, can be removed from the problem, as long as an accurate, first-principles method such as that underlying RECPs can be employed. Major advances in all-electron methods, together with technological advances in supercomputing, may make them competitive with pseudopotential-based methods in the future. However, concomitant advances in the latter raise questions regarding the necessity for incorporation of the additional cost and complexity mandated by all-electron approaches. In this context, the present volume presents techniques that will be in use for the foreseeable future, and it provides one of the best sources for detailed background material. The last section of Chapter 4 discusses two approximate methods that are becoming more generally used: the local density functional and semiempirical approaches.

The last chapter is the jewel of the volume and the one of most value to active researchers in the field. Entitled Double-Group Symmetry and the Classification of Relativistic Electronic States, it fills an enormous void in the available reference literature. Theoretical chemists and molecular spectroscopists will be pleased to have access to the development presented here. That the electron angular momentum coupling of molecular electronic states, especially those of molecules containing one or more heavy elements, is intermediate in nature is a fact not generally appreciated nor understood by the chemical and molecular physics community. Balasubramanian admirably develops this problem, beginning with discussions of double group symmetry in the first five sections. The 12 tables comprised of double group character tables, electronic states derived from separated atoms, molecular term symbols, nonrelativistic–relativistic correlations, and direct products are invaluable for the construction and analysis of relativistic molecular wave functions for diatomics. The same information is presented for polyatomics in Sections 6 and 7. The section includes double group character tables for all of the important molecular point groups. The chapter concludes with a section on symmetry-adapted spin functions for electronic states. This subject is especially important in the context of the increasingly popular spin–orbit configuration interaction and related methods whereby initial (active-space) wave functions are defined in terms of nonrelativistic angular momentum coupling, i.e., molecular orbitals built as linear combinations of atomic spin orbitals, and the final Hamiltonian matrix is constructed in the presence of spin–orbit coupling operators. (This method is to be contrasted with those employing atomic basis sets of four- or two-component spinors.) The author shows how double group symmetry-adapted configuration sets are constructed for polyatomic systems using the proper combinations of  $\alpha$  and  $\beta$  spin functions. This chapter is of practical value to the researcher involved with the calculation and analysis of electronic states of molecules that contain heavy elements.

This book can be used as an introduction to relativistic quantum chemistry for advanced graduate students. I would be inclined to use it as a text for such a graduate course. In particular, the material contained in Chapter 3 condenses much of the subject matter presented in advanced treatises or relativistic quantum mechanics texts into a form appropriate for the classroom. The detailed solution of the relativistic hydrogen atom is especially well-conceived. The incorporation of some of the language of relativistic quantum chemistry is, at long last, finding its way into new physical chemistry, inorganic

chemistry, and even general chemistry textbooks. The insightful work of such pioneers as Kenneth Pitzer and Pekka Pyykkö inspired the quantitative developments that are in extensive use today. This book is a good introduction to the general subject and presents, together with Balasubramanian's second volume (*Part B: Applications*), an extensive treatise on the methods used by the author and his applications to a vast number of molecules and clusters containing heavy elements. This book is a valuable addition to the literature dealing with relativistic quantum chemistry and is highly recommended.

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**HPLC and CE: Principles and Practice.** By Andrea Weston (Dionex) and Phyllis R. Brown (University of Rhode Island). Academic Press: San Diego. 1997. xiv + 280 pp. \$69.95. ISBN 0-12-136640-5.

This book is unique in that it covers the basic principles, instrumentation, method development, and applications of both HPLC and capillary electrophoresis. (Similar books invariably deal with either a single technique or several.) Although the coverage of this volume is supposedly aimed at both novices and users, it is particularly suitable for use in teaching upper level undergraduate courses in analytical chemistry and instrumental analysis, and for individuals from other scientific disciplines who need to do separations but have no previous experience or basic knowledge of chromatography or capillary electrophoresis.

The first three chapters deal with HPLC. Chapter 1 covers fundamentals and principles. Chapter 2 deals with the different types of separations and the different modes of LC (affinity, chiral, hydrophobic interaction, reversed phase, and so on). Chapter 3 covers all the components of instrumentation (solvent delivery system, inlet, the column, and the various detectors), and also includes a rather extensive section on trouble-shooting. Trouble-shooting information is always very useful, but it is usually found only in handbooks intended for use in the laboratory.

The next three chapters, 4, 5, and 6, cover CE following the same organization as for HPLC, i.e., principles, modes of separation, and instrumentation. Again, each chapter concludes with a summary of major concepts, and the instrumentation section ends with several pages on trouble-shooting.

The final two chapters, 7 and 8, cover data manipulation and miniaturization for both HPLC and CE. Data manipulation in this case deals with the various methods of peak identification (by retention factors, UV and MS libraries, spiking with standards, etc.), and also includes methods of quantitative measurement. Miniaturization covers the various practical aspects of designing an HPLC or CE system based on chips, micromachining, and so on.

The material in each chapter is presented in a well-organized and easy to understand style. Everything is expressed in a manner that makes it easy for the reader to follow, to learn, and to remember. At the end of each chapter there is a section summarizing the major concepts. Because this is a compact book, it tends to provide information that is mainly of immediate and practical use to the practitioner (or the student). At the same time the book takes no shortcuts to provide the "reason why" in addition to the "how to". For example, in describing MECC (micellar electrokinetic capillary chromatography), it explains why this technique is commonly performed with anionic surfactants and why SDS (sodium dodecyl sulfate) is the preferred surfactant.

*HPLC and CE: Principles and Practice* is a well-organized and well-written handbook useful to anyone, but the expert, who is doing or planning to do HPLC or CE analysis.

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