



## Methods in Computational Chemistry: Volume 2 Relativistic Effects in Atoms and Molecules (Paperback)

By -

Springer-Verlag New York Inc., United States, 2011. Paperback. Condition: New. Language: English . Brand New Book \*\*\*\*\* Print on Demand \*\*\*\*\*. This volume is devoted to methods for the study of the effects of relativity on the electronic structure of atoms and molecules. The accurate description of relativistic effects in heavy atoms has long been recognized as one of the central problems of atomic physics. Contemporary relativistic atomic structure calculations can be performed almost routinely. Recent years have seen a growing interest in the study of the effects of relativity on the structure of molecules. Even for molecular systems containing atoms from these second rows of the periodic table the energy associated with relativistic effects is often larger than that arising from electron correlation. For molecules containing heavier atoms relativistic effects become increasingly important, and for systems containing very heavy atoms relativity is known to dominate many chemical properties. In this volume, one of the pioneers of relativistic atomic structure calculations, Jan P. Grant, provides a detailed survey of the computational techniques employed in contemporary studies of the effects of relativity on atomic structure. This is an area of research in which calculations can often lead to a particularly impressive degree of agreement between theory and experiment. Furthermore, these atomic studies have provided many of the foundations of a fully relativistic quantum chemistry. However, the spherical symmetry of atoms allows significant simplifications to be made in their quantum mechanical treatment, simplifications which are not possible in studies of molecules. In particular, as is well known from non-relativistic theories of molecular electronic structure, it is almost obligatory to invoke the algebraic approximation in molecular work and use finite basis set expansions. The problem of describing relativistic effects in molecules is addressed in Chapter 2 by Stephen Wilson. This chapter is devoted to a brief relativistic molecular structure calculation in which all electrons are explicitly considered. The problem of including relativistic effects in molecular studies is also addressed in Chapters 3 and 4. In Chapter 3, Odd...



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