



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

By -

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tionofrelativisticeffectsinheavyatomshaslongbeenrecognizedasoneof the central problems of atomic physics. Contemporary relativistic atomic structure calculations can be performed almost routinely. Recent years have seen agrowing interestin the study of the effects of relativity on the structure of molecules. Even for molecular systems containing atoms from

thesecondrowoftheperiodictable theenergy associated with relativistic effects is often larger than that arising from electron correlation. For molecules containing heavier atoms relativistic effects become increasingly

important,andforsystemscontainingveryheavyatomsrelativityisknown todominatemanychemicalproperties. In this volum~, one of the pioneers of relativistic atomic structure calculations,lan P. Grant,providesadetailedsurveyofthecomputational techniquesemployedincontemporarystudiesoftheeffectsofrelativityon atomicstructure. Thisisanareaofresearchinwhichcalculationscanoften lead to a particularly impressive degreeofagreement between theoryand experiment. Furthermore, theseatomicstudies haveprovided manyofthe foundations of a fully relativistic quantum chemistry. However, the spherical symmetry ofatoms allows significantsimplifications to bemade in their quantum mechanical

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