Relativity and Electron Correlation in Molecules. Calculation of Molecular Properties Using the Dirac-Coulomb-Breit Hamiltonian

L. Visscher

Department of Chemistry, Vrije Universiteit Amsterdam, De Boelelaan 1083, NL-1081 HV Amsterdam, The Netherlands

I will discuss recent developments in the calculation of molecular properties, based on the Dirac-Coulomb-Breit Hamiltonian with inclusion of electron correlation. First, I will analyse the current capabilities and limitations of methods for the calculation of Nuclear Quadrupole Coupling Constants[1]. Second, I will present the recent implementation of the Fock space Coupled Cluster formalism in the molecular coupled cluster code RELCCSD and its application to calculate electron affinities and ionisation energies of molecules[2].

[1]. M. Pernpointner and L. Visscher, Nuclear Quadrupole Moments for ^{27}Al and ^{69}Ga derived from four-component molecular coupled cluster calculations, J. Chem. Phys., in press.

[2] L. Visscher, E. Eliav, and U. Kaldor, Formulation and implementation of the relativistic Fock-space coupled cluster method for molecules, to be published.