FINITE DIFFERENCE HARTREE-FOCK METHOD: DEVELOPMENTS AND APPLICATIONS

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Numerical methods have always been prevalent in solving the Hartree-Fock equations of atomic electronic structure problems. It has just been the opposite in the case of their molecular counterparts where lack of spherical symmetry rendered the methods difficult to implement or computationally intractable. Diatomic molecules are the only molecular systems which have been routinely treated numerically. The finite difference Hartree-Fock method is the most frequently used approach to calculate Hartree-Fock-limit values of various diatomic properties.

Currently the main and most important application of this method is the development of sequences of universal even-tempered and polarization consistent Gaussian basis sets which support total Hartree-Fock energies to an accuracy approaching μhartree level. The basis sets thus obtained have been shown to yield accurate values of equilibrium distances, electric moments and polarizabilities. This approach can also be used to study the dependence of the basis set truncation errors on the number and type of functions in order to test basis set extrapolation techniques.

A summary of recent developments of the finite difference Hartree-Fock method and several examples of its applications will be presented.