

Accurate calculation of molecular properties using explicitly correlated wave functions

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Recent developments of explicitly correlated coupled-cluster and multireference electron correlation methods in our group are reviewed. Benchmarks are presented for ground and excited states and various properties of molecules and elementary reactions. The explicitly correlated (F12) terms very much reduce the basis set incompleteness errors for many different properties, and typically at least quintuple-zeta quality is achieved already with triple-zeta basis sets. We present a new implementation of analytical CCSD(T)-F12 one-electron properties. This is applied to study the convergence of quantities such as dipole moments and dipole polarizabilities with basis set size. It is shown that the F12 terms significantly improve convergence of the correlation contributions, but for polarizabilities the Hartree-Fock basis set error dominates unless at least doubly augmented basis sets are used. The convergence of the Hartree-Fock contribution can be much improved using the CABS singles correction.