

Title: Study of Diradicals by Explicitly Correlated Multireference Coupled Cluster Methods

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Abstract: Total energies of cyclopropane, trimethylene, and propylidene were calculated with conventional post-HF CCSD(T), BWCCSD(T), MkCCSD(T) methods and their explicitly correlated alternatives. Main aims of the thesis were to compare the basis set convergence of total energies and relative energies between cyclopropane and trimethylene/propylidene, both at the conventional and the explicitly correlated levels. It was shown that use of explicit correlation accelerates the convergence of the total energy by one order of basis set quality, resulting in considerable savings in computational times. Also, the MkCCSD(T)-F12/QZ and the BWCCSD(T)-F12/QZ calculations belong to the most sophisticated approaches employed for estimation of the relative energies of cyclopropane and trimethylene/propylidene to date.

Keywords: explicitly correlated, coupled cluster, multi-reference, cyclopropane isomerisation, trimethylene, propylidene