

The performance of explicitly correlated CCSD in the High accuracy Extrapolated *Ab initio* Thermochemistry (HEAT) protocol

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The performance of several approximations to explicitly correlated coupled-cluster singles and doubles (CCSD-F12) [1] is investigated in the framework of the High accuracy Extrapolated *Ab initio* Thermochemistry (HEAT) [2] protocol. Extrapolated CCSD correlation energies are benchmarked against their explicitly correlated counterparts, while the remaining contributions to the thermochemical protocol are kept constant. The resulting total atomization energies are compared with those obtained with the conventional HEAT scheme and reference values from the active thermochemical tables (ATcT) [3].

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