Implementation of the incremental scheme

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A fully automated parallelized implementation of the incremental scheme[1-4] for coupled-cluster singles-and-doubles (CCSD) energies has been extended to treat MP2-F12 and CCSD(F12) energies [5] and to treat molecular (unrelaxed) first-order one-electron properties such as the electric dipole and quadrupole moments [6]. The convergence and accuracy of the incremental approach for the dipole and quadrupole moments has been studied for a variety of chemically interesting systems.
For the explicitly correlated methods the numerical accuracy of the approach is explored for a set of 15 chemical reactions using the limiting case of single orbital one-site domains as a worst case scenario. The results are analyzed by the maximum absolute deviation, the mean absolute error and the root mean squared error, with respect to the standard MP2-F12 and CCSD(F12) results.

Literature:

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