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Abstract

Application of the Scaled MP3 method for calculation of non-covalent interactions.

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Scaled MP3 interaction energies calculated as a sum of MP2/CBS (Complete Basis Set limit) and a scaled third order energy contribution obtained in small or medium basis set agree closely with the estimated CCSD(T)/CBS for the test set of 22 hydrogen-bonded, dispersion controlled non-covalent complexes from the S22 data set. Performance of so-called MP2.5 (third-order scaling factor scaled by 0.5) is also tested for 33 hydrogen-bonded and stacked nucleic acid base pairs and various geometries of porphine dimer. In all tests, performance of MP2.5 is shown to be superior to various SCS-MP2 (scaled spin component) versions, liked SCS(MI)-MP2 or SCSN-MP2 and to DFT methods augmented with the empirical dispersion correction. Main advantage of MP2.5 is that it employs only single empirical parameter a is biased by two rigorously defined, asymptotically correct *ab-initio* methods, MP2 an MP3. Another advantage, compared to the CCSD(T), is its reduced scaling with the system size, N^6, and a possibility for almost perfect parallelization. In combination with Cholesky Decomposition of 2-electron integrals or density fitting, MP2.5 is applicable for systems with more than 100 correlated orbitals and more than 1000 AO basis functions.

1. M. Pitoňák, P. Neogrády, J. Černý, S. Grimme and P. Hobza, ChemPhysChem **10**(1) 282-289 (2009).