BENCHMARK CALCULATIONS OF THE CORRELATION MATRIX RENORMALIZATION METHOD FOR A MOLECULE TEST SET

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ABSTRACT

We report benchmark results of our recently developed correlation matrix renormalization (CMR) method [1,2,3] on the neutral molecules of G2 test set. The binding energy curves, as well as the energy components from CMR calculations are compared favorably with the results from full configuration interactions calculations based on quasi-atomic minimal basis set orbitals [4]. We will also discuss the CMR calculation results on chromium dimer, which is a well-established example showing significant electron correlation effects.

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