The MP2-F12 method in the Turbomole program package

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I. Introduction

The implementation of the explicitly correlated second-order Møller-Plesset perturbation theory (MP2-F12) method [1,2] in the Turbomole program package [2,3] is presented and discussed. A brief introduction to explicitly correlated coupled-cluster methods, as implemented in Turbomole, is also given [4].

II. MP2-F12 theory

Turbomole’s MP2-F12 implementation makes use of density fitting, which greatly reduces the prefactor for integral evaluation. Methods are available for the treatment of ground states of open- and closed-shell atoms and molecules, using unrestricted as well as restricted (open-shell) Hartree–Fock reference determinants [5]. The implementation has been parallelized.

III. Performance assessment

The performance of the Turbomole implementation is assessed by performing calculations on the molecule ethylenedioxytetrafulvalene, on a cluster model for the adsorption of methanol on the zeolite H-ZSM-5, and on the (antirheumatic) drugs leflunomide, prednisone, and methotrexate.

Basis sets of varying size (from aug-cc-pVDZ to aug-cc-pV5Z) are used, including correlation-consistent basis sets optimized for explicitly correlated calculations. The largest calculation was performed in a basis set with 3652 basis functions.