

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.

[1] W. Klopper, F.R. Manby, S. Ten-no, and E.F. Valeev, *Int. Rev. Phys. Chem.* **2006**, *25*, 427–468.

[2] R.A. Bachorz, F.A. Bischoff, A. Glöß, C. Hättig, S. Höfener, W. Klopper, and D.P. Tew, *J. Comput. Chem.* **2011** (in press).

[3] Turbomole V6.3, a development of Universität Karlsruhe (TH) and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007. See <http://www.turbomole.com>. For information on license schemes, prices, and how to order the TURBOMOLE program package, please contact COSMOlogic GmbH & Co. KG in Leverkusen, Germany, via turbomole@cosmologic.de.

[4] C. Hättig, W. Klopper, A. Köhn, and D.P. Tew, *Chem. Rev.* (in preparation).

[5] D.P. Tew and W. Klopper, *Mol. Phys.* **2010**, *108*, 315–325.