# Analytical energy gradients for explicitly correlated second-order Møller–Plesset perturbation theory

Werner Győrffy, Gerald Knizia, and Hans-Joachim Werner

Institut für Theoretische Chemie, Universität Stuttgart, Germany

We present algorithms for computing analytical energy gradients for explicitly correlated second-order Møller–Plesset perturbation theory (MP2-F12) using the 3*A and the 3*C approximations with fixed amplitude ansatz. In order to simplify the formulation of the theory, equations are derived without using the complementary auxiliary basis set (CABS) approach. A variant of the 3*A approximation has been derived from the 3*C approximation to avoid computing the troublesome commutator integrals. It is identical to the common 3*A approximation within the assumption that the resolution-of-the-identity (RI) space is complete. For efficiency, the density fitting (DF) approximation is used for evaluating all two-electron integrals and their derivatives.