Analytical nuclear gradients for RI-MP2-F12

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We present analytical nuclear gradients for explicitly correlated MP2 using density fitting (RI-MP2-F12) in Turbomole [1-2]. Compared to previous results of Kordel *et al.* [3], the implementation has been accomplished in Turbomole for Ansatz 2^* [4] without coupling terms, standard approximation A using CABS, a Slater-type geminal (STG-6G), and robust density-fitting. Additionaly, a second-order perturbation theory correction for single excitations into a complementary auxiliary basis set (CABS singles) is included to reduce the Hartree-Fock error [5]. Smooth convergence towards the basis set limit is observed for all investigated molecules. For dimers to be computed with small basis sets, RI-MP2-F12 outperforms conventional RI-MP2 clearly, since basis set superposition errors (BSSE) are avoided.

Literature:

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