

Coupled Cluster Method with Explicitly Correlated Gaussian Functions

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The coupled cluster (CC) method can be applied using the basis set of explicitly correlated Gaussian (ECG) functions. The first such application was published in 1984 at the double excitation level (CCD) [1] and then single excitations (CCSD) were included in 1999 [2]. While the CCSD/ECG approach is more time consuming than the popular CCSD-F12 methods, its advantage is that it avoids the approximations that are an inherent part of CCSD-F12. Therefore it can be used to establish correlation energy benchmarks with arbitrary accuracy given sufficient computer resources.

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- [1] B. Jeziorski, H. J. Monkhorst, K. Szalewicz, and J. G. Zabolitzky, *J. Chem. Phys.* **81**, 368 (1984).
[2] R. Bukowski, B. Jeziorski, and K. Szalewicz, *J. Chem. Phys.* **110**, 4165 (1999).