

# Can Density Cumulant Functional Theory Describe Static Correlation Effects?

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We evaluate the performance of density cumulant functional theory (DCT) for capturing static correlation effects. In particular, we examine systems with significant two-determinant character of the electronic wavefunction, such as the beryllium dimer, diatomic carbon, *m*-benzyne, and 2,6-pyridyne. We compute optimized geometries, harmonic vibrational frequencies, dissociation energies, and adiabatic excitation energies using the ODC-12 and DC-12 variants of DCT and compare these results to coupled cluster theory with single and double excitations (CCSD), as well as perturbative triples [CCSD(T)]. For all systems the DCT methods show intermediate performance between that of CCSD and CCSD(T), with significant improvement over the former method. Our results suggest that the DC-12 and ODC-12 methods are capable of describing emerging static correlation effects of two-configurational nature, but should be used cautiously when highly accurate results are required.