Transition Moments for STEOM-CCSD with Core Triples

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Similarity transformed equation-of-motion coupled cluster theory (STEOM-CC) is an alternative approach to equation-of-motion coupled cluster theory for excited states (EOMEE-CC) which uses a second similarity transformation of the Hamiltonian, followed by diagonalization in a small (CI singles-like) excitation space even when single and double excitations are included in the transformation. In addition to vertical excitation energies, transition moments measure the strength of the interactions between states governing absorption, emission, and other processes. In STEOM-CCSD, transition moments are calculated in a straight-forward manner as biorthogonal expectation values using both the left- and right-hand solutions, with the main difference with respect to EOMEE-CC being the inclusion of the transformation operator. We recently developed an extension of STEOM-CCSD to core excitations, CVS-STEOM-CCSD+cT, which includes triple excitations and the well-known core-valence separation for the core ionization potential calculations. In this work, we derived transition moments for core-excited states with core triple excitations, including both ground-to-core-excited and valence-to-core-excited transitions. The improvement of the computed transition moments of standard CVS-STEOM-CCSD and CVS-EOMEE-CCSD is measured on our previously published small molecule benchmark set.