The Performance of CCSD(T)(a) for Core-Excitations and -Ionizations

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The accuracy of the recently-developed CCSD(T)(a) method and its non-iterative counterpart CCSD(T)(a)* is examined for core-excitation and -ionization processes relevant to XPS and NEXAFS spectroscopies. The equation-of-motion excitation and ionization (EOMEE and EOMIP) variants of these methods are employed in conjunction with the core-valence separation (CVS) ansatz. CCSD(T)(a) is compared to standard CVS-EOM-CCSD and -CCSDT as well as other iterative and non-iterative triples approximations. This method is shown to recover a large portion of the triples contribution for predominantly single-excitation character states, such as primary shape resonances in the X-ray region.