SCALAR RELATIVISTIC EQUATION-OF-MOTION COUPLED CLUSTER CALCULATIONS OF CORE-IONIZED/EXCITED STATES

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Scalar relativistic equation-of-motion coupled cluster (EOMCC) calculations of core ionization/excitation energies for a set of benchmark molecules are reported. The Arnoldi algorithm as well as the core-valence-separation (CVS) scheme have been used to expedite the convergence of the wave function for the core-ionized/excited states. Scalar relativistic effects have been accounted for using the spin-free exact two-component theory in its one-electron variant (SFX2C-1e) and their importance are assessed. Preliminary calculations of ligand core excitation spectra of transition-metal containing compounds are also presented.