Equation-of-motion coupled cluster method for ionized states with partial inclusion of connected triples: assessment of the accuracy in regular and explicitly-correlated approaches

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Equation-of-motion coupled cluster method for ionized states with partial inclusion of connected triples is implemented within both regular and explicitly-correlated approaches. The computational scaling of proposed scheme is N^6, so the IP-EOM part is not more expensive then the underlying neutral-state CCSD calculation. Numerical results for the set of molecules and their ionized states are in good agreement with highly-accurate IP-EOM-CCSDT results. Comparison of predicted and experimental results for target ionization potentials shows good agreement between two sets with average deviation of ~ 0.2 e.V. The most significant discrepancies may be related to the not enough accurate values of vertical ionization potentials, restored from experimental data.