ANALYTIC RELATIVISTIC COUPLED-CLUSTER CALCULATIONS OF TIME-REVERSAL VIOLATING PARAMETERS

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We report an analytic scheme for relativistic exact two-component coupled-cluster singles and doubles with a noniterative triples [X2C-CCSD(T)] calculations of electric effective field, ε_{eff}, a time-reversal symmetry-violating parameter that plays a key role in the interpretation of experimental precision measurement of paramagnetic atoms and molecules for electron electric dipole moment (eEDM) search. Benchmark X2C-CCSD(T) calculations for the ε_{eff} values of twenty-one heavy-metal containing small molecules demonstrate the efficacy and accuracy of the present scheme. The computational results show that metal methoxides including $BaOCH_3$, $YbOCH_3$, and $RaOCH_3$ possess large ε_{eff} values similar to those of the corresponding fluorides and hydroxides, supporting the recent proposal of using nearly degenerate rotational states of these symmetric-top molecules to enhance the sensitivity of eEDM measurement. The present analytic scheme enables fast and reliable initial screening of candidate molecules for the eEDM search.