

CALCULATION AND UNCERTAINTY EVALUATION OF THE P,T-ODD ENHANCEMENT FACTORS OF POLY-ATOMIC MOLECULES

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The Standard Model of particle physics (SM) is the most complete theory nowadays; this model predicts all known fundamental particles and explains their interactions unifying three of the four fundamental forces. There are still many open questions that cannot be explained by the SM, such as the matter-antimatter asymmetry. The electron electric dipole moment (eEDM) is one of the most sought-after phenomena as a non-zero value violates Parity and Time Reversal Symmetries and could provide a clue to the origin of the matter-antimatter asymmetry. Experiments searching for the eEDM have been performed over the last 50 years and the latest upper limit was determined on ThO molecule^a. Spectroscopy with high resolution and high sensitivity has developed enormously over the past years, enabling the observation of tiny optical effects induced by novel interactions. Now the focus of interest is shifting to polyatomic molecules. In this work we perform computational investigations of polyatomic molecules in the context of the search for the eEDM, using as the example AcOH^+ and AcOCH_3^+ . The aim of this work is to provide values of effective electric field (E_{eff} - system-dependent relativistic enhancement factor that describes the interaction of the EDM of the unpaired electron with the molecular internal electric field) of AcOH^+ and AcOCH_3^+ on the highest level of theory currently available for heavy many-electron systems. Additionally we performed investigation of the influence of various computational parameters on the results. We analyzed the influence of the basis sets^b by checking the description of the valence and core regions and varying amount of diffuse or tight functions. Separately we investigated the effects of the electron correlation, like limiting number of active and virtual orbitals and the influence of perturbative triple excitations. Based on these calculations we are able to assign uncertainties on our predictions.

^aAndreev V. et al. *Nature*, 562, 355-360, 2018.

^bDyall K.G. *The Journal of Phys. Chem. A*. 113, 12638-12644, 2009.