

INFLUENCE OF VIBRATIONS ON THE SENSITIVITY OF RAOH AND YBOH MOLECULES TO THE P, T-VIOLATION

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To find a new physics beyond the Standard Model (SM), it is necessary to investigate effects that violate the invariance with respect to spatial reflections and time reversal, such as the electric dipole moment of an electron (eEDM) and the scalar-pseudoscalar electron-nuclear interaction. Triatomic molecules that we study in this paper combine the advantages of the opposite parity closely spaced levels (l -doublets) and the possibility of laser cooling that makes them promising species for high-precision experiments. The average value of the operators responsible for the violation of spatial and temporal parity can be affected by the vibrational modes of molecules, which were not previously taken into account in theoretical calculations. We computed the parameters of \mathcal{P} , \mathcal{T} -odd interactions of E_{eff} and E_s for nonlinear configurations of the RaOH^a and YbOH molecules with subsequent averaging over the vibrational wave function. We also obtained the value of l -doubling, that determines the value of the external field necessary for the maximum sensitivity of the molecule to \mathcal{P} , \mathcal{T} -odd effects. We obtained molecular orbitals by the Dirac-Hartree-Fock method implemented in Dirac 19 software package. Potential surfaces were calculated by the coupled cluster method taking into account triple excitations (CCSD(T)). To describe the electronic structure of heavy atoms, we used a generalized effective core potential with the restoration of the correct behavior of four-component spinors in the core region. This method was extended by us to complex molecular spinors. The vibrational wave functions were obtained in the Born-Oppenheimer approximation by the coupled channel method.

^aA. Zakharova, A. Petrov, P,T-odd effects for RaOH molecule in the excited vibrational state, arXiv:2012.08427 [physics.atom-ph]