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Study of nuclear magnetic quadrupole moments at triatomic molecules

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Search for spatial parity and time-invariance violation is one of the most topical fields of particle physics. Observation of P,T-invariance violation at atomic and molecular physics may lead to some new restrictions for Standard Model extensions and even be indirect evidence of unknown particles existence. So, precise theoretical and experimental study of molecular electronic structure is necessary for construction of fundamental physical interactions theory.

At the present work the electronic structure of ytterbium monohydroxide molecule YbOH [1] and its iso-electonics is considered. Recent suggestion to perform this kind of experiments on triatomic molecules [2,3] promises to lead to new restrictions for electron electric dipole moment (eEDM) and other P,T-odd constants. Here we consider nuclear magnetic quadrupole moment (NMQM) of 173Yb nucleus as such a constant. Its interaction with molecular electrons leads to energy shift, which is proptional to NMQM value. Calculation of proportionality constant is the main goal of the work, however, expected value of the energy shift is also estimated.

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