High Precision Ab Initio Calculations of the Polarizability of BaOH: Towards a Competitive eEDM Measurement

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The electron electric dipole moment (eEDM) has in recent years been measured with rapidly increasing precision, with the current upper bound at $O(10^{-30})$ e cm [1]. The NL-eEDM collaboration is currently designing an experiment to lower this limit by making use of barium monohydroxide molecules (BaOH) [2]. BaOH is laser-coolable and MOT-trappable and allows the suppression of certain systematic effects. For optimal laser-cooling and trapping, the electronic structure and properties of BaOH must be known to high precision.

We present high precision *ab initio* calculations of the static and dynamic polarizabilities of BaOH, employing the state-of-the-art coupled cluster computational method (CCSD(T)). Uncertainties on the calculated values are estimated by investigating dependence on basis set, complete basis set limit, CCSD(T) active space, and level of treatment of relativistic effects. Since BaOH in the ground state is a linear molecule, the polarizabilities both parallel and perpendicular to the molecular axis were determined. The parallel and perpendicular components of the static polarizability were found to be 198.2(1.8) and 292.5(5.3) (a.u.) respectively, and the parallel and perpendicular dynamic polarizability at the frequency of the laser in the proposed experiment (ω = 1064 nm) were found to be 363(35) and 735(51) (a.u.) respectively.

References

[1] T.S. Roussy et al, *Science* (2023), **381**, 46-50.
[2] R. Bause et al. (2025), *Manuscript in preparation*.