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Theoretical study of properties of AcF – Canceled

Heavy diatomic molecules are currently considered to be among the most sensitive systems used in the search for the P,T-violating effects and in probing of the Standard Model of particle physics. In certain molecules effects resulting from both parity violation and time-reversal violation (P,T- odd effects) are considerably enhanced with respect to atomic systems. The strength of these interactions grows with atomic number, nuclear spin and nuclear deformation. Molecules with atomic nuclear octupole deformation are sensitive for investigating of parity and time-reversal violating effects, in particular nuclear EDM. Diatomic molecule AcF has been proposed to be sensitive to the Schiff moment of the Ac nucleus[1,2]. Nowadays different laboratories plan to perform experimental study of radioactive AcF in aim to measure isotopologue shifts and hyperfine structure and achieve first successful measurements of the Schiff moment.
Pursuing studies on AcF can also provide insight into dynamics of molecular extraction of Ac, as a pathway to delivering a wider range of actinium isotopes for experiments.
This work aims to determine AcF molecular properties at the highest possible level of computational accuracy using the couple cluster in relativistic framework.
The ionization potential, excitation energies, and spectroscopic constants of AcF will be presented and the uncertainty of the predicted values will be discussed.

References:

1. D. Cho, K. Sangster, and E. Hinds. Phys. Rev. A, 44:164–164, 1991.
2. V. Flambaum and V. Dzuba. Phys. Rev. A, 101:42504, 2020.

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