THEORETICAL STUDY OF THE PbF AND PbO MOLECULES[a]

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Planned experiments to search for the simultaneous violation of the time-reversal invariance (T) and space parity (P) have motivated interest to the theoretical study of the PbF and PbO molecules. In this work we use the configuration interaction method with the generalized relativistic effective core potential for calculation of the spin-rotational Hamiltonian for the ground $^2\Pi_{1/2}$ and the first excited $A^2\Sigma^+_{1/2}$ states of the PbF including *P,T*-odd and *P*-odd terms. In particular, we have obtained hyperfine constants on the ^{207}Pb nucleus. For the $^2\Pi_{1/2}$ state $A_\perp = -6859.6$ MHz, $A_\parallel = 9726.9$ MHz and for the $A^2\Sigma^+_{1/2}$ $A_\perp = 1720.8$ MHz, $A_\parallel = 3073.3$ MHz. Our values are in good agreement with recent experimental data. The effective electric field on the electron, which is required for interpretation of the results of the planned experiment in terms of eEDM is found to be $3.3 \times 10^{10} \mathrm{V/cm}$. The same method was used for calculation of the PbO molecule. The main goal is to clarify role of interaction with the nearest electronic state $^3\Sigma^+_{0^-}$ on the hyperfine structure and magnetic properties of the $a(1)[^3\Sigma^+_1]$ state of PbO. The accounting for this contribution leads to the difference between g-factors of the $J = 1$ Ω-doublet levels, $\Delta g = 37 \times 10^{-4}$, which is in good agreement with the experimental data $\Delta g = 30(8) \times 10^{-4}$. The contribution of this interaction rapidly grows with J. For $J = 30$ the difference of g-factors of Ω-doublet states reaches 100%; for hyperfine constants it reaches 18%. These differences also depend on the electric field, and for $E = 11$ V/cm for ^{207}PbO the difference in g-factors turns to zero. The latter is important for suppressing systematic effects in the electron electric dipole moment search experiment.

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