HYPERFINE INTERACTION IN DIATOMICS AS A TOOL FOR SUPPRESSION OF SYSTEMICS AND VERIFICATION OF THEORETICAL VALUES FOR THE EFFECTIVE ELECTRIC FIELD ON ELECTRON FOR THE ELECTRON EDM EXPERIMENTS

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An important feature of the effective electric field ($E_{\rm eff}$) acting on electrons is that it cannot be obtained in an experiment and the electronic structure calculation is required for its evaluation[b]. Therefore, an accuracy check must be provided by calculating the experimentally known hyperfine constants which, similarly to $E_{\rm eff}$, depend on the electron spin density near heavy nuclei. As was shown[c] the knowledge of the $A_{\parallel}$ and $A_{\perp}$ constants for molecules with dominant one-electron s-p mixed molecular orbital contribution ($\Omega = 1/2$) provide the most important information for the $E_{\rm eff}$ accuracy check. However, the hyperfine structure for the $\Omega = 1$ molecules, for a good approximation, is mainly determined by only one constant, $A_{\parallel}$. We show, nevertheless, that perturbation of the hyperfine structure of the $^3\Delta_1$ state of WC, HfF^+ and others molecules can be detected in an experiment giving missing information for the $E_{\rm eff}$ accuracy check.

Besides we show that the difference between g-factors for the Omega-doublet levels in diatomics with hyperfine structure can be converged to zero for some electric field[d]. The latter is important for suppressing systematic effects and is one of the factors which determines the sensitivity limit in the eEDM search experiments.

We show that in order to reproduce the experimental hyperfine structure of PbF[e] obtained with high accuracy one must take into account the dependence of the hyperfine constants on the internuclear distance.

[a] SPbU Fundamental Science Research grant from Federal budget N 0.038.652.2013 and RFBR grant 13-02-01406 are gratefully acknowledged

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