Impact of the ligand deformation on the $\mathcal{P},\mathcal{T}$-violation effects in the YbOH molecule

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The ytterbium monohydroxide is a promising molecule for a new physics searches. It is well known that levels of the opposite parity, separated by the energy split, so-called $l$-doublets, define the experimental electric field strength required for the molecule polarization. In addition, in our previous paper\textsuperscript{2} we have shown that the value of $l$-doubling directly influences the sensitivity of linear triatomic molecules to the $\mathcal{P},\mathcal{T}$-odd effects. In our work\textsuperscript{2} we have calculated the value of $l$-doubling for the YbOH molecule with approximation of fixed O-H bond length. Accounting the importance of this property, in the present study, we consider the additional degree of freedom corresponding to the ligand (OH) deformation.

I. INTRODUCTION

Symmetry breaking with respect to the spatial reflection ($\mathcal{P}$), the time inversion ($\mathcal{T}$), and the charge conjugation ($\mathcal{C}$) are embedded in the Standard model (SM)\textsuperscript{[4]} One of the possible sources of the strong $\mathcal{P},\mathcal{T}$-violation in the SM is $\theta$ term, that however is negligible\textsuperscript{[5,6]}. The observed source of the $\mathcal{P}$ and $\mathcal{C}$ non-conservation comes from the weak interaction, that affects only the left components of the lepton and quark spinors. This fact means that $\mathcal{P}$, and $\mathcal{C}$ symmetries are broken separately\textsuperscript{[7]}. However, the combined $\mathcal{CP}$ parity could be conserved. But in SM there is a Cabibbo-Kobayashi-Maskawa (CKM)\textsuperscript{[8,9]} matrix, which is associated with the interaction of quarks and $W^{\pm}$-bosons, and Pontecorvo–Maki–Nakagawa–Sakata matrix (PMNS)\textsuperscript{[10,11]} which is associated with the interaction of leptons with $W^{\pm}$-bosons. When these matrices have complex components, they violate $\mathcal{CP}$, which is manifested in neutral kaon and $B^{0}-\bar{B}^{0}$-meson decays\textsuperscript{[12]}. Because of the $\mathcal{CPT}$ theorem, $\mathcal{CP}$ combination is equivalent to time reversal $\mathcal{T}$.

The probable effect of the $\mathcal{CP}$-symmetry violation in the Standard model can be found in the electron electric dipole moment ($\text{eEDM}$) and scalar-pseudoscalar electron-nucleon interaction ($\text{S-PS}$)\textsuperscript{[13]} parametrized correspondingly by $d_e$ and $k_s$ constants. In the SM the predicted values for these constants are very small. Nevertheless, there are many extensions of the SM that can lead to the considerable increase of the $d_e$ and $k_s$ constants\textsuperscript{[14,15]}. To investigate the $\mathcal{CP}$-violating physics, tabletop experiments with atoms and molecules can be employed\textsuperscript{[16,17]}. The current limit on the electron electric dipole moment (the ACME II experiment), $|d_e| < 1.1 \times 10^{-29}$ e·cm (90% confidence), was set by measuring the spin precession using thorium monoxide (ThO) molecules in the metastable electronic H$^3\Delta_1$ state\textsuperscript{[18]}. In its turn, cold polar molecules provide unique opportunities for further progress in search for effects of symmetry violation\textsuperscript{[19]}. The strength of polyatomic species as probes of the parity-violating physics lies in a possibility of laser-cooling that does not interfere with the existence of the parity doublets\textsuperscript{[20]}. Unlike the diatomic molecules, polyatomic ones possess the distinctive rovibrational spectrum with additional energy levels of opposite parity. The transverse vibrations of triatomic molecules result in $l$-doublets\textsuperscript{[21,22]}. For symmetric top molecules nonvibrational $K$-doublets, associated with rotation of the molecule around its axis, appear\textsuperscript{[23,24]}.

One dimensional laser-cooling was made for SrOH, CaO, CaOCH\textsubscript{3}\textsuperscript{[30,31]}, and the YbOH\textsuperscript{[33,34]} molecules. Recently, the magneto-optical trapping and cooling of the CaOH molecule was achieved\textsuperscript{[35]}. The molecule we are considering, ytterbium monohydroxide, is a good candidate for the eEDM search\textsuperscript{[27,29]}.

For triatomic molecules, the external fields are mixing the opposite parity levels, and due to this, the molecule is polarized to a degree determined by a coefficient $\Delta E_{\mathcal{P},\mathcal{T}}$\textsuperscript{[11,36]}. If the electron has eEDM and interacts with the nucleus by the S-PS, the $\mathcal{P},\mathcal{T}$-nonconservation emerges in the energy difference between levels with opposite projection of the total angular momentum on the field’s axis:

$$\Delta E_{\mathcal{P},\mathcal{T}} = P(2E_{\text{eff}}d_e + 2E_kk_s),$$

Knowing the enhancement coefficients $E_{\text{eff}}$, $E_k$ and $P$ one may extract the value of the constants $d_e$ and $k_s$ from this energy splitting\textsuperscript{[30,35]}.

Recently, we have calculated the enhancement factors $E_{\text{eff}}$ and $E_k$ for the RaOH, YbOH, and the symmetric top molecule RaOCH\textsubscript{3}\textsuperscript{[27,30,39]} the rovibrational wavefunctions were obtained\textsuperscript{[27,30,39]} on the CCSD level. Our computational approach, that does take into account the rotational and anharmonic effects, allowed us to calculate $l$-doubling for the triatomic molecules RaOH and YbOH. We have

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also determined the value of the polarization coefficient $P$ for the YbOH molecule\cite{1}. In our work\cite{2} we have shown that the $l$-doubling structure is, in general, different from $\Omega$-doubling of diatomics, and the $P$ value tends to approach 50% value for most of the ground rotational levels of the first excited $v_2 = 1$ bending mode of YbOH. For some levels a maximum of the polarization $P_{\text{max}}$ value as a function of electric field with $1/2 < |P|_{\text{max}} < 1$ is observed. The smaller the $l$-doubling, the larger is the $|P|_{\text{max}}$. Thus, the value of $l$-doubling directly influences the sensitivity of linear triatomic molecules to the $\mathcal{P}, \mathcal{T}$-odd effects.

However, when calculating $l$-doubling, in our preceding work\cite{2} we assumed that the deformations of the ligand may be neglected as the corresponding vibrational frequency is much higher than the frequencies for bending and stretching of the whole molecule. The aim of the present paper is to take into account the change of the ligand’s bond length (i.e., of the equilibrium ligand size and its vibrational frequency) due to the interaction with bending and stretching modes of the YbOH.

II. POTENTIAL SURFACE INTERPOLATION

To obtain the potential surface we used the Dirac 19 program suite\cite{3}. The PNPI\cite{4} 42-valence electron basis was used to describe the Ytterbium atom. Moreover, to simplify calculations with a heavy atom, we employed the 28-electron generalized relativistic effective potential, also developed by the PNPI Quantum Chemistry Laboratory\cite{5,6}. For oxygen and hydrogen atoms, we used cc-pVTZ basis sets. Active space for the coupled cluster computations comprises 21 active and 30 frozen electrons.

We obtain the CCSD and CCSD(T) potential surface $V$ on the grid of coordinates $(R_i, r_j, \theta_k)$,

\begin{align*}
\{R_i\} &= 3.3, 3.5, \ldots 4.3 \text{ a.u.} \quad (2) \\
\{r_j\} &= 1.632, 1.732, \ldots 2.032 \text{ a.u.} \quad (3) \\
\{\theta_k\} &= 0^\circ, 5^\circ, 10^\circ, 15^\circ, 20^\circ, 25^\circ, 55^\circ, 90^\circ, 122^\circ, 155^\circ \quad (4)
\end{align*}

At the first step we approximate the dependence on $r$ for each $(R_i, \theta_k)$ by the Morse potential

\[ V(r) = V_0 + D(1 - e^{-\alpha(r-r_{eq})})^2 \quad (5) \]

where $r_{eq}$ is the equilibrium ligand size, $D$ – dissociation energy, $\alpha$ is the exponent parameter, and $V_0$ is the energy of the minimum. The values for $V_0$ and $r_{eq}$ parameters for various configurations of YbOH are presented on Fig. 1 and Fig. 2 correspondingly.

At the second step, for each $R_i$ we interpolate the dependence of this set of parameters $V_0(R_i, \theta_k)$, $r_{eq}(R_i, \theta_k)$, $D(R_i, \theta_k)$, and $\alpha(R_i, \theta_k)$, on $\theta$ by the Akima splines.

Then, using Akima splines, obtained at the previous step, we take the values at the zeros of the $(\lambda_{\text{max}}+1)$-th Legendre polynomial $P_{\lambda_{\text{max}}+1}(x)$, where $x = \cos \theta$. For each $R_i$, we then use the Gauss-Legendre method to rep-
To solve eq. (12) we use the expansion
\[ \psi_{\text{nuc}}(\vec{R}, \vec{r}) = \sum_{\lambda=0}^{\lambda_{\text{max}}} \sum_{j=0}^{l_{\text{max}}} \sum_{m=0}^{m_{\text{max}}} F_{JjLm}(R) \Phi_{JjLM}(\vec{R}, \vec{r}) f_n(r), \]
where
\[ \Phi_{JjLM}(\vec{R}, \vec{r}) = \sum_{m_{L,j} m_j} C_{Lm_{L,j} m_j}^{Jm} Y_{Lm_{L}}(\vec{R}) Y_{jm}_j(\vec{r}) \]
is coupled to conserved total angular momentum \( J \) basis set, \( Y_{Lm_{L}} \) is a spherical function, \( f_n(r) \) is a solution of
\[ \left( -\frac{1}{2\mu_{\text{OH}}} \frac{\partial^2}{\partial \vec{r}^2} + V(R, r, \theta) \right) f_n(r) = \epsilon_n f_n(r), \]
where \( R_i \) and \( \theta_i \) are some fixed values. To test the approximation \( (13) \) we perform our computations for different sets of \((R_i, \theta_i)\).

Substituting wavefunction \( (13) \) to eq. \( (12) \) one gets the system of close-coupled equations for \( F_{JjLm}(R) \).

III. METHODS

We use the Born-Oppenheimer approximation to separate wavefunction to \( \psi_{\text{nuc}} \), responsible for the nuclear motion in the adiabatic potential of the electrons, and the \( \psi_{\text{elec}} \), corresponding to the electronic motion in the field of heavy nuclei
\[ \psi_{\text{total}} \approx \psi_{\text{nuc}}(\vec{R}, \vec{r}) \psi_{\text{elec}}(\vec{R}, \vec{r} q), \]
where \( q \) are the generalized coordinates of the electrons, \( \vec{R} \) is the vector from the Ytterbium atom to the center of mass of the OH ligand, \( \vec{r} \) is the vector from the Oxygen to the Hydrogen atom.

The Hamiltonian of nuclei takes the form,
\[ \hat{H}_{\text{nuc}} = -\frac{1}{2\mu} \frac{\partial^2}{\partial \vec{R}^2} - \frac{1}{2\mu_{\text{OH}}} \frac{\partial^2}{\partial \vec{r}^2} + \frac{\hat{L}^2}{2\mu R^2} + \frac{\hat{j}^2}{2\mu_{\text{OH}} r^2} + V(R, r, \theta), \]
where \( \theta \) is the angle between vectors \( \vec{R} \) and \( \vec{r} \) (so that \( \theta = 0 \) corresponds to the Yb-O-H linear configuration), \( \mu \) is the Yb-OH reduced mass, \( \mu_{\text{OH}} \) is the reduced mass of the ligand, \( \hat{L} \) and \( \hat{j} \) are the angular momentum of the whole system rotation and the OH angular momentum correspondingly. Directions of axes \( \hat{r} \) and \( \hat{R} \) are represented in Fig. \( 3 \). \( V \) is the electronic potential surface obtained on the CCSD or CCSD(T) level and depending only on the relative Jacobi coordinates \( (R, r, \theta) \).

The nuclear wavefunction \( \psi_{\text{nuc}}(\vec{R}, \vec{r}) \) is the solution of the Schrödinger equation
\[ \hat{H}_{\text{nuc}} \psi_{\text{nuc}}(\vec{R}, \vec{r}) = E \psi_{\text{nuc}}(\vec{R}, \vec{r}). \]

To solve eq. \( (12) \) we use the expansion

IV. RESULTS

The parameters obtained from the spectrum of the nuclear wavefunctions \( \psi_{\text{nuc}} \) compared with the results from the rigid ligand approximation and experimental values are presented in the Table \( I \). One can see that taking into account the ligand deformation improves the agreement with experiments. To test our method and codes, which now take into account the ligand deformation, we performed calculations with two different sets of the parameters \( R_i \) and \( \theta_i \) from eq. \( (15) \). The Set 1 corresponds to \( R_1 = 3.9 \text{ a.u}, \theta_1 = 0 \) and and Set 2 corresponds to \( R_2 = 4.2 \text{ a.u}, \theta_1 = 0.5 \text{ radians} \). In Table \( I \) one can see that results with Set 1 and Set 2 converge to each other as quantum number \( n_{\text{max}} \) (see eq. \( (13) \)) increases. Table \( I \) also show that for purposes of the present paper it is sufficient to use \( n_{\text{max}} = 2 \). Probably inclusion of the noniterative triple excitations to the coupled cluster computations and using more extensive basis sets are necessary to reach the accuracy of the calculation on the order of \( 5 \text{ cm}^{-1} \) for the vibrational frequencies, what is out of scope of the current work.

However, to estimate the actual value of the \( l \)-doubling one can note the following. The decrease of the \( l \)-doubling
value together with the increase of the $\nu_2$ frequency is consistent with the estimate,

$$q \simeq \frac{B^2}{\nu_2} \left( 1 + 4 \sum_{k=1,3} \frac{\xi_k^2}{k^2 \nu_2^2} \right) (v + 1), \quad \Delta E = 2q.$$

(16)

where $\xi_k$ are Coriolis coefficients. As the current experimental data for the $\nu_2$ frequency fall into a rather wide range $319 - 339 \text{ cm}^{-1}$, we sum up our results for $l$-doubling with the estimate of $\Delta E_{l=1} \simeq 24 - 26 \text{ MHz}$.

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AUTHOR DECLARATIONS

Conflict of interest

The authors have no conflicts to disclose.

AVAILABILITY OF DATA

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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TABLE I. Rovibrational spectrum parameters

| Parameter                  | Rigid ligand, CCSD(T) | CCSD | CCSD(T) | Experiment |
|----------------------------|-----------------------|------|---------|------------|
| Stretching mode $\nu_1$, cm$^{-1}$ | 550                   | 545  | 536     | 529.34 (1) |
| Bending mode $\nu_2$, cm$^{-1}$     | 319                   | 351  | 342     | 319(5) (2) |
| Ligand mode $\nu_3$, cm$^{-1}$       | -                     | 4055 | 4030    | -          |
| Rotational constant $B(\nu_1 = 0, \nu_2 = 0, \nu_3 = 0)$, cm$^{-1}$ | 0.2461               | 0.2456 | 0.2468 | 0.24543(13) (2) |
| Rotational constant $B(\nu_1 = 1, \nu_2 = 0, \nu_3 = 0)$, cm$^{-1}$ | -                     | 0.2437  | 0.2443  | 0.243977(35) (2) |
| $l$-doubling $\Delta E_{J=1} = 2q$, MHz | 26                    | 23   | 24      | -          |

$a$ The number in parentheses denotes $2\sigma$ deviation

TABLE II. Convergence of the results with $n_{\text{max}}$ (see eq. (13)) for different sets of parameters $R_i$ and $\theta_i$ (see eq. (15)) for CCSD(T) calculations

| Parameter                  | Set of $R_i, \theta_i$ | $n_{\text{max}} = 1$ | $n_{\text{max}} = 2$ | $n_{\text{max}} = 3$ |
|----------------------------|-----------------------|----------------------|----------------------|----------------------|
| Bending mode $\nu_2$, cm$^{-1}$ | 1                     | 344.0892             | 341.9777             | 341.9655             |
|                            | 2                     | 340.9922             | 341.9698             | 341.9671             |
| $l$-doubling $\Delta E_{J=1} = 2q$, MHz | 1                     | 23.520               | 24.247               | 24.257               |
|                            | 2                     | 23.712               | 24.235               | 24.256               |

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