Rovibrational structure of the Ytterbium monohydroxide molecule and the \( \mathcal{P},\mathcal{T} \)-violation searches

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The spectrum of triatomic molecules with close rovibrational opposite parity levels is sensitive to the \( \mathcal{P},\mathcal{T} \)-odd effects. This makes them a convenient platform for the experimental search of a new physics. Among the promising candidates one may distinguish the YbOH as a non-radioactive compound with a heavy atom. The energy gap between levels of opposite parity, \( l \)-doubling, is of a great interest as it determines the electric field strength required for the full polarization of the molecule. Likewise, the influence of the bending and stretching modes on the sensitivities to the \( \mathcal{P},\mathcal{T} \)-violation requires a thorough investigation since the measurement would be performed on the excited vibrational states. This motivates us to obtain the rovibrational nuclear wavefunctions, taking into account the anharmonicity of the potential. As a result, we get the values of the \( E_{\text{eff}} \) and \( E_s \) for the lowest excited vibrational state and determine the \( l \)-doubling

I. INTRODUCTION

The violation of the charge conjugation (C), spatial reflection (P), and time reversal (T) symmetries is the striking feature of the Standard model (SM)\(^{1,2}\). The sources of the charge-parity (CP) nonconservation in the SM are Cabibbo-Kobayashi-Maskawa (CKM)\(^{3,4}\) and Pontecorvo–Maki–Nakagawa–Sakata (PMNS) matrices\(^{5,6}\), and, possibly, the \( \theta \) term of the strong interaction\(^{7,8}\). One of the CPT theorem consequences is that nonconservation of CP is equal to the violation of T-symmetry.

One of the possible manifestation of the CP-nonconservation is the electron electric dipole moment (eEDM). In the Standard model the eEDM appears only in the multiloop processes with a high order of the weak coupling constant and, thus, the predicted value is very small. On the other hand, some models of the physics beyond the Standard Model (SM) forecast new CP-violation sources that can lead to the significant increase of the eEDM\(^{9,10}\). The presence of the particle superpartners in the Supersymmetry theory (SUSY) would provide new \( \mathcal{P}, \mathcal{T} \)-violation sources. Besides, the fluctuations of the \( \theta \) parameter, the axion, in the Peccei–Quinn theory may result in the CP-violating processes. Furthermore, the matter-antimatter ratio in the observable universe\(^{11,12}\) may imply new sources of the charge-parity violation.

The high precision molecular experiments provide a powerful way to investigate the CP-violating physics\(^{13,14}\).

As for now, the best experimental bound on the eEDM was obtained for diatomic molecules with closely spaced \( \Omega \)-doublets such as ThO\(^{15,16}\) and HfF\(^{17,18}\). These experiments also put constraints on the scalar-pseudoscalar nucleon-electron interaction\(^{19,20}\). Experiments for searching other \( \mathcal{P}, \mathcal{T} \)-odd effects, including nuclear magnetic quadrupole moment\(^{21,22}\) and axion mediated interaction\(^{23,24}\) are planned.

The vibrational modes of the polyatomic molecules create unique spectral characteristics not possessed by diatomic molecules. For instance, the triatomic species can simultaneously allow laser-cooling\(^{25}\) and possess levels with opposite parity, the so-called \( l \)-doublets\(^{26,27}\).

The levels of opposite parities constituting the \( l \)-doublet are mixed when the external electric field applied so that the molecule becomes polarized. The \( \mathcal{P}, \mathcal{T} \)-violation is manifested in the energy splitting, \( \Delta E_{\mathcal{P},\mathcal{T}} \), between the levels with opposite values \( \pm M \) of total angular momentum projection on the electric field axis.

If the electron has EDM \( d_e \) and is affected by the scalar-pseudoscalar interaction with nuclei characterized by the coupling constant \( k_s \), these \( \mathcal{P}, \mathcal{T} \)-odd effects can be estimated from the maximum splitting between levels with opposite values of \( M \) given by,

\[
\Delta E_{\mathcal{P},\mathcal{T}} = 2E_{\text{eff}}d_e + 2E_s k_s, \tag{1}
\]

The parameters \( E_{\text{eff}} \) and \( E_s \) are determined by the molecular electronic structure\(^{28,29}\).

The laser-cooling in one dimension was achieved for alkaline earth metal monohydroxides such as SrOH\(^{30}\) and, recently, the YbOH\(^{31,32}\). The latter is considered a promising candidate for the future experiments searching eEDM\(^{33}\).

The sensitivity of the YbOH molecule to the eEDM was previously computed\(^{34}\) within the relativistic coupled cluster method. However, the vibrational motion, including the bending modes, of excited vibrational states may influence the value of this parameter. In\(^{35}\) \( E_{\text{eff}} \) was studied for different nonlinear configurations and strong dependence on the bending angle already at

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Dirac-Hartree-Fock (DHF) level was stressed. This claim is inconsistent with the results of Refs. that used the complex generalized Hartree-Fock and Kohn-Sham methods within zeroth-order regular approximation and also has given the harmonic estimate for $E_{\text{eff}}$ at the $v = 1$ vibrational level.

Previously we obtained the rovibrational wavefunctions for the molecule RaOH$^{23}$. This allowed us not only to compute the $E_{\text{eff}}$ and $E_s$ parameters for the first vibrational levels but also to obtain the value of the $l$-doubling that determines the external electric field required for the complete polarization of the molecule. In this paper, we apply the techniques we developed to perform a similar analysis for the YbOH molecule.

II. METHODS

We assume that the wavefunction of the molecule can approximately be factorized into the nuclear and electronic parts,

$$\Psi_{\text{total}} \simeq \Psi_{\text{nuc}}(Q) \psi_{\text{elec}}(Q|q),$$  \quad (2)

where $Q$ denotes generalized coordinates of the nuclei and $q$ - generalized coordinates of the electrons. Within the Born-Oppenheimer approximation the electronic part $\psi_{\text{elec}}(Q|q)$ is the solution of the Dirac-Coulomb equation for the electrons in the field of the nuclei fixed at coordinates $Q$. To describe the configuration of the triatomic molecule we choose $Q$ as the Jacobi coordinates represented in Fig. 1: $\hat{r}$ and $\hat{R}$ are unit vectors directed along the OH axis and Yb - OH center of mass (c.m.) axis respectively, $\theta$ is the angle between above axes, $\hat{R}$ is the distance between Yb and the c.m. of OH. As the frequency of OH vibrational mode is about one order of magnitude larger than other vibrational frequencies in YbOH, we fix OH ligand stretch at the equilibrium distance $r = 1.832 \text{ a.u.}^{19}$

The nuclear part of the wavefunction $\Psi_{\text{nuc}}$ satisfies the Schrödinger equation,

$$\hat{H}_{\text{nuc}} \Psi_{\text{nuc}}(R, \hat{R}, \hat{r}) = E \Psi_{\text{nuc}}(R, \hat{R}, \hat{r}).$$  \quad (3)

The nuclear Hamiltonian takes the form,

$$\hat{H}_{\text{nuc}} = -\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + \frac{\hat{L}^2}{2\mu R^2} + \frac{\hat{j}^2}{2\mu_{\text{OH}}^2} + V(R, \theta),$$  \quad (4)

where $\mu$ is the the Yb – OH reduced mass, $\mu_{\text{OH}}$ is the the OH ligand reduced mass, $\hat{L}$ is the angular momentum of the Yb-OH system rotation around its c.m., $\hat{j}$ is the ligand angular momentum, and $V(R, \theta)$ is the effective adiabatic potential obtained from the electronic structure calculations.

The sensitivity of the spectrum to the $P$, $T$-odd interactions for the fixed configurations can be described by the parameters,

$$E_{\text{eff}}(R, \theta) = \frac{\langle \psi_{\text{elec}}(R, \theta)|\hat{H}_d|\psi_{\text{elec}}(R, \theta)\rangle}{\rho_s \text{sign}(\Omega)},$$  \quad (5)

that can be understood as the expectation values for the eEDM and scalar-pseudoscalar nucleon-electron interaction terms in the $P$, $T$-odd interaction Hamiltonian

$$\hat{H}_d = \hat{H}_d + \hat{H}_s,$$  \quad (6)

$$\hat{H}_d = 2d_e \sum_i \left( \begin{array}{ccc} 0 & 0 & 0 \\ 0 & \sigma_i & 0 \\ 0 & 0 & 0 \end{array} \right),$$  \quad (7)

$$\hat{H}_s = i k_s \frac{G_F}{\sqrt{2}} \sum_{j=1}^{N_{\text{elec}}} \sum_{i=1}^{N_{\text{nuc}}} \rho_I (r^j) Z_I \gamma^0 \gamma^5,$$  \quad (8)

where $\rho_I$ is the normalized charge density of the $I$-th nucleon, $G_F$ is Fermi constant, $\sigma$ are Pauli matrices, $E_i$ is the internal molecular electric field that acts on ith electron.

For the total molecular wavefunction (2) these parameters should be averaged over the nuclear wavefunction,

$$E_{\text{eff,s}} = \int dR d\hat{r} \rho_s \langle |\Psi_{\text{nuc}}(R, \hat{R}, \hat{r})|^2 E_{\text{eff,s}}(R, \theta).$$  \quad (9)

The Ytterbium atom was described by a 28-electron generalized relativistic effective core potential (GRECP) and a 42-valence electron basis set developed by the PNPI Quantum Chemistry Laboratory. The cc-pVTZ basis was used for H and O atoms. The calculations were performed on a grid of Jacobi coordinates. The $R$ coordinate ranges from 2.6 a.u. to 4.3 a.u. with step 0.1 a.u. The $\theta$ angle values are $0^\circ$, $5^\circ$, $10^\circ$, $15^\circ$, $20^\circ$, $25^\circ$, $75^\circ$, $90^\circ$, $122^\circ$, $155^\circ$ and $180^\circ$. Extra points near the equilibrium were added to better describe the region most relevant for the lowest vibrational levels.

The molecular two-component pseudospinors were obtained using the Hartree-Fock self-consistent field (SCF)
method implemented in the Dirac 19 software. The pseudospinors are smoothed in the inner core region, so that the electronic density in this region is not correct. The operators in eqs. (3) are heavily concentrated near the nucleus and are therefore strongly affected by the wave function in the inner region. The four-component molecular spinors must therefore be restored in the inner region of Yb. The MOLGEP program was used to apply the method of one-center restoration of the correct four-component spinors in the core region with help of the equivalent basis set. The matrix elements of $H_d$ and $H_s$ were computed in the basis of the restored spinors $\tilde{\psi}_i$.

Restoration of the basis begins with the creation of an equivalent basis set of atomic (one-center) four-component spinors:

$$\{ \left( f_{nlj}(r)\chi_{ljm}, g_{nlj}(r)\chi'_{ljm} \right) \}, \quad (11)$$

and two-component pseudospinors $\{ f_{nlj}(r)\chi_{ljm} \}$. Here $f$ - large component, $g$ - small component, $\chi$ - spin-angular part, $n$ - principal quantum number, $j$ and $m$ - total electronic momentum and his projection in internuclear axis, $l$ and $l'$ - orbital moment, and $l' = 2j - l$.

For the numerical four-component and two-component atom calculations, the HFD and HFJ/GRECP programs were used to create two equivalent basis sets for reconstruction. Molecular pseudo-orbitals then decompose in the basis of two-component single-center atomic pseudospinors,

$$\tilde{\phi}_i(r) \approx \sum_{l=0}^{L_{\text{max}}} \sum_{j=|l-1/2|}^{l=|l+1/2|} \sum_{nm} c_{nljm} f_{nlj}(r)\chi_{ljm}. \quad (12)$$

Then two-component pseudospinors are replaced by equivalent four-component spinors:

$$\phi_i(r) \approx \sum_{l=0}^{L_{\text{max}}} \sum_{j=|l-1/2|}^{l=|l+1/2|} \sum_{nm} c_{nljm} \left( f_{nlj}(r)\chi_{ljm}, g_{nlj}(r)\chi'_{ljm} \right). \quad (13)$$

Molecular four-component spinors constructed in this way are orthogonal to the core spinor Yb, since atomic basis functions in the equation were calculated for frozen inner core electrons. For the current calculation we put $L_{\text{max}} = 3$, what is enough for accurate calculation of $E_{\text{eff}}$ at CCSD level with help of the MRCC program suite. The density matrix is then contracted with $E_{\text{eff}}$ and $E_s$ matrix elements to obtain the values of the correlation corrections for the linear configurations,

$$E_{\text{eff},s}(R, \theta) = \frac{1}{N_{\text{elec}}} \sum_{i,j=1}^{N_{\text{orb}}} \frac{P_{ij}^{(1)}}{d_c \text{sign}(\Omega)}. \quad (14)$$

FIG. 2. Potential surface $V(R, \theta)$

the close-coupled equations obtained as a decomposition of $[3]$ in terms of the eigenfunctions of the molecular and ligand angular momenta. For the details of our approach we refer the reader to our previous work. This way we take into account the anharmonicities of the potential and interaction between the rotational and vibrational degrees of freedom without resorting to the perturbative techniques.

For the property calculations of the linear configuration we get the one-electron density matrix $P_{ij}^{(1)}$ at CCSD level with help of the MRCC program suite. The density matrix is then contracted with $E_{\text{eff}}$ and $E_s$ matrix elements to obtain the values of the correlation corrections for the linear configurations,

$$E_{\text{eff},s}(R, \theta) = \frac{1}{N_{\text{elec}}} \sum_{i,j=1}^{N_{\text{orb}}} \frac{P_{ij}^{(1)}}{d_c \text{sign}(\Omega)}. \quad (14)$$

Regrettably, the Dirac-MRCC interface works only for the symmetry groups with real representations (such as $C_{2v}$) but not with ones with complex representations (such as $C_s$) of the nonlinear molecules. Therefore the CCSD correction was obtained only for the linear configurations and are depicted on Fig. [4]. Since these corrections constitute only about 1% of the SCF values near minimum reaching 6% far from equilibrium point, we assumed that, as a first approximation, it is reasonable to approximate the CCSD correction for the nonlinear molecule by the result computed for the linear molecule:

$$E_{\text{eff},s}^{(\text{total}, l)}(R, \theta) = E_{\text{eff},s}^{(\text{ccsd})}(R, 0^\circ) + \left( E_{\text{eff},s}^{(\text{ccs})}(R, \theta) - E_{\text{eff},s}^{(\text{ccs})}(R, 0^\circ) \right). \quad (15)$$

In other words, the dependence of $E_{\text{eff},s}(R, \theta)$ on $\theta$ was calculated at SCF level. To test the validity of
our approximation, we made a finite field computation of $E_{\text{eff},s}$ by CCSD method for the near equilibrium value of $R = 3.9$ a.u. and different angles. Because this computation is very expensive we were able to obtain the values only for the single value of $R$.

### III. RESULTS AND DISCUSSION

The spectrum of the nuclear wavefunctions $\Psi_{\text{nuc}}$ is characterized by the parameters we present in the Table I. The agreement between the computed and the experimental values of frequencies is rather good.

Our $l$-doubling value is consistent with an estimate[21,22]

$$ q \simeq \frac{B^2}{\nu_2} \left( 1 + \frac{2 \Omega_{21}^2 \nu_2^2}{\nu_1^2 - \nu_2^2} \right) (v + 1) . \quad (16) $$

Comparing with our results, we can find Coriolis coefficient, $\Omega_{21} = 0.265$. The value of $l$-doubling for YbOH is greater than our result for RaOH molecule, $\Delta E_{l=1} = 2q = 14.5$ MHz [23] as expected from the smaller momentum of inertia of the YbOH molecule.

The dependence of the $E_{\text{eff},s}$ on the bending and stretching is depicted on the Fig. 3. As with RaOH [21,22], we do not confirm the oscillatory behavior claimed in [25].

As described in previous section, the full dependence of $E_{\text{eff},s}(R, \theta)$ on $\theta$ was calculated at SCF level. The finite field computation was performed only for the single value of $R = 3.9$ a.u.. In the Table I we compare the deviations from the equilibrium value of $E_{\text{eff}}(0^\circ)$ for the SCF and correlation corrections results. The changes of the correlation correction happen to be of the same magnitude as the changes of the SCF values. The deviation becomes significant for large bending angles and, while this does not affect the average values on the rovibrational levels considered, it may become important for the higher excited levels. The similar analysis was made for the $E_s$ values in the Table III. Unlike SCF values the correlation correction for $E_s$ have a different angular dependence from $E_{\text{eff}}$.

To take the angular dependence of the correlation correction $\Delta E_{\text{eff},s}^{\text{corr}}$ into account using the available data we use the following approximation,

$$ E_{\text{eff},s}^{(\text{total,II})}(R, \theta) = E_{\text{eff},s}^{(\text{ccsd})} (R, 0^\circ) + $$

$$ + \left( E_{\text{eff},s}^{(\text{scf})} (R, \theta) - E_{\text{eff},s}^{(\text{scf})} (R, 0^\circ) \right) $$

$$ + \left( E_{\text{eff},s}^{(\text{ccsd})} (3.9 \text{ a.u., } \theta) - E_{\text{eff},s}^{(\text{scf})} (3.9 \text{ a.u., } \theta) \right) $$

$$ - \left( E_{\text{eff},s}^{(\text{ccsd})} (3.9 \text{ a.u., } 0^\circ) - E_{\text{eff},s}^{(\text{scf})} (3.9 \text{ a.u., } 0^\circ) \right). \quad (17) $$

We summarize the results for the $P,T$-odd parameters and confront them with the preceding work in the Table IV. The sensitivities to $P,T$-odd effects is more than two times smaller than for the RaOH molecule [25]. Our results are in concordance with the previous estimates for the fixed geometries. While for the lower levels vibrations do not strongly affect the $E_{\text{eff}}$ and $E_{s}$ parameters, for higher levels it may become significant.

### TABLE I. Rovibrational spectrum parameters

| Computation     | Experiment |
|-----------------|------------|
| Stretching mode $\nu_1$ | $550$ cm$^{-1}$ | $529.341(1)$ cm$^{-1}$ |
| Bending mode $\nu_2$   | $319$ cm$^{-1}$ | $339(5)$ cm$^{-1}$ |
| Rotational constant $B$ | $0.2461$ cm$^{-1}$ | $0.245434(13)$ cm$^{-1}$ |
| $l$-doubling $\Delta E_{l=1}$ | $= 2q$ | $26$ MHz |

$a$ The number in parenthesis denotes $2\sigma$ deviation
TABLE II. The deviations of $E_{\text{eff}}$ for $R = 3.9 \text{ a.u.}$ from the equilibrium values in the finite field approach

| Angle | SCF, GV/cm | CCSD correction, GV/cm |
|-------|------------|------------------------|
| $5^\circ$ | -0.006 | 0.003 |
| $10^\circ$ | -0.025 | -0.024 |
| $15^\circ$ | -0.055 | -0.066 |
| $20^\circ$ | -0.096 | -0.117 |
| $25^\circ$ | -0.149 | -0.173 |
| $30^\circ$ | -0.205 | -0.257 |
| $35^\circ$ | -0.257 | -0.309 |
| $40^\circ$ | -0.309 | -0.361 |
| $45^\circ$ | -0.361 | -0.413 |
| $50^\circ$ | -0.413 | -0.465 |

TABLE III. The deviations of $E_s$ for $R = 3.9 \text{ a.u.}$ from the equilibrium values in the finite field approach

| Angle | SCF, GV/cm | CCSD correction, GV/cm |
|-------|------------|------------------------|
| $5^\circ$ | -0.006 | 0.001 |
| $10^\circ$ | -0.022 | 0.002 |
| $15^\circ$ | -0.049 | 0.005 |
| $20^\circ$ | -0.086 | 0.008 |
| $25^\circ$ | -0.132 | 0.010 |
| $30^\circ$ | -0.188 | 0.027 |
| $35^\circ$ | -0.244 | 0.046 |
| $40^\circ$ | -0.300 | 0.067 |
| $45^\circ$ | -0.356 | 0.087 |
| $50^\circ$ | -0.412 | 0.108 |

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AUTHOR DECLARATIONS

Conflict of interest

The authors have no conflicts to disclose.

TABLE IV. Sensitivities to the $P$, $T$-odd effects for YbOH

| Equilibrium geometry | $E_{\text{eff}}, \text{GV/cm}$ | $E_s, \text{kHz}$ |
|----------------------|-------------------------------|-----------------|
| Angular dependence as in $^{15}$ |                         |                 |
| $v = 0$ state        | 23.810                        | 20.602          |
| $v = 1$ state        | 23.740                        | 20.540          |
| Angular dependence as in $^{17}$ |                         |                 |
| $v = 0$ state        | 23.716                        | 20.608          |
| $v = 1$ state        | 23.576                        | 20.548          |

Ref. $^{12}$ FSCC+Gaunt
Ref. $^{13}$ QZ CCSD
Ref. $^{14}$ GHF
Ref. $^{14}$ cGHF
Ref. $^{14}$ cGKS

* For the value of $\Omega = 0.495$.

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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FIG. 4. SCF (dashed) and CCSD (solid) $\mathcal{P}_J\mathcal{T}$-odd parameters for linear configurations of YbOH