

Electronic matrix elements for parity doubling in the YbOH molecule

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The YbOH molecule is one of the most sensitive systems for electron electric dipole moment (eEDM) searches. The eEDM-induced energy shift is proportional to the polarization P of the molecule. Petrov and Zakharova [A. Petrov and A. Zakharov, *Phys. Rev. A* **105**, L050801 (2022)] showed that the value of l doubling and spin-rotation splitting directly influence the maximum value of P . Recently, Jadbabaie *et al.* [A. Jadbabaie, Y. Takahashi, N. H. Pilgram, C. J. Conn, Y. Zeng, C. Zhang, and N. R. Hutzler, *New J. Phys.* **25**, 073014 (2023)] determined the corresponding energy levels experimentally. We introduce electronic matrix elements in the Hund’s case c coupling scheme to reproduce experimental energy levels and calculate P as a function of external electric field.

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I. INTRODUCTION

Measuring the electron electric dipole moment (eEDM) is now considered a most promising test for the existence of physics beyond the standard model [1–4]. The current constraint for the eEDM $|d_e| < 4.1 \times 10^{-30} e \text{ cm}$ (90% confidence) was obtained using trapped $^{180}\text{Hf}^{19}\text{F}^+$ ions [5] with the spinless ^{180}Hf isotope. Cold polar triatomic molecules provide opportunities for further progress in the search for the effects of \mathcal{T} , \mathcal{P} -symmetry violation, where \mathcal{T} is time reversal and \mathcal{P} is space parity [6]. In such molecules the sensitivity of the experiments can be strongly enhanced due to laser cooling and increasing the coherence time [7].

Next, the triatomic molecule with the linear equilibrium configuration possesses two degenerate bending (distorting linear configuration) vibrational modes in orthogonal planes. For the excited $v = 1$ (v is a vibrational quantum number) mode two alternative basis functions $|m\rangle$ having definite projections $m = \pm 1$ of vibrational momenta l on the molecular axis can be considered. The Coriolis interaction with stretching (preserving the linear configuration) modes results in a small splitting of energies (ΔE_1 and ΔE_3 in Fig. 2 below) between $1/\sqrt{2}(|m = +1\rangle + |m = -1\rangle)$ and $1/\sqrt{2}(|m = +1\rangle - |m = -1\rangle)$ states with opposite parities. This effect is known as l doubling (or parity doubling), and the corresponding states are called l doublets. The effect of l doubling is partially similar to the Ω -doubling one in diatomic molecules. The existence of l doublets of the excited $v = 1$ bending vibrational mode helps to suppress many systematics and allows us to polarize the molecule in a rather small electric field (see Fig. 3 below) [8,9].

Great progress was achieved recently in both theoretical and experimental studies of triatomics. In Ref. [10], using

the photon cycling transition $\tilde{A}^2\Pi(000) \rightarrow \tilde{X}^2\Sigma^+(000)$ [11,12], one-dimensional Doppler and Sisyphus cooling of a beam of $^{174}\text{YbOH}$ below 600 μK was achieved. In Ref. [13] quantum control of trapped triatomic molecules for eEDM searches was demonstrated. In Ref. [14] detailed spectroscopy of the eEDM-sensitive l doublets of the ground rotational $N = 1$ level of the excited $v = 1$ bending vibrational mode of $^{174}\text{YbOH}$ was performed. Unusually large asymmetric parity doubling of the $J = 1/2$ and $J = 3/2$ manifolds compared to other metal hydroxides was revealed. As noted in Ref. [14] further study is required to determine in detail the nature of this asymmetry. In Ref. [9] a method to compute the energy levels and different properties of triatomic molecules was developed. The method was applied to the calculation of the sensitivity of the $^{174}\text{YbOH}$ molecule to eEDM in the ground rotational $N = 1$ level of the first excited $v = 1$ bending mode in external electric field. In calculations (see below for details) the matrix elements of $v = 1$ were assumed to be equal to those for $v = 0$ and taken from Ref. [15]. In this approximation there was no asymmetry in the parity doubling of $J = 1/2$ and $J = 3/2$. In Ref. [9] we showed that the value of l doubling and spin-rotation splitting directly influence the maximum degree of \mathcal{T} , \mathcal{P} -odd polarization and thus influence the sensitivity of linear triatomic molecules to the \mathcal{T} , \mathcal{P} -odd effects. Therefore, in the current work we modify and introduce different *electronic* matrix elements in the Hund’s case c coupling scheme, which allows us to reproduce the experimental energy levels and, in particular, the asymmetry of the $J = 1/2$ and $J = 3/2$ manifolds. As opposed to Hund’s case b , using the Hund’s case c coupling scheme will help us in the future to calculate this effect *ab initio* because many modern quantum chemical packages allow us to include the spin-orbit interaction in all orders. Using the obtained electronic matrix elements, we recalculated the sensitivity of the $^{174}\text{YbOH}$ molecule to the eEDM in the external electric field.

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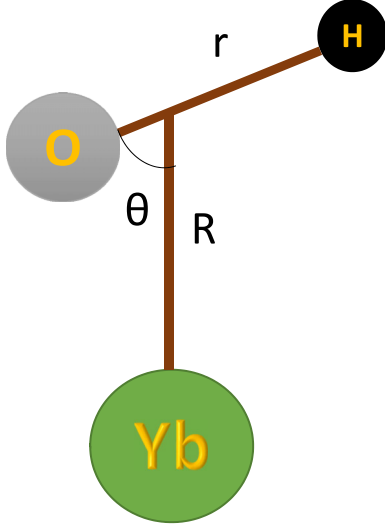


FIG. 1. Jacobi coordinates.

It is worth noting that beyond the eEDM the YbOH molecule was proposed to measure the nuclear magnetic quadrupole moment [16–18] and coupling constants of the interaction of electrons and the nucleus mediated by axionlike particles [19].

II. METHOD

Following Ref. [9], we present our Hamiltonian in the molecular reference frame as

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_{\text{mol}} + \hat{\mathbf{H}}_{\text{hfs}} + \hat{\mathbf{H}}_{\text{ext}}, \quad (1)$$

where

$$\hat{\mathbf{H}}_{\text{mol}} = \frac{(\hat{\mathbf{J}} - \hat{\mathbf{J}}^{e-v})^2}{2\mu R^2} + \frac{(\hat{\mathbf{J}}^v)^2}{2\mu_{\text{OH}} r^2} + V(\theta) \quad (2)$$

is the molecular Hamiltonian; μ is the reduced mass of the Yb-OH system; μ_{OH} is the reduced mass of OH; $\hat{\mathbf{J}}$ is the total electronic, vibrational, and rotational angular momentum; $\hat{\mathbf{J}}^{e-v} = \hat{\mathbf{J}}^e + \hat{\mathbf{J}}^v$ is the electronic-vibrational momentum; $\hat{\mathbf{J}}^e$ is the electronic momentum; $\hat{\mathbf{J}}^v$ is the vibrational momentum; R is the distance between Yb and the center of mass of OH; r is the OH bond length; and θ is the angle between OH and the axis (the z axis of the molecular frame) directed from Yb to the OH center of mass. The condition $\theta = 0$ corresponds to the linear configuration where the O atom is between Yb and H atoms. R , r , and θ are the so-called Jacobi coordinates (Fig. 1).

In the current work we have fixed R and r in such a way that $\frac{\hbar^2}{2\mu R^2} = 7329$ MHz to reproduce the experimental value for the rotation constant [14] and $\frac{\hbar^2}{2\mu_{\text{OH}} r^2} = 19.6$ cm⁻¹ to fit the experimental value of 24 MHz for l doubling [14]. Previously, the same value was also obtained in *ab initio* calculations [20]. In this approximation we neglect the influence of the stretching (associated with R) and OH ligand (associated with r) modes but, nevertheless, take into account the bending ones (associated with θ) with fixed R and r . $V(\theta)$ is the potential-energy curve obtained in the electronic structure calculations [21].

$\hat{\mathbf{H}}_{\text{hfs}}$ and $\hat{\mathbf{H}}_{\text{ext}}$ are the hyperfine interaction with the H nucleus and the Stark interaction with the external electric field, respectively, as described in Ref. [9].

Wave functions, rovibrational energies, and hyperfine structure were obtained by numerical diagonalization of the Hamiltonian (1) over the basis set of the electronic-rotational-vibrational-nuclear-spin wave functions

$$\Psi_{\Omega} P_{lm}(\theta) \Theta_{M_J, \omega}^J(\alpha, \beta) U_{M_I^H}^H. \quad (3)$$

Here $\Theta_{M_J, \omega}^J(\alpha, \beta) = \sqrt{(2J+1)/4\pi} D_{M_J, \omega}^J(\alpha, \beta, \gamma=0)$ is the rotational wave function, α and β correspond to the azimuthal and polar angles of the z axis, $U_{M_I^H}^H$ is the hydrogen nuclear-spin wave function, M_J is the projection of the molecular (electronic-rotational-vibrational) angular momentum $\hat{\mathbf{J}}$ on the laboratory axis, ω is the projection of the same momentum on the z axis of the molecular frame, M_I^H is the projections of the nuclear angular momenta of hydrogen on the laboratory axis, $P_{lm}(\theta)$ is the associated Legendre polynomial, l is the vibration angular momentum, m is its projection on the molecular axis, and Ψ_{Ω} is the electronic wave function (see Ref. [9] for details).

In this calculation functions with $\omega - m = \Omega = \pm 1/2$, where $l = 0-30$ and $m = 0, \pm 1, \pm 2$, and $J = 1/2, 3/2, 5/2$ were included in the basis set (3). The ground vibrational state $v = 0$ corresponds to $m = 0$, the first excited bending mode $v = 1$ (the focus of this paper) corresponds to $m = \pm 1$, the second excited bending mode $v = 2$ has states with $m = 0, \pm 2$, etc.

Provided that the *electronic-vibrational* matrix elements are known, the matrix elements of $\hat{\mathbf{H}}$ between states in the basis set (3) can be calculated with the help of the angular momentum algebra [9,22] mostly in the same way as for the diatomic molecules [23].

The required matrix elements associated with H-nucleus magnetic hyperfine interaction were taken from Ref. [9]. The dipole moment operator

$$\langle \Psi_{\Omega} | D_z | \Psi_{\Omega} \rangle = -0.850 \text{ a.u.} \quad (4)$$

determining the interaction with the external electric field was taken from Ref. [14].

Special attention is given to the matrix element of the $J_+^e = J_x^e + iJ_y^e$ operator which, in particular, ensures the asymmetry of the l doubling of the $J = 1/2$ and $J = 3/2$ manifolds. We set

$$\frac{1}{\mu R^2} \langle \Psi_{\Omega=1/2} | J_+^e | \Psi_{\Omega=-1/2} \rangle = p_0 + p_1 P_{l=1m=0}(\theta), \quad (5)$$

$$\frac{1}{\mu R^2} \langle \Psi_{\Omega=-1/2} | J_+^e | \Psi_{\Omega=+1/2} \rangle = p_2 P_{l=2m=2}(\theta). \quad (6)$$

Here we take into account that pure electronic matrix elements, in general, depend on θ , and the selection rules for the quantum number Ω can be violated [9]. It is assumed that Ψ_{Ω} are chosen in such a way that $\langle \Psi_{\Omega=1/2} | \partial/\partial\theta | \Psi_{\Omega=-1/2} \rangle = 0$. Note that here Ω is the projection of the total electronic angular momentum on the molecular axis z for the *linear* configuration. The equation $\hat{J}_z^e \Psi_{\Omega}(\theta) = \hbar \Omega \Psi_{\Omega}(\theta)$ is not satisfied [as seen from Eq. (6)] for the bending configuration with $\theta \neq 0$. The selection rules for the quantum number ω

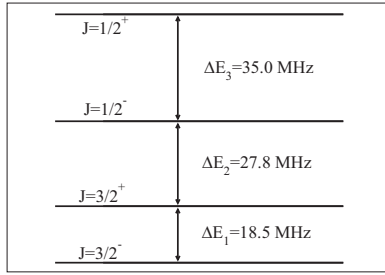


FIG. 2. Experimental energies of the ground rotational $N = 1$ level of the excited $v = 1$ bending vibrational modes of $^{174}\text{YbOH}$ [14]. The parity of the states is shown as a superscript. Unusually large asymmetry of the parity doubling of the $J = 1/2$ (ΔE_3) and $J = 3/2$ (ΔE_1) manifolds is observed. Hyperfine structure is not shown.

are rigorous and are the same as for the quantum number Ω for the linear configuration.

III. RESULTS

A. Energy levels for field-free case

The rotational levels of the excited $v = 1$ bending vibrational mode of YbOH are well described by the Hund's case b coupling scheme [14]. Electron spin $S = 1/2$ for a good approximation is an integral of motion. Its interaction (spin rotation) with the rovibrational momentum $\mathbf{N} = \mathbf{J} - \mathbf{S}$ gives rise to the splitting between the energy levels with total $J = N \pm 1/2$ momenta. Each level has two parity eigenstates: l doublets. l doubling is, in general, different for the $J = N + 1/2$ and $J = N - 1/2$ levels. The experimental energy levels obtained in Ref. [14] for the ground rotational level $N = 1$ are depicted in Fig. 2.

The p_0 value used in the Hund's case c coupling scheme can be obtained with the equation [24]

$$p_0 = \frac{\hbar^2}{\mu R^2} - \gamma = 0.492 \text{ cm}^{-1}, \quad (7)$$

where $\gamma = -88.7$ MHz determines spin-rotation interaction $\gamma(\hat{\mathbf{S}} \cdot \hat{\mathbf{N}} - S_z N_z)$ in the Hund's case b coupling scheme [14]. Using the p_0 and γ correlated by Eq. (7) gives the same energy levels in both Hund's case coupling schemes. In this approximation (corresponding to the calculations in Ref. [9]) l doubling is the same for $J = N \pm 1/2$ levels ($\Delta E_1 \approx \Delta E_3$; see Table I and Fig. 2 for the definition of ΔE_i). To reproduce the experimental energy levels we also set

$$p_1 = -37.0 \text{ MHz}, \quad (8)$$

$$p_2 = 125.9 \text{ MHz}. \quad (9)$$

Table I gives the calculated values of ΔE_1 , ΔE_2 , and ΔE_3 for the cases with $p_0 = 0.492 \text{ cm}^{-1}$, $p_1 = 0.0$ MHz, and $p_2 = 0.0$ MHz (case A); $p_0 = 0.492 \text{ cm}^{-1}$, $p_1 = 0.0$ MHz, and $p_2 = 125.9$ MHz (case B); and $p_0 = 0.492 \text{ cm}^{-1}$, $p_1 = -37.0$ MHz, and $p_2 = 125.9$ MHz [case C; corresponding to optimal matrix elements (7)–(9)].

Accounting for the p_2 constant leads to the asymmetry of the l doubling of $J = 1/2$ (ΔE_3) and $J = 3/2$ (ΔE_1)

TABLE I. The calculated ΔE_1 , ΔE_2 , and ΔE_3 energy splittings (MHz) for the p_0 , p_1 , and p_2 parameters corresponding to cases A, B, and C. In case A only the p_0 constant is taken into account. In case B the p_1 constant is added. In case C all three constants are taken into account. See text for details. Case C reproduces experimental values for ΔE_1 , ΔE_2 , and ΔE_3 . For case B the parentheses show the increment from case A, and for case C they show the increment from case B.

	Case A	Case B	Case C
ΔE_1	23.9	18.5 (−5.4)	18.5 (0.0)
ΔE_2	42.4	39.7 (−2.7)	27.8 (−11.9)
ΔE_3	24.1	35.0 (10.9)	35.0 (0.0)

manifolds. One can see that the increments ($\delta \Delta E_i$) for ΔE_i energy splittings when the constant p_2 is taken into account have ratios $\delta \Delta E_1 / \delta \Delta E_2 = 2$ and $\delta \Delta E_3 / \delta \Delta E_2 = -4$. The ratios for the Hamiltonian $p_G/2(N_+ S_+ e^{-i2\phi} + N_- S_- e^{+i2\phi})$ used in Ref. [14] for the Hund's case b coupling scheme are exactly the same. Therefore, one should associate the constants p_G and p_2 . From Eq. (6) one can see that the constant p_2 is nonzero when the quantum number Ω is violated for the bending configuration.

Accounting for the constant p_1 leads only to the increment of ΔE_2 . This is the same effect as for the Hamiltonian $\gamma_G N_z S_z$ used in Ref. [14]. Therefore, one should associate the constants γ_G and p_1 . From Eq. (5) one can see that the constant p_1 can be nonzero without violating the quantum number Ω .

Beyond conservation, for a good approximation, of the electron spin S and rotational quantum number N (discussed at the beginning of the section), one can consider Hund's case b to be a case when the energy splitting due to the spin-dependent interactions ($\sim \gamma = 89$ MHz for YbOH) is small compared with the energy differences between the rotational levels ($\sim \frac{\hbar^2}{2\mu R^2} = 7329$ MHz for YbOH). In Hund's case c the situation is the reverse [22]. Hence, in case b , at first glance, one can first obtain rotational structure, neglecting the spin-dependent interactions, and then the latter must be taken into account in the basis set of electronic-rotational functions. However, this approach cannot be considered a complete solution of the problems considered in this paper. For example, to calculate the constant p_G , it is assumed that formulas like (16) from Ref. [25] are used. Such formulas imply summation over the entire spectrum (which is difficult to implement) and take into account the spin-orbit interaction only in the second order. Meanwhile, for molecules containing atoms of heavy elements, for high-precision calculations, spin-orbit interactions must be taken into account in all orders. In case c , we first solve the electronic structure problem for nuclei at rest. For this step many modern quantum chemical packages, e.g., DIRAC [26], MRCC [27], and EXP-T [28], allow us to include the spin-orbit interaction in all orders. Then the motion of the nuclei is taken into account, and the rovibrational structure appears. This scheme, without any approximation, can actually be applied for case b as well. However, one should remember that large (comparable to the rotational constant) nonadiabatic matrix elements (5) and (6) have to be taken into account, as done in this paper. To the best of our knowledge, calculations

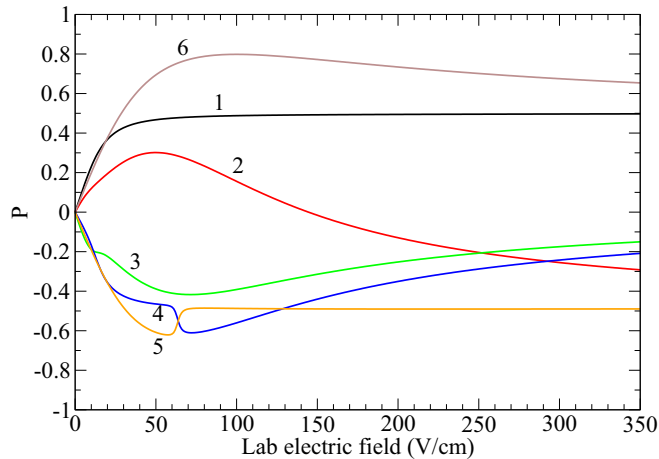


FIG. 3. Calculated polarization P [see Eq. (10)] for the $M_F = M_J + M_I = 1$ hyperfine sublevels of the lowest $N = 1$ rotational level of the first excited $v = 1$ bending vibrational mode of $^{174}\text{YbOH}$ as a function of the external electric field. The colors (numbering) of the lines correspond to the colors (numbering) of the lines in Fig. 4.

of the constants p_1 and p_2 are not currently available in public quantum chemical codes and should be a goal for further development.

B. Sensitivity to the eEDM

Any eEDM experiment searches for an eEDM-induced Stark shift

$$\delta E = PE_{\text{eff}}d_e, \quad (10)$$

where d_e is the value of the electron electric dipole moment, E_{eff} is the *effective electric field* acting on an electron in the molecule, and P is the polarization of the molecule by the external electric field. (We note that P is not equal to the mean value of the projection of the unit vector \hat{z} along the molecular axis in the direction of the external electric field.) To extract $d_e = \delta E / (E_{\text{eff}}P)$ from the measured shift δE , one needs to know PE_{eff} . E_{eff} was the subject of molecular calculations [21,29–31].

In this work to calculate P we also include hyperfine interaction with the hydrogen nucleus. The hydrogen nucleus has a nonzero nuclear spin $I = 1/2$, which gives rise to

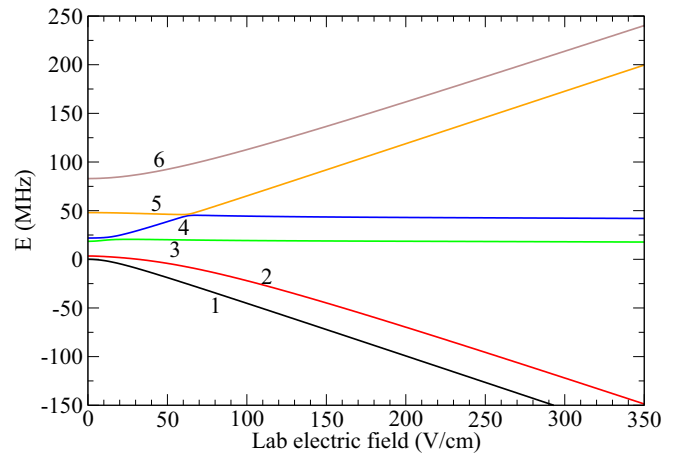


FIG. 4. Calculated energies for the $M_F = M_J + M_I = 1$ hyperfine sublevels of the lowest $N = 1$ rotational level of the first excited $v = 1$ bending vibrational mode of $^{174}\text{YbOH}$ as a function of the external electric field. The colors (numbering) of the lines correspond to the colors (numbering) of the lines in Fig. 3.

the hyperfine energy splitting between the levels with total (electronic-vibrational-rotational-nuclear-spin) angular momentum $F = J \pm 1/2$ (not shown in Fig. 2). Figure 3 gives the calculated polarizations P for six $M_F = M_J + M_I = 1$ hyperfine sublevels of the lowest $N = 1$ rotational level of the first excited $v = 1$ bending vibrational mode of $^{174}\text{YbOH}$ as a function of the external electric field. The maximum of polarization $P = 0.80$ is reached for the sixth level at an electric field of 100 V/cm, in agreement with data in Ref. [14]. Figure 4 presents the corresponding calculated energy levels.

IV. CONCLUSION

We determined the electronic matrix element in the Hund's case c coupling scheme to reproduce experimental energy levels and, in particular, asymmetry in the l -doubling structure of the ground rotational level of the first excited bending vibrational mode of $^{174}\text{YbOH}$. Matrix elements can be associated with the parameters of the effective Hamiltonian in the Hund's case b coupling scheme. \mathcal{T} , \mathcal{P} -odd polarization determining the sensitivity to the eEDM was calculated as a function of the external electric field. The maximum value $P = 0.8$ was found for electric field $E = 100$ V/cm.

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