

# Hexatomic molecule $\text{RaOCH}_3$ as a platform for studying interactions with the Dark Matter halo

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The interaction of the electronic shell of a hexatomic „symmetric top“ molecule with the Dark Matter halo is studied under the assumption that it is formed by a condensate of the pseudoscalar axion field. In the linear order, the contribution of the corresponding interaction vanishes for non-chiral molecules in equilibrium configurations, that's why chiral molecules were previously considered for its search. In this paper, we point out the possibility of this interaction for non-chiral molecules of the „symmetric top“ type through transitions between excited rovibrational, and consider it using the example of the  $\text{RaOCH}_3$  molecule. For this molecule, the effect is strongly suppressed, but the mechanism considered can lead to the observable effects in other molecules of this type.

**Keywords:** axion, symmetric top molecule, opposite parity levels, self-consistent field.

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## 1. Introduction

An important problem of fundamental physics is the nature of Dark Matter, whose existence is known from galaxy rotation curves and gravitational lensing data by galaxy clusters. It is also necessary to describe structure formation in the early Universe and the observed inhomogeneities of the cosmic microwave background radiation.

Potential candidates for dark matter particles are pseudoscalar particles called axions. Such particles in a certain mass range can solve the strong  $\mathcal{CP}$ -problem [1], which remains unresolved in the Standard Model (SM) of particle physics [2,3]. The discrete  $C$  transformation denotes symmetry with respect to charge conjugation,  $\mathcal{P}$  is related to spatial inversion. Violation of symmetry with respect to  $\mathcal{CP}$  transformation is equivalent to violation of time-reversal symmetry  $\mathcal{T}$  [4]. In the SM, all known parity violations occur in weak interactions related to mixing of the Cabibbo-Kobayashi-Maskawa quark matrices [5,6] and the Pontecorvo-Maki-Nakagawa-Sakata neutrino matrices [7,8]. Some physical effects, such as the electron electric dipole moment, are strongly suppressed in the Standard Model [9–12]. However, certain New Physics scenarios, such as supersymmetry, predict much larger values for these effects. The existence of new sources of  $\mathcal{CP}$ -violation may also be necessary to explain the baryon asymmetry problem of the Universe [13].

Molecular experiments make it possible to investigate effects related to violations of  $\mathcal{P}$  and  $\mathcal{T}$ -parities [10,14–17]. For example, a limit on the electron electric dipole moment was obtained in an experiment with the diatomic molecule

$\text{HfF}^+$  [18]. Theoretical calculations are required to estimate parameters of  $\mathcal{P}$ - and  $\mathcal{T}$ -arity violation for these effects [19].

Among studies of effects induced by new interactions with axions on molecules, works on axion exchange effects between electrons and nuclei as well as between electrons can be distinguished [20,21]. The sensitivity of the chiral molecule  $\text{CHBrClF}$  to interactions with cosmic fields of axions and dark photons, forming the Dark Matter halo, was previously considered in [.] Interaction symmetries imply that this effect can be nonzero only for chiral configurations. However, even achiral molecules in equilibrium configurations can be chiral in non-chiral configurations. In particular, molecules of the „symmetric top (rotator)“ type, such as  $\text{RaOCH}_3$ . In this work, we show how these interaction effects with background Dark Matter fields can manifest in transitions between excited vibrational states.

Hexatomic molecules are characterized by a rich rovibrational spectrum that contains various levels of opposite parity. In addition to doublets associated with rotation of the electronic shell, triatomic linear molecules possess  $l$ -doublets [23–25]. Hexatomic molecules of the „symmetric top“ type exhibit additional doublets connected with rotation of the  $\text{CH}_3$  ligand in two opposite directions [26]. Thus, in a molecule such as  $\text{RaOCH}_3$  both  $l$  and  $K$  doublets can be studied, which allows suppression of many systematic effects in an experiment.

$\mathcal{P}$ ,  $\mathcal{T}$  odd effects were previously studied also in molecules of the „symmetric top“ type. The molecule of interest  $\text{RaOCH}_3$  was studied in work [26]. In addition, several other molecules were investigated in works [27–30]. Laser cooling in polyatomic molecules

has been theoretically predicted [31–34] and experimentally demonstrated [35,36]. Large values of experimental sensitivity parameters for radium-containing molecules of the „symmetric top“ type to  $\mathcal{CP}$  and  $\mathcal{P}$ -symmetry violating effects were obtained earlier for:  $\text{RaOCH}_3$  [26],  $\text{RaOCH}_3^+$  and  $\text{RaCH}_3^+$  [37].

## 2. Interaction of Dark Matter fields with molecular electronic shells

Assume that the Dark Matter halo is generated by a Bose-Einstein condensate of pseudoscalar axion particles described by the field  $a$ . Thanks to the high density of the axion condensate and the small coupling constant of interaction with ordinary particles [38], its coherence is maintained even over cosmological times. Thus, ordinary particles interact coherently with such a condensate, so it can be considered a classical field. Moreover, the Dark sector may include additional fields such as a new vector field  $A^\mu$  known as the Dark photon. The following  $\mathcal{P}$ - and  $\mathcal{T}$ -interaction terms are considered among proposed interactions of these Dark sector fields with SM fields [22]:

$$\mathcal{L}^a = -\frac{g_{a\bar{e}e}}{m_e} (\partial_\mu a) \bar{\psi}_e \gamma^\mu \gamma^5 \psi_e, \quad \mathcal{L}^{\tilde{A}} = -\frac{g_{\tilde{A}\bar{e}e}}{m_e} \tilde{A}^\mu \bar{\psi}_e \gamma^\mu \gamma^5 \psi_e, \quad (1)$$

where  $g_{a\bar{e}e}$  and  $g_{\tilde{A}\bar{e}e}$  are the coupling constants of interaction with leptons of the axion field and the dark photon field, respectively.

We consider that on the scale of the solar system, the axion condensate density changes little. It can be expected that the velocity of axions composing the halo relative to the galaxy center should not exceed the galaxy's second cosmic velocity  $\sim 550$  km/s, which combined with the solar system velocity  $\sim 200$  km/s gives relative velocities of molecules and axions much less than the speed of light. These two assumptions imply that the axion condensate density  $a$  can be considered dependent only on  $t$  and its gradient  $\partial_\mu a$  is directed along the time axis. The  $a$  field must obey the Klein-Gordon-Fock equation for the corresponding mass  $m_a$ . Consequently, the axion field can be considered oscillating with a frequency determined by its mass:

$$a(t) = a_0 \cos m_a t. \quad (2)$$

Similarly, the vector potential of the dark photon will be considered directed along the time axis:

$$\tilde{A}^\mu(t) = \tilde{A} \delta_0^\mu \cos m_{\tilde{A}} t. \quad (3)$$

For molecular electronic states with fixed electron number, these interaction terms lead to the following additions to the effective molecular Hamiltonian:

$$\hat{H}_{\text{eff}}^a = \frac{g_{a\bar{e}e}}{m_e} m_a a_0 \gamma^5 \cos m_a t, \quad \hat{H}_{\text{eff}}^{\tilde{A}} = \frac{g_{\tilde{A}\bar{e}e}}{m_e} \tilde{A} \gamma^5 \cos m_{\tilde{A}} t. \quad (4)$$

Thus, the total molecular Hamiltonian can be represented as

$$\hat{H}_{\text{mol}} = \hat{H}_{\text{mol}}^{\mathcal{PT}} + \hat{H}_{\text{eff}}^a + \hat{H}_{\text{eff}}^{\tilde{A}}, \quad (5)$$

where  $\hat{H}_{\text{mol}}^{\mathcal{PT}}$  is the molecular Hamiltonian without New Physics effects and is  $\mathcal{P}$ ,  $\mathcal{T}$ -symmetric. We consider contributions of new effects as a small perturbation  $\hat{H}_{\text{mol}}^{\mathcal{PT}}$  to the Hamiltonian. Then the molecular Hamiltonian in the basis of unperturbed molecular wavefunctions  $|\Psi_{\text{tot},i}\rangle$  can be written as the matrix

$$H^{ij} = E_i \delta_{ij} + g_{a\bar{e}e} W_a^{ij} + g_{\tilde{A}\bar{e}e} W_{\tilde{A}}^{ij}, \quad (6)$$

where  $E_i$  is the energy of state  $|\Psi_{\text{tot},i}\rangle$  for the unperturbed molecular Hamiltonian  $\hat{H}_{\text{mol}}^{\mathcal{PT}}$  and the matrix elements are given by averaging the interaction Hamiltonians over unperturbed states:

$$W_{a,\tilde{A}}^{ij} = \frac{1}{g_{a,\tilde{A}\bar{e}e}} \langle \Psi_{\text{tot},i} | \hat{H}_{\text{eff}}^{a,\tilde{A}} | \Psi_{\text{tot},j} \rangle, \quad (7)$$

As can be seen, both interactions are described by the same effective one-electron operator  $\gamma_5$ .

In the Born-Oppenheimer approximation, the total molecular wavefunction can be represented as the product of the nuclear wavefunction with degrees of freedom  $\{Q_I\}$  and the electronic wavefunction with degrees of freedom  $\{q_i\}$  for a fixed molecular configuration:

$$\Psi_{\text{tot}} = \Psi_{\text{nuc}}(\{Q_I\}) \psi_{\text{elec}}(\{q_i\} | \{Q_I\}), \quad (8)$$

where the electronic state for a given configuration  $\{Q_I\}$  is also denoted as  $|\psi_{\text{elec}}, \{Q_I\}\rangle$ . Restricting consideration to only the ground electronic state, the matrix elements of the new interactions can be represented as

$$W_{a,\tilde{A}}^{ij} = \int \prod_I dQ_I \Psi_{\text{nuc},i}^*(\{Q_I\}) \Psi_{\text{nuc},j}(\{Q_I\}) W_{a,\tilde{A}}(\{Q_I\}), \quad (9)$$

where parameters characterizing the sensitivity of the electronic shell to new interactions for a fixed molecule configuration are introduced:

$$W_{a,\tilde{A}}(\{Q_I\}) = \frac{1}{g_{a,\tilde{A}\bar{e}e}} \langle \psi_{\text{elec}}, \{Q_I\} | \hat{H}_{\text{eff}}^{a,\tilde{A}} | \psi_{\text{elec}}, \{Q_I\} \rangle, \quad (10)$$

i.e., the task breaks down into calculating properties for fixed molecular configurations with subsequent averaging over the rovibrational nuclear wavefunction.

Under reflection of the molecule configuration, the operator  $\gamma_5$  is odd. For non-chiral molecular configurations

$$\mathcal{P}|\psi_{\text{elec}}, \{Q_I\}\rangle = P_\psi |\psi_{\text{elec}}, \{Q_I\}\rangle, \quad P_\psi = \pm 1, \quad (11)$$

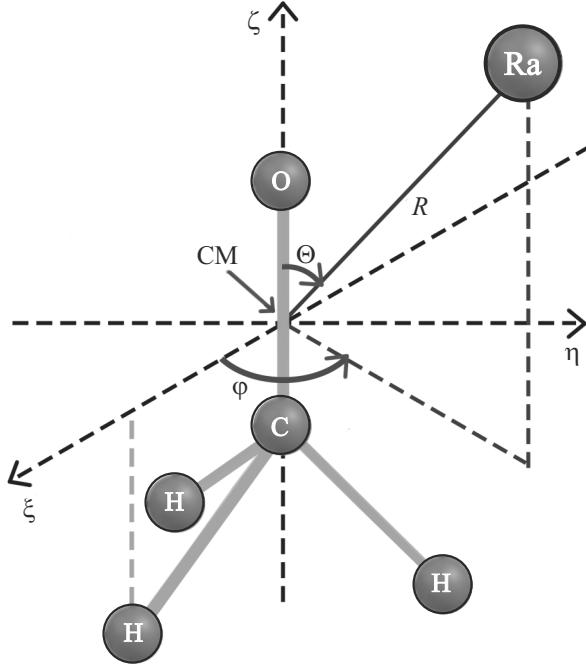
and the oddness of operator  $\mathcal{P}\gamma_5\mathcal{P} = -\gamma_5$  means that

$$\begin{aligned} \langle \psi_{\text{elec}}, \{Q_I\} | \gamma_5 | \psi_{\text{elec}}, \{Q_I\} \rangle &= \\ &= \langle \psi_{\text{elec}}, \{Q_I\} | \mathcal{P}^2 \gamma_5 \mathcal{P}^2 | \psi_{\text{elec}}, \{Q_I\} \rangle \\ &= P_\psi^2 \langle \psi_{\text{elec}}, \{Q_I\} | \mathcal{P} \gamma_5 \mathcal{P} | \psi_{\text{elec}}, \{Q_I\} \rangle \\ &= -\langle \psi_{\text{elec}}, \{Q_I\} | \gamma_5 | \psi_{\text{elec}}, \{Q_I\} \rangle = 0. \end{aligned} \quad (12)$$

Thus,  $\gamma_5$  contributes only for non-chiral configurations.

Geometry of ligand  $\text{OCH}_3$ 

Parameter	Value
$r(\text{O-C})$	2.600 a.u.
$r(\text{C-H})$	2.053 a.u.
$\angle(\text{O-C-H})$	$110.73^\circ$

Geometry of molecule  $\text{RaOCH}_3$ .

### 3. Molecular structure

The molecule  $\text{RaOCH}_3$  can be considered as a system consisting of a heavy radium atom and  $\text{OCH}_3$  ligand. Vibration frequencies corresponding to ligand deformations are much larger than the vibration frequencies of this system, so we will consider the  $\text{OCH}_3$  ligand as rigid. We use the same geometry of the  $\text{OCH}_3$  ligand as in article [26], the parameters of which are given in the table. The ligand  $\text{OCH}_3$  itself is a symmetric top with a moment of inertia

$$I_{\text{OCH}_3} = \text{diag}\{I_\xi, I_\xi, I_\xi\}, \quad I_\xi > I_z. \quad (13)$$

For a rigid ligand, the molecular configuration in the Space-Fixed Frame can be specified by the following parameters: a vector  $\mathbf{R} \equiv \mathbf{R} \cdot \hat{\mathbf{R}}$  connecting the ligand's center of mass to the heavy atom; Euler angles  $\alpha, \beta, \gamma$  defining the ligand orientation in LCS. Angles  $\alpha$  and  $\beta$  define the unit vector  $\hat{\mathbf{r}}$  corresponding to the primary axis direction of the ligand C-O, and the angle  $\gamma$  is chosen such that for  $\alpha = 0, \beta = 0, \gamma = 0$  one of the O-C-H planes coincides with the plane  $xz$ .

The molecular configuration can also be described using the Body-Fixed Frame by the distance  $R$  from the ligand's

center of mass (CM, indicated by a straight arrow in the figure) to the heavy atom, the angle  $\theta$  between vector  $\mathbf{R}$  and the C-O axis, and the angle  $\varphi$  between the R-O-C plane and one of the O-C-H planes (see figure). The molecule is non-chiral for the equilibrium configuration  $\theta = 0$ , as well as for nonzero values of  $\theta$  at angles  $\varphi = 0^\circ, 60^\circ, 120^\circ, 180^\circ, 240^\circ, 300^\circ$  where the Ra-O-C plane coincides with any of the O-C-H planes. However, at other values of  $\varphi$  the molecular configuration becomes chiral and sensitive to perturbation by the operator  $\gamma_5$ .

Within the Born-Oppenheimer approximation, the molecular wave function factorizes into the product of the nuclear motion wave function and the electronic wave function:

$$\Psi_{\text{total}} \simeq \Psi_{\text{nuc}}(R, \hat{\mathbf{R}}, \hat{\mathbf{r}}, \gamma) \psi_{\text{elec}}(\{\mathbf{r}_i\} | \mathbf{R}, \theta, \varphi), \quad (14)$$

where  $\psi_{\text{elec}}$  is computed for a fixed molecular geometry  $(R, \theta, \varphi)$ , and  $\Psi_{\text{nuc}}$  is the eigenfunction of the nuclear motion Hamiltonian.

Formula (9) takes the form:

$$W_{a,\hat{A}}^{ij} = \int_0^{+\infty} dR \int_0^\pi d\theta \sin \theta \int_0^{2\pi} d\varphi \times \Psi_{\text{nuc},i}^*(R, \theta, \varphi) \Psi_{\text{nuc},j}(R, \theta, \varphi) W_{a,\hat{A}}(R, \theta, \varphi), \quad (15)$$

where  $W_{a,\hat{A}}(R, \theta, \varphi)$  is obtained by averaging the Hamiltonian of the new interaction over the electronic wave function at fixed molecular configuration.

In the harmonic approximation, the nuclear motion Hamiltonian can be represented as [26]:

$$\hat{H}_{\text{nuc}} \simeq \frac{1}{2}(\hat{\mathbf{J}} - \hat{\pi}) \cdot \mathcal{M}(\hat{\mathbf{J}} - \hat{\pi}) + \hat{H}_{\parallel} + \hat{H}_{\perp}. \quad (16)$$

The first term is the Hamiltonian of a symmetric top with total angular momentum  $\hat{\mathbf{J}}$  and vibrational angular momentum  $\hat{\pi}$ . The inertia moment matrix in the first approximation can be considered equilibrium  $\mathcal{M} \simeq I_{\text{tot}}^{(\text{eq})}$ . Quantum numbers for projections  $\hat{\mathbf{J}}$  on the SFF and BFF axes are denoted as  $M$  and  $K$ , respectively. The second term  $\hat{H}_{\parallel}$  is the Hamiltonian of a one-dimensional harmonic oscillator for longitudinal vibrations:

$$\hat{H}_{\parallel} = -\frac{1}{2} \frac{\partial^2}{\partial q_{\parallel}^2} + \frac{\omega_{\parallel}^2 q_{\parallel}^2}{2}, \quad q_{\parallel} = \sqrt{\mu} \delta R, \quad (17)$$

where  $\delta R = R - R_{\text{eq}}$  and  $\mu = m_{\text{Ra}} m_{\text{OCH}_3} / (m_{\text{Ra}} + m_{\text{OCH}_3})$ . The occupation number of  $\hat{H}_{\parallel}$  is denoted as  $v_{\parallel}$ . In [26] the value  $\omega_{\parallel} = 345.17 \text{ cm}^{-1}$  was obtained. The third term  $\hat{H}_{\perp}$  is the Hamiltonian of a two-dimensional harmonic oscillator for transverse vibrations:

$$\hat{H}_{\perp} = -\frac{1}{2} \frac{\partial^2}{\partial q_x^2} - \frac{1}{2} \frac{\partial^2}{\partial q_y^2} + \frac{\omega_{\perp}^2 (q_x^2 + q_y^2)}{2}, \quad (18)$$

depending on variables,

$$q_x = \sqrt{\mathcal{J}} \theta \cos \varphi, \quad q_y = \sqrt{\mathcal{J}} \theta \sin \varphi, \quad \mathcal{J} = \frac{\mu R_{\text{eq}}^2 I_\xi}{\mu R_{\text{eq}}^2 + I_\xi}. \quad (19)$$

In [26] the value  $\omega_{\parallel} = 151.32 \text{ cm}^{-1}$  was found. The eigenstates of  $\hat{H}_{\perp}$  can be characterized by the occupation number  $v_{\perp} = 0, 1, \dots$  and vibrational angular momentum  $l = -v_{\perp}, -v_{\perp} + 2, \dots, v_{\perp}$ . In the considered approximation, the eigenstates of the nuclear motion Hamiltonian can be approximately described as:

$$|JMKv_{\parallel}v_{\perp}l\rangle \mapsto \Psi_{\text{nuc}} \simeq D_{MK}^J(\alpha_m, \beta_m, \gamma_m) \times \phi_{v_{\parallel}}(q_{\parallel})\Phi_{v_{\perp}l}(q_x, q_y), \quad (20)$$

where  $D_{MK}^J$  is the Wigner function depending on Euler angles describing the orientation of MCS relative to BFF;  $\phi_{v_{\parallel}}$  is the eigenfunction of the one-dimensional harmonic oscillator;  $\Phi_{v_{\perp}l}$  is the eigenfunction of the two-dimensional harmonic oscillator, which depends on  $\varphi$  as

$$\Phi_{v_{\perp}l} = F_{v_{\perp}l}(\theta)e^{il\varphi}. \quad (21)$$

In the harmonic approximation, a large degeneracy of the spectrum

$$E \simeq BJ(J+1) + (A-B)K^2 + \omega_{\parallel}\left(v_{\parallel} + \frac{1}{2}\right) + \omega_{\perp}(v_{\perp}+1) \quad (22)$$

is observed, which is broken when taking into account anharmonic contributions and rotational effects. In particular, states with opposite signs of  $l$  should form split doublets of states of opposite parity:

$$\begin{aligned} & \left| \pm, \{JMKv_{\parallel}v_{\perp}l\} \right\rangle \\ &= \frac{1}{\sqrt{2}} \left( \left| JMKv_{\parallel}v_{\perp} + l \right\rangle \pm \left| JM, -K, v_{\parallel}v_{\perp}, -l \right\rangle \right). \end{aligned} \quad (23)$$

Note that in molecules of the symmetric top type,  $K$  is not fully determined by  $l$  due to additional contributions from the rotation of ligand  $\text{OCH}_3$ .

The oddness of the operator  $\gamma_5$  under reflections of the molecular configuration means that properties defined in (10) are antisymmetric in  $\varphi$ , i.e.  $W_{a,\tilde{A}}(R, \theta, \varphi) = -W_{a,\tilde{A}}(R, \theta, -\varphi)$ . On the other hand, from the symmetry of the molecular equilibrium configuration, it follows that  $W_{a,\tilde{A}}(R, \theta, \varphi + 2\pi/3) = W_{a,\tilde{A}}(R, \theta, \varphi)$ . From these two facts, we obtain that averages over electronic states should have the following dependence on molecular geometry:

$$W_{a,\tilde{A}}(R, \theta, \varphi) = \sum_{n=1}^{+\infty} W_{a,\tilde{A}}^{(n)}(R, \theta) \sin 3n\varphi. \quad (24)$$

We are interested in matrix elements between closely spaced states, i.e., those with identical  $J$ ,  $K = 0$ ,  $v_{\parallel}$  and  $v_{\perp}$ . The requirement  $K = 0$  in the harmonic approximation follows from the orthogonality of Wigner functions with nonzero  $K = \pm|K|$  in the nuclear wave function (20). From (21) and (24) it can be obtained that the following matrix

elements may be nonzero:

$$\begin{aligned} & \left\langle JM, K = 0, v_{\parallel}v_{\perp}, l + 3n \left| W_{a,\tilde{A}} \right| \right. \\ & \left. \times JM, K = 0, v_{\parallel}v_{\perp}, l \right\rangle \equiv W_{a,\tilde{A}}^{JKv_{\parallel}v_{\perp}, l, l+3n}, \end{aligned} \quad (25)$$

and its sign-opposite counterpart

$$\left\langle JMKv_{\parallel}v_{\perp}, l \left| W_{a,\tilde{A}} \right| JMKv_{\parallel}v_{\perp}, l+3n \right\rangle = -W_{a,\tilde{A}}^{JKv_{\parallel}v_{\perp}, l, l+3n}. \quad (26)$$

Note that since in a multiplet with identical  $v_{\perp}$  there are states with  $l$  differing only by even values, contributions in (24) with odd  $n$  cannot provide the matrix elements of interest. Therefore, the leading contribution is expected from the term with  $\sin 6\varphi$ . The lowest states in which this term can induce transitions are the doublet  $\left| \pm, \{J = 3, K = 0, v_{\parallel} = 0, v_{\perp} = 3, l = 3\} \right\rangle$  hereafter denoted as  $|\pm\rangle$ .

## 4. Discussion of Results

Electronic calculations were performed using the Dirac-Hartree-Fock self-consistent field method implemented in the DIRAC19 software package. For the radium atom, a full-electron 3z Dyal basis with diffuse functions (aee3z) was used. For atoms O, C, and H, cc-pVTZ basis sets were employed.

Neglecting the time dependence of Dark fields, note that the property values are expressed through the average value  $\gamma^5$ :

$$W_a(R, \theta, \varphi) = \frac{1}{m_e} m_a a_0 \langle \gamma^5 \rangle (R, \theta, \varphi), \quad (27)$$

$$W_{\tilde{A}}(R, \theta, \varphi) = \frac{1}{m_e} \tilde{A} \langle \gamma^5 \rangle (R, \theta, \varphi), \quad (28)$$

where most parameters characterize background Dark fields, and the molecule-specific value is  $\langle \gamma^5 \rangle$  obtained by averaging the corresponding one-electron operator over the electronic wave function for a fixed configuration:

$$\langle \gamma^5 \rangle (R, \theta, \varphi) = \langle \psi_{\text{elec}}, \{R, \theta, \varphi\} | \gamma^5 | \psi_{\text{elec}}, \{R, \theta, \varphi\} \rangle. \quad (28)$$

Calculations were conducted for a fixed distance from the center of mass of ligand  $\text{OCH}_3$  to the heavy radium atom  $R_{\text{eq}} = 5.7 \text{ a.u.}$  corresponding to the equilibrium value. Angular coordinates were considered on grids of values  $\theta = 0^\circ, \dots, 25^\circ$  and  $\varphi = 0^\circ, \dots, 60^\circ$  with step  $5^\circ$ .

The results are well described (deviations within the machine precision of calculations) by the formula:

$$\langle \gamma_5 \rangle (R_{\text{eq}}, \theta, \varphi) = (8.619 \cdot 10^{-8} \theta^2 + 2.947 \cdot 10^{-7} \theta^4) \sin 3\varphi, \quad (29)$$

where  $\theta$  and  $\varphi$  are given in radians.

Formula (29) for  $\theta = 12^\circ$  (corresponding to the probability density peak for the state  $|v = 3, l = 3\rangle$ ) and  $\varphi = 30^\circ$  (corresponding to the maximum of property  $W_a$ ) gives the value  $\langle \gamma_5 \rangle = 4.35 \cdot 10^{-9}$ . This value is comparable in order

of magnitude to  $\langle \gamma_5 \rangle = -8.28 \cdot 10^{-9}$  obtained in [22] for the ground state of the chiral molecule  $\text{CHBrClF}$ . Nevertheless, for our mechanism, sufficiently large contributions  $\sin 6\varphi$  are required. In our calculations, such contributions were negligibly small.

It should be noted that calculations were performed only for the self-consistent field method. Correlation effects can significantly influence the value and qualitative behavior of  $\langle \gamma_5 \rangle$  as a function of  $(\theta, \varphi)$ . Calculating average values considering correlation effects requires the finite field method, in which the molecular Hamiltonian is augmented with the property operator multiplied by a coefficient  $\epsilon$  and its average value can be obtained from the formula for energy  $E \simeq E_0 + \epsilon \langle \gamma_5 \rangle$ . In our case, coupled cluster method calculations showed very poor convergence, so we do not present these results.

Additionally, according to estimates in [22] with increasing nuclear charge  $Z$  the average property value scales like  $\langle \gamma_5 \rangle \sim c_1 \alpha^5 Z_A^2 Z_B^2 + c_2 \alpha^3 Z_A^3 + c_3 \alpha^3 Z_B^3$ . In our case, the heavy radium atom provides a large value  $Z_{\text{Ra}} = 88$  but the molecular chirality is ensured by the light hydrogen atoms with  $Z_{\text{H}} = 1$ . One may suppose that for molecules of the symmetric top type with heavier atoms, such as  $\text{RaOCF}_3$  this effect may be significantly enhanced.

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## Conflict of interest

The author declares that he has no conflict of interest.

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