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P-ODD DIFFERENCE OF HYPERFINE STRUCTURE CONSTANTS IN OPTICAL ISOMERS

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ABSTRACT

The existence of the difference between the hyperfine structure constants in optical isomers due to the parity non-conserving nuclear spin-dependent weak interaction of an electron with nucleus is demonstrated in a model. For heavy radicals with $Z \sim 80$ the effect may exceed 10 Hz, so that its observation is sufficiently realistic with modern experimental technics.

P-odd energy difference between optical isomers is under discussion already for many years. The full list of papers concerning this topic is too large to be presented in this short note. Unfortunately, neither of discussed phenomena of this kind has been experimentally discovered up to now.

In the present work we consider the contribution to the energy difference between isomers caused by the P-odd nuclear spin-dependent interaction of an electron with nucleus. This effect was discussed previously in Refs. [1,2]. In the first of them (see also Ref. [3]) the possibility to observe the corresponding energy difference in optically isomeric crystals by means of the Mössbauer effect was considered. In the second one the order of magnitude estimates were given for the P-odd effects in optical isomers, both in molecules and radicals, with and without magnetic field.

The present note pursues two aims. The first is to demonstrate in a simple model the existence of the P-odd energy difference between optical isomers caused by the weak interaction of an electron with nuclear spin. Second, I wish to turn attention to the fact that the observation of the effect in radicals with a heavy atom is sufficiently realistic with modern experimental technics.

As to the first aim, such a model consideration seems to be appropriate at least because the very existence of such effects was questioned repeatedly. We shall use here the same model of a molecule that was used in Refs. [1,3] to demonstrate the existence of the nuclear spin-independent splitting. Suppose a heavy atom with external electron in the $p_{3/2}$ state is surrounded by three other atoms that differ both from it and from one another. The interaction with one of the neighbouring atoms, which we shall call atom 3, is taken into account by assuming that the levels having different moduli of a projection μ of the angular momentum onto the axis passing through the heavy atom and atom 3 are not degenerate. We shall consider the fields of the other two neighbouring atoms (more, precisely, ions) as the Coulomb perturbations with the charges Z_1 and Z_2. Since the weak interaction of an electron with nucleus mixes the states $s_{1/2}$ and $p_{1/2}$

only (see, e.g., Ref. [3]), just these states should be admixed at any rate by the Coulomb perturbation to the initial one $|p_{3/2}, \mu\rangle$. The state arising when these admixtures are taken into account looks as follows [1,3]:

$$|\tilde{\mu}\rangle = |p_{3/2}, \mu\rangle + \frac{4}{3}\frac{\sqrt{4\pi}\,Ry}{E_s}\sum_{i=1,2} Z_i Q_1(r_i)\sum_{q,\mu'}(-1)^{1/2-\mu'}\begin{pmatrix} 3/2 & 1 & 1/2 \\ \mu & q & -\mu' \end{pmatrix} Y^*_{1q}(\underline{n}_i)|s_{1/2}, \mu'\rangle + \frac{4}{5}\frac{\sqrt{4\pi}\,Ry}{E_p}\sum_{i=1,2} Z_i Q_2(r_i)\sum_{q,\mu'}(-1)^{1/2-\mu'}\begin{pmatrix} 3/2 & 2 & 1/2 \\ \mu & q & -\mu' \end{pmatrix} Y^*_{2q}(\underline{n}_i)|p_{1/2}, \mu'\rangle. \quad (1)$$

Here E_s and E_p are the energies of the admixed s and p states reckoned from the initial $p_{3/2}$ level; $Ry = m\alpha^2/2$ is the Rydberg constant; Y_{kq} are spherical functions; the expressions $\begin{pmatrix} j & k & j' \\ \mu & q & -\mu' \end{pmatrix}$ are $3j$ symbols. The quantities $Q_k(r_i)$ correspond to the multipoles of the Coulomb field of the ions 1 and 2, they are expressed in the following way through the nonrelativistic radial wave functions $R_{3/2}$ and $R_{1/2}$ for the ground and admixed states of the heavy atom:

$$Q_k(r_i) = a\int_0^\infty dr\, r^2 R_{3/2}(r) R_{3/2}(r)\left[\theta(r-r_i)\frac{r_i^k}{r^{k+1}} + \theta(r_i - r)\frac{r^k}{r_i^{k+1}}\right] \quad (2)$$

Here a is the Bohr radius.

Consider now the wave functions of the molecule taking into account magnetic hyperfine (hf) interaction. It can be easily seen that at $\mu = \pm 3/2$ this interaction, being a vector both in electron and nuclear variables, does not mix to the zeroth order in the Coulomb perturbation Q different states of the kind

$$|\tilde{\mu}\rangle|I, \nu\rangle \quad (3)$$

where $|I, \nu\rangle$ are wave functions of a nucleus with angular momentum I and its projection ν. It means that with the accuracy of interest to us the molecular wave function with hf structure taken into account is described by the expressions (3). Note that the hf splitting at $\mu = \pm 3/2$ to the zeroth order in Q is

$$A\mu\nu \quad (4)$$

where A is a constant.

At $\mu = \pm 1/2$ the hf interaction mixes the states $|p_{3/2}, {}^{1}/_{2}\rangle|I, \nu\rangle$ and $|p_{3/2}, -{}^{1}/_{2}\rangle|I, \nu+1\rangle$ to the zeroth order in Q already so that the molecular wave function is not factorized in electron and nuclear variables. This case is somewhat more complicated than $\mu = \pm 3/2$, and we do not consider it here.

We pass now to the parity nonconserving nuclear spin-dependent interaction of an electron with nucleus. As it was shown in Refs. [4,5], it is caused mainly by the electromagnetic interaction of the electron with P-odd anapole moment (am) of nucleus. This interaction can be presented as

$$H = \frac{G}{\sqrt{2}}\varkappa_a \frac{K\underline{I}\,\underline{\alpha}}{I(I+1)}\delta(\underline{r}), \quad K = (-1)^{I+1/2-l}(I+1/2). \quad (5)$$

Here G is the Fermi weak interaction constant; l is the orbital angular momentum of the external nucleon in the nucleus; $\underline{\alpha}$ is the Dirac matrix of an electron; $\varkappa_a$ is a dimensionless characteristic of the am, in heavy nuclei with odd Z it is close to 0.3. The matrix element of the mixing of the

states $s_{1/2}$ and $p_{1/2}$ due to this interaction constitutes (see, e.g., [3])

$$\langle s_{1/2}|H|p_{1/2}\rangle = i\frac{Gm^2\alpha^2Z^2R}{\sqrt{2}\pi(\nu_s\nu_p)^{3/2}}\frac{2r+1}{3}\mathcal{X}_a Ry \times$$
$$\times\frac{K}{I(I+1)}2(\underline{I}\underline{j}). \qquad (6)$$

Here m is the electron mass, $\alpha = 1/137$, $r=\sqrt{1-Z^2\alpha^2}$, ν_s and ν_p are the effective principal quantum numbers of the mixing states, R is a relativistic enhancement factor close to 10 at $Z\sim 80$. Now by means of elementary calculations one can get the following expression for the discussed correction to the energy of the molecule:

$$\frac{8}{15}Z_1Z_2\left([\underline{n}_1\times\underline{n}_2]\underline{n}_3\right)\left([Q_1(r_1)Q_2(r_2)\underline{n}_2 - Q_1(r_2)Q_2(r_1)\underline{n}_1]\underline{n}_3\right)\times \qquad (7)$$
$$\times\frac{Gm^2\alpha^2Z^2R}{\sqrt{2}\pi(\nu_s\nu_p)^{3/2}}\frac{2r+1}{3}\frac{(Ry)^3}{E_sE_p}\mathcal{X}_a\frac{K}{I(I+1)}\mu\nu.$$

In essence, this quantity is just a pseudoscalar correction to the constant A of the molecular hf structure (cf.(4)), a correction which sign depends on the molecule being a right or left isomer.

Having demonstrated by this example the existence of the discussed effect, we turn now to the second question, concerning the feasibility of its observation. The order of magnitude estimate of the splitting looks evidently as follows:

$$\Delta E \sim \frac{Gm^2\alpha^2Z^2R}{\sqrt{2}\pi(\nu_s\nu_p)^{3/2}}Ry\,\theta\,\mathcal{X}_a \qquad (8)$$

where θ is a characteristic angle of the twist that distinguishes a right molecule from a left one. Numerically at $Z\sim 80$ the discussed effect constitutes

$$\Delta E \sim (10-100)\,Hz\cdot\mathcal{X}_a. \qquad (9)$$

We try to be cautious in this estimate, so that the value (9) proves to be 10-100 times smaller than the corresponding estimates in Refs. [1-3]. Nevertheless, the measurement of frequency splitting at the level of 10 Hz in the transitions between the hf structure components seems to be a sufficiently realistic task. It should be stressed however that the estimate (9) refers to a radical as an optical isomer. In the case of a molecule where total electron angular momentum is zero, the magnitude of P-odd nuclear spin-dependent splitting is much smaller [2].

It is necessary here also that the wave function of the odd electron in a radical should be sufficiently localized on the heavy centre, first, and should feel the structure asymmetry, second.

The observation of the discussed effect would be extremely interesting not only by itself. It would allow to discover P-odd nuclear moments-anapoles that have not been observed up to now. In principle a possibility arises to compare the am of different isotopes, and molecular calculations are not necessary for such a comparison, evidently.

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