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PARITY VIOLATION EFFECTS IN DIATOMIC MOLECULES

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1. Introduction

As it is known, there are very close levels of the opposite parity in diatomic molecules. These are the so-called Λ-doubling or Ω-doubling of the rotational level with a given total angular momentum J. In this paper the enhancement mechanism of T- and P-odd effects is presented which is based on this nearness. When this work was over, we made acquaintance with the paper by L.N.Labzovsky /1/ devoted to the calculation of P-odd effects in molecules. It turned out that our results dealing with the enhancement of P-odd effects are consistent, in principle, with those of Labzovsky. However, since we discuss the experiments of another type, more promising from our point of view, and since we treat the enhancement of an electric dipole moment (EDM) of the electron, publication of this paper seems worthwhile.

In molecules the part of weak interaction which is due to product of the electron vector current and nucleon axial one proves to be enhanced. The contribution of this interaction increases with an increase of a nucleus charge as Z^2 /2/. The enhancement factor of EDM increases as Z^3/3,4,5/. Therefore, we shall consider the molecules where one of the atoms is heavy. The spin-orbit interaction in such molecules is comparable to splitting between the states with different Λ (the case intermediate between a and c, according to Hund /6/) and it is convenient to carry out the classification of electron terms on the basis of the projection Ω of the total electronic angular momentum on the axis of a molecule.

Remind the origin of the splittting of opposite-parity levels. Consider first of all the simplest case $|\Omega| = 1/2$. For

crude estimates one can assume that the total angular momentum of electrons is $j = 1/2$ (the case c, according to Hund). The levels with $\Omega = 1/2$ and $\Omega = -1/2$ are degenerate, therefore the electronic momentum $j = 1/2$ is decoupled from the axis of a molecule, i.e. it may be quantized on any axis. Let L be the angular momentum of the nuclei. It is clear that at a given total angular momentum there are two states of different particles: $L_1 = J - 1/2$ and $L_2 = J + 1/2$. A typical splitting $\Delta E \sim B L_1(L_1+1) - B L_2(L_2+1) = 2B(J+\frac{1}{2})$, $B = \hbar^2/2I$, where I is the moment of inertia of the molecule. For example, for the BiS molecule $\Delta E = 0.11\,(J + 1/2)$ cm^{-1} /7/, i.e. ΔE is 4-6 orders of magnitude less than the distance between the opposite-parity levels in heavy atoms.

For accurate calculations it is convenient to express the wave function of a diatomic molecule via D-functions of the symmetric top /6,8/

$$|JM\omega\eta\rangle = \sqrt{\frac{2J+1}{8\pi}}\left\{D^J_{\omega M}(\varphi,\theta,0)|\omega\rangle + \eta(-1)^{J-\omega} D^J_{-\omega M}(\varphi,\theta,0)|-\omega\rangle\right\} \quad (1)$$

$\omega \equiv |\Omega|$

Here J and M are the total angular momentum and its projection on the z-axis, Ω is the projection on the axis of the molecule, η is the parity of the state ($\eta = \pm 1$); $|\omega\rangle$ and $|-\omega\rangle$ are the corresponding internal states of the molecule. The centrifugal energy operator is of the form

$$H_B = B(\vec{J} - \vec{j})^2 \quad (2)$$

The matrix elements for the states (1) are calculated in a standard way /6,8/. In the first order in H the splitting between

the levels of opposite parity is as follows:

$$\Delta E = E_+ - E_- = 2\cdot(-1)^{J+\omega}\cdot B(J+\omega)\langle\omega|j_+|-\omega\rangle \quad (3)$$

$j_+ = j_x + i j_y$ is a component of the operator j in the body-fixed frame [redacted]. It is obvious that $\Delta E \neq 0$ only at $\omega = 1/2$. At $\omega > 1/2$ the splitting differs from zero in a higher order in H_B /6/

$$\Delta E \sim B\cdot J^{2\omega}(B/\varepsilon)^{2\omega-1} \quad (4)$$

ε is the characteristic distance between electronic terms of molecule. $B/\varepsilon \sim m_e/M_{mol}$ Stress that we discuss the molecules with strong spin-orbit interaction. Otherwise, an additional smallness can arise in the splitting.

II. T-Odd Effects. Enhancement of an Electric Dipole Moment of Electron

P- and T-odd interaction of an EDM of the electron with an electric field of the molecules H_d results in the mixing of opposite-parity states. The matrix elements of the interaction H_d over the states (1) are reduced, by means of a standard technique /6,8/, to the matrix elements over the states of a molecule at rest $\langle\Omega|H_d|\Omega\rangle$ and $\langle\Omega|H_d|-\Omega\rangle$. Since H_d is T-odd and pseudoscalar,

$$\langle\Omega|H_d|\Omega'\rangle \sim \delta_{\Omega\Omega'}\,\Omega \equiv \delta_{\Omega\Omega'}\,(\vec{J}\vec{n}) \quad (5)$$

$\vec{n}$ is the direction of the axis of molecule. We shall present concrete estimates for the BiS molecule ($\omega = 1/2$) whose spectrum is well known /7/. In this case, only T-odd interac-

tion between the electron and the nucleus of Bi is essential. According to /7/, one can assume that in the ground state of BiS there is *one* unpaired electron concentrated mostly on the Bi atom. An electric field of another atom leads to mixing of different electronic states

$$|1/2\rangle = a|s_{1/2}, J_z=\tfrac{1}{2}\rangle + b|p_{1/2}, J_z=\tfrac{1}{2}\rangle + c|p_{3/2}, J_z=\tfrac{1}{2}\rangle + \dots \qquad (6)$$

The coefficiencts a, b, c are real and $a \sim b \sim c$. Using the results of Ref. /5/, it is possible to write down the matrix element of H_d in the form

$$\langle \tfrac{1}{2}|H_d|\tfrac{1}{2}\rangle \approx -2ab\,\frac{4(z\alpha)^2 z|e|d_e}{\gamma(4\gamma^2-1)\,a_B^2\,(\nu_s\nu_{p_{1/2}})^{3/2}} \qquad (7)$$

Here ν_i is the effective principal quantum number of the electron, $\gamma = \sqrt{1-(z\alpha)^2}$, d_e is the dipole moment of the electron, e is the electron charge, a_B is the Bohr radius. There is no term $\sim ac$ in /7/ because H_d conserves the angular momentum.

The fact that the polar molecule has its intrinsic dipole moment d_M, does not lead by itself to a linear Stark-effect in the stationary state with fixed total angular momentum $\vec{J}$. However, P- and T-odd mixing of rotational states (1) results in the fact that $\vec{d}_M$ proves to be correlated with the total momentum $\vec{J}$. Thus, a dipole moment arises in a stationary state

$$\vec{d} = \frac{2\omega d_M \langle\omega|H_d|\omega\rangle}{\Delta E_{J,\eta}}\,\frac{\vec{J}}{J(J+1)} \qquad (8)$$

For the BiS molecule $\Delta E_{J,\eta} = \eta\cdot(-1)^{J+1/2}\cdot(J+\frac{1}{2})\,0.11\cdot\mathrm{cm}^{-1}$. The matrix element of mixing is given by the formula (7). For numerical estimates take $-2ab = 1$, $d_M = 0.5|e|a_B$, $\nu_s = \nu_p = 1.5$ (these are the characteristic values of ν for external electrons in Bi). Thus the enhancement factor for a dipole moment of electron is equal to

$$R = \frac{d}{d_e} = 3\cdot 10^7\,\eta\,\frac{(-1)^{J+1/2}}{(J+1/2)(J+1)} \qquad (9)$$

From the experimental point of view, the circumstance that R changes its sign in the transition to the level of opposite parity η or in variation of J by unity, may be important.

Let us consider now the case $\omega > 1/2$. The energy denominator ΔE in formula (8) quickly falls down with an increase of ω (see (4)). Therefore, already at $\omega = 1$ R may reach 10^{11}. Of course, there are limitations on a minimal possible value of ΔE. The most obvious from them consists in the fact that at large ω the levels will be pushed apart by an external electric field. At a fixed ΔE this condition gives the limitation on the field. For BiS $E \lesssim 10^4 \cdot J^2$ v/cm.

Note that there is some correspondence between the enhancement mechanism of an EDM of the electron which has been considered in this paper and the method of measuring an EDM of the proton which was proposed by Sandars in /9/ (the measurements were carried out in /10/). Sandars' idea was: if one polarizes the TlF molecule by an external electric field, then a strong intramolecular field will be directed along the external field, i.e. the external field seems to be enhanced. It is clear that the enhancement mechanisms discussed in /9/ and in the present paper belong correspondingly to the cases of strong and weak, in comparison

with rotational intervals, interactions with an external electric field.

Usually the experiments on the search for a dipole moment are carried out with atomic and molecular beams, by measuring a linear Stark effect. Let us mention the principal possibility to detect T-odd effects, by observing the optical activity of atomic or molecular vapors in electric field (an analogue of the Faraday effect).

III. P-Odd Effects. Circular Polarization of Photons and Optical Activity of Molecular Vapors

P-odd effects in molecules are enhanced, as well as T-odd effects, due to mixing of the rotational states (1) of different parity. Taking into account that the weak interaction Hamiltonian H_w is T-even and hermitian, it can be easily seen that $\langle\Omega|H_w|\Omega\rangle=0$, while the nondiagonal matrix element $\langle\Omega|H_w|-\Omega\rangle$ differs from zero. The operator H_w has the parts which are dependent and independent of the spin of nucleus /2/, i.e.

$$H_w = S + \vec{V}\,\vec{I}_N \qquad (10)$$

It is evident that the matrix element $\langle\Omega|H_w|-\Omega\rangle$ is distinct from zero only at $\omega = 1/2$ and only the second term contributes to it, being a vector in electronic variables. Thus, in molecules the weak interaction part connected with the product of the electron vector current and the nucleon axial current one turns out to be enhanced.

Using the wave functions (6) and the results of Ref./2/, one can write down the matrix element of the weak interaction

as follows:

$$\langle\tfrac{1}{2}|V_+|-\tfrac{1}{2}\rangle = 2i\,ab\,g_I\cdot\frac{2\gamma+1}{3}\cdot\frac{6\,m_e^2\alpha^2Z^2R}{\pi(\gamma_s\gamma_{p_{1/2}})^{3/2}}\cdot\frac{m_e e^4}{2\hbar^2} \qquad (11)$$

Here $V_+ = (-V_x - iV_y)/\sqrt{2}$, $R = 4\cdot\left(\frac{2r_0 Z}{a_B}\right)^{2\gamma-2}\Big/\left[\Gamma(2\gamma+1)\right]^2$ is the relativistic factor, r_0 is the nucleus radius, $g_I = \varkappa_W\langle\beta_N\rangle$, $\langle\beta_N\rangle$ is the expectation value of the spin of external nucleon, $\varkappa_W$ is the constant of the weak interaction between the electron vector and nucleon axial currents which should be experimentally determined. In Bi $R = 9.4$, $\langle\beta_p\rangle=\frac{2}{11}$; in Weinberg model $\varkappa_p = (2\sin^2\theta - 1/2)\lambda$, λ is the renormalization constant of the axial current; $\sin\theta$ is a parameter of the model.

Further calculations are carried out by means of standard technique /8/. The states of opposite parity $|F, J'=J\pm 0, 1; -\eta\rangle$ are admixed to the level $|F, J, \eta\rangle$ ($\vec{F}=\vec{J}+\vec{I}_N$). We do not write down here the expressions for mixing coefficients since they are cumbersome.

Consider now the transitions between the hyperfine structure components of the ground and first excited electronic states (X and A , respectively) of the BiS molecule. The wavelengths of appropriate transitions lie in the range of 5500-8000 Å, depending on between which oscillating and rotational terms the transition occurs. According to the electronic selection rules, the transition $X\to A$ may take place both as E1 and M1. If we consider a transition between the rotational levels of the same parity $(\eta\to\eta)$, then this is a M1-transition. Correspondingly, the transition $\eta\to-\eta$ is a E1-transition. Let us consider now the optical activity of BiS vapors near M1 transitions. Due to the already mentioned mixing of opposite-

parity levels, a small admixture of E1 is added to M1-amplitude in the ground state of the BiS molecule. The numerical estimates show that in the excited state the mixing is small and may be neglected. Calculations of M1 and E1 amplitudes are carried out with the standard technique of the angular momentum theory /8/. For numerical estimates we take the following values of electronic matrix elements:

$$\langle A, \tfrac{1}{2} | \mathcal{D}_z | X, \tfrac{1}{2} \rangle = e a_B \ , \langle A, \tfrac{1}{2} | M_+ | X, -\tfrac{1}{2} \rangle = \mu_B \qquad (12)$$

In BiS the matrix elements $\langle A, \frac{1}{2} | \mathcal{D}_+ | X, -\frac{1}{2} \rangle$ and $\langle A, \frac{1}{2} | M_z | X, \frac{1}{2} \rangle$ are suppressed due to the structure of electronic states /7/. The largest value of square of the overlapping of oscillating wave functions (Frank-Gordon factor) is $\sim$ o.2 (transitions V_X = = 0,1 $\rightarrow$ V_A = 6, 7, 8). As far as rotational and hyperfine states are concerned, the transitions $|X, J, F = J + I_N\rangle \rightarrow |A, J\pm1, F' = J\pm1+I_N\rangle$ are best suited to observation of optical activity. The degree of circular polarization

$$P = -2\, Im \frac{\langle \mathcal{D} \rangle}{\langle M \rangle} \qquad (13)$$

reaches $\sim 5\cdot10^{-4}\, \chi_p/(J+1)$ in these transitions. The angle of rotation of light polarization plane in BiS is independent of J at large J and constitutes $\Psi \sim 0.7\cdot10^{-7}\, \chi_p$ rad/m at temperature 1200°C and vapor pressure 100 mm[1]. At small J $\Psi \sim 2\cdot10^{-7}\chi_p$ rad/m.

Note that optical activity of BiS vapors is one order of magnitude less than the optical activity of Bi vapors /11/, although the degree of circular polarization in BiS is 3-4 orders

1) For definiteness, we assume that collisional line-broadening is smaller than Doppler one.

of magnitude larger than in Bi. This circumstance is associated with the fact that at T = 1200°C large number of the rotational levels of the molecule are excited

$$Z = (2I+1)\sum_v e^{-\frac{\hbar\omega v}{T}} \sum_J (2J+1) e^{-\frac{B J(J+1)}{T}} \approx 2{,}8\cdot10^5 \qquad (14)$$

and, therefore, the population of any fixed level from which the transition goes is small. The BiS molecule which we have considered as an example, is not apparently optimal from the experimental point of view, even among the molecules with ω = 1/2. The effect in it is suppressed approximately by one order of magnitude because of a large spin of the Bi nucleus. Most of the molecules have ω = 0 in the ground state. However, if in the excited state to which the transition goes, ω = 1, then the effect will be of the same order of magnitude as in a molecule with ω = 1/2. Indeed, the matrix element of the mixing is of the form:

$$\frac{\langle 1 | H_w | 0 \rangle \langle 0 | H_B | -1 \rangle}{E_1 - E_0} \sim \langle \tfrac{1}{2} | H_w | -\tfrac{1}{2} \rangle \frac{B}{\mathcal{E}} J \qquad (15)$$

H_B is the centrifugal energy operator (2). The smallness of $B/\mathcal{E}$ in the matrix element is however compensated by the same smallness in splitting of the opposite parity levels (see Introduction).

Note that at ω = 1 the tensor weak interaction $H_T = T_{ik} I_i I_k$ arising due to nonsphericity of the nucleus can prove to be essential. The point is that this interaction can lead to mixing of the states Ω = 1 and Ω = -1 in the first order of perturbation theory, i.e. the matrix element $\langle 1 | H_T | -1 \rangle$ has

no smallness $\mathcal{B}/\mathcal{E}$. It is possible to evaluate this matrix element using the magnitude of mixing of one-electron atomic states $S_{1/2}$ and $P_{1/2}$ by weak interaction (mixing of $\Omega = 1$ and $\Omega = -1$ can be connected with the transition $P_{3/2}$ -electron with $j_z = 3/2$ to $S_{1/2}$ with $j_z = -\frac{1}{2}$). This mixing is by a factor of $\alpha_\beta / Z\gamma_0$ smaller than the mixing of $S_{1/2}$ and $P_{1/2}$, induced by vector weak interaction (10,11). Nevertheless, in the molecule with heavy atom $Z\gamma_0/\alpha_\beta \sim 10^{-2} \gg \frac{\beta}{\mathcal{E}} \sim 10^{-5}$, i.e. the tensor interaction can dominate . I.B.Khriplovich attracted our attention to the fact that the tensor weak interaction has no smallness $Z\gamma_0/\alpha_\beta$, if the electron has "weak" anomalous magnetic moment.

Turn attention to the fact that the optical activity of molecules can be also stidued in the radidiapazon in transitions between the rotational levels and the hyperfine structure ones.

In conclusion, note that the two-centre system similar to the molecule in a definite rotational state is formed during the fission of nuclei. In such a system, as it is shown in this paper, T-odd effects are considerably enhanced. As to P-odd effects in the fission, the mechanism considered by us is not applicable to this phenomenon due to strong spin-spin interaction.

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