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Calculation of the spin-rotational Hamiltonian including P- and P, T-odd weak interaction terms for HgF and PbF molecules

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The spin-rotational Hamiltonian parameters for the ground states of HgF and PbF molecules are evaluated on the basis of the ab initio effective core potential calculations. The term corresponding to the electric dipole moment of the electron as well as several other P- and P, T-odd terms are included.

1. Introduction

In this paper we report the results of the calculation of the effective spin-rotational Hamiltonian parameters for two heavy radicals – HgF and PbF. It was shown in a number of papers that these molecules can be used in the experimental search for the break of time-reversal invariance [1–3]. The latter can be caused either by P, T-odd electron–nucleus interaction or by the existence of the multipole moments of the particles that break the inversion symmetry P and the time-reversal symmetry T. In particular, the most interesting is the electric dipole moment (EDM) of the electron [4].

In order to treat these phenomena we have introduced several P, T-odd terms into the spin-rotational Hamiltonian H_{sr}. The corresponding constants are evaluated in terms of the EDM of the electron d_e, the magnetic quadrupole moment of the nucleus M and the constant of the scalar electron–nucleus neutral currents interaction $\kappa_{P,T}$. One more term in H_{sr} is connected with the anapole moment of the nucleus κ_P and is P-odd but T-even [5,6].

Our results are in reasonable agreement with earlier calculations [7,8] and with the experimental data on the hyperfine structure, the Zeeman effect and the

ω-doubling constant. On these grounds we conclude that the accuracy of our calculation of the P-odd and P, T-odd terms of the H_{sr} operator is close to 20%. This is much better than in the case of the TlF molecule, where the P, T-odd effect is connected with the EDM of the proton and the so-called Schiff moment of the Tl nucleus and where the computational accuracy cannot be controlled [9,10].

The structure of the paper is as follows. In the second section the effective Hamiltonian H_{sr} is defined and its constants are expressed in terms of the electronic matrix elements (MEs). The third section is devoted to the description of the SCF calculations of the molecular wave function (WF). The results of the calculation are reported in the fourth section. The discussion follows in the fifth section of the paper.

2. Spin-rotational Hamiltonian

Electronic states of diatomic radicals are classified according to the the projections Λ and ω of the orbital and total electronic angular momenta on the molecular axis. The ground states for the HgF and PbF molecules are $^2\Sigma_{1/2}$ ($\Lambda=0$, $|\omega|=\frac{1}{2}$) and $^2\Pi_{1/2}$ ($|\Lambda|=1$, $|\omega|=\frac{1}{2}$) respectively.

It is convenient to describe the spin-rotational spectrum of the ground electronic state in terms of the effective spin-rotational Hamiltonian H_{sr}. Two electronic states with different signs of ω are degenerate. In this subspace one can define the effective electron spin S', $S' = \frac{1}{2}$. Then the Hamiltonian H_{sr} can be written in the same manner for both molecules [11]:

$$H_{sr} = BJ^2 + \Delta S' \cdot J + S' \cdot A \cdot I$$
$$+ \mu_0 S' \cdot G \cdot B - D n \cdot E$$
$$+ W_P \kappa_P n \times S' \cdot I + (W_{P,T} \kappa_{P,T} + W_d d_e) S' \cdot n$$
$$- \frac{M}{4I(2I-1)} [I_i I_k + I_k I_i - \tfrac{2}{3} \delta_{i,k} I(I+1)]$$
$$\times [2W_M^1 S'_i n_k + 2W_M^2 (S' \cdot n) n_i n_k] . \tag{1}$$

The first line of this expression corresponds to the rotational structure with ω- or spin-doubling and the hyperfine interaction of the electron spin with nuclear spin I. B is the rotational constant, J is the electron-rotational angular momentum, Δ is the ω-doubling constant. For the $^2\Sigma_{1/2}$ molecules a transition to the standard notations follows by the substitutions $\gamma = \Delta - 2B$ and $N = J - S'$, where γ is the spin-doubling constant and N is the rotational angular momentum.

The second line describes the interaction of the molecule with the external fields B and E (n is the unit vector directed from the heavy nucleus to the light one).

The two last lines of eq. (1) correspond to P, T-odd weak interactions of the electrons with the heavy nucleus and to the interactions caused by the P- or P, T-forbidden electromagnetic moments of the electron and the nucleus. The corresponding electron operators are given below. A detailed discussion of these subjects can be found in ref. [12] by Khriplovich and the recent review of Hunter [13].

The parameter Δ, the tensors A and G, the molecular dipole moment D and the constants W_i are expressed in terms of the one-electron MEs.

Below we shall restrict ourselves to the single-particle approximation. Then for the $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$ states there is only one unpaired electron. As far as all electron operators of interest here are spin-dependent, contributions of the closed shells to the MEs turn to zero. (The exceptions are the rotational con-

stant B and the molecular dipole moment D which are calculated in a standard manner.) So we have to know only the WF of the unpaired electron.

The quantum number Δ is good in the nonrelativistic approximation but it is not valid for molecules with such atoms as mercury and lead. Moreover, as will be seen later, the MEs of interest are very sensitive to the spin–orbital mixing. We assume that the main mixing takes place between the two lower states. For both molecules they are $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$ [14]. In this approximation the WF of the unpaired electron can be written in the form [7,8]

$$|\omega\rangle = \xi|\pi, \omega\rangle + \eta|\sigma, \omega\rangle , \tag{2}$$

where $\omega = \pm \frac{1}{2}$, $|\pi, \omega\rangle$ and $|\sigma, \omega\rangle$ are the WFs of the unpaired electrons in the $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$ states. One can expect that for HgF $|\xi| \ll 1$, while for PbF $|\eta| \ll 1$.

Now we can write the ME for the ω-doubling constant Δ:

$$\Delta/2B = -\sqrt{2} \langle \omega = \tfrac{1}{2} | j_1^e | \omega = -\tfrac{1}{2} \rangle$$
$$= \eta^2 - 2\sqrt{2} \, \xi\eta \langle \pi | l_1 | \sigma \rangle , \tag{3}$$

where j^e and l are the total and orbital angular momenta of the electron.

The tensors A and G are diagonal in the molecular frame of reference, the two components perpendicular to the molecular axis being equal to each other. For the tensor G one has

$$G_\| = 2 \langle \tfrac{1}{2} | l_0 + 2S_0 | \tfrac{1}{2} \rangle = 2\eta^2 ,$$
$$G_\perp = -\sqrt{2} \langle \tfrac{1}{2} | l_1 + 2S_1 | -\tfrac{1}{2} \rangle$$
$$= 2\eta^2 - 2\sqrt{2} \, \xi\eta \langle \pi | l_1 | \sigma \rangle . \tag{4}$$

It is seen from eqs. (3), (4) that the constants Δ, $G_\|$ and $G_\perp$ are very sensitive to spin–orbital mixing (2). For the pure $^2\Sigma_{1/2}$ state $\xi = 0$ and $\Delta/2B = G_\| = G_\perp = 2$, while for the $^2\Pi_{1/2}$ state $\eta = 0$ and $\Delta/2B = G_\| = G_\perp = 0$.

Consider the hyperfine tensor A and the constants W_i. These parameters arise from the electron operators that are singular in the vicinity of the nucleus. In this region the WF is relativistic and has a strong Z dependence. As a result, the corresponding MEs are enhanced for the heavy nuclei. (That is why we did not include the same terms for the fluorine nucleus in (1).) Let us expand the WF (3) over the

basis of the relativistic atomic orbitals of the heavy atom,

$$|\omega\rangle = C_{-1}|6s_{1/2}, \omega\rangle + 2\omega C_1|6p_{1/2}, \omega\rangle$$
$$+ C_{-2}|6p_{3/2}, \omega\rangle + 2\omega C_2|5d_{3/2}, \omega\rangle$$
$$+ C_{-3}|5d_{5/2}, \omega\rangle . \tag{5}$$

In this expansion we took into account only the orbitals of the valence shells. The accuracy of this approximation will be discussed below. The factors $2\omega = \pm 1$ arise from symmetry considerations [7]. The expansion coefficients C_k are numerated by the relativistic quantum number $k = (l-j)(2j+1)$.

The standard form of the atomic WF is

$$\psi_{nljm} = \frac{1}{r}\begin{pmatrix} P_{nlj}(r)\Omega_{km}(\vartheta, \varphi) \\ iQ_{nlj}(r)\Omega_{-km}(\vartheta, \varphi) \end{pmatrix}, \tag{6}$$

where Ω_{km} is the spherical spinor. Taking into account that the hyperfine interaction operator can be written as (atomic units are used throughout)

$$H_{hf} = \frac{\mu_N}{I}\frac{I \cdot \alpha \times n}{r^2}, \quad \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \tag{7}$$

where μ_N is the nuclear magnetic moment, we can express the components of tensor **A** in terms of expansion (5) as

$$A_{\parallel} = \tfrac{4}{3}(C^2_{-1}h_{-1,-1} - C^2_1 h_{1,1})$$
$$+ \tfrac{8}{15}(C^2_{-2}h_{-2,-2} - C^2_2 h_{2,2}) + \tfrac{24}{35}C^2_{-3}h_{-3,-3}$$
$$+ \tfrac{4}{3}\sqrt{2}\,(C_{-1}C_2 h_{-1,2} - C_1 C_{-2}h_{1,-2})$$
$$- \tfrac{8}{5}\sqrt{3}\,C_2 C_{-3}h_{2,-3}, \tag{8}$$

$$A_{\perp} = \tfrac{4}{3}(C^2_{-1}h_{-1,-1} + C^2_1 h_{1,1})$$
$$+ \tfrac{16}{15}(C^2_{-2}h_{-2,-2} + C^2_2 h_{2,2}) + \tfrac{36}{35}C^2_{-3}h_{-3,-3}$$
$$- \tfrac{2}{3}\sqrt{2}\,(C_{-1}C_2 h_{-1,2} + C_1 C_{-2}h_{1,-2})$$
$$- \tfrac{2}{5}\sqrt{6}\,C_2 C_{-3}h_{2,-3}, \tag{9}$$

$$h_{k',k} = \frac{\mu_N}{I}\int_0^\infty (P_{k'}Q_k + P_k Q_{k'})\frac{dr}{r^2}. \tag{10}$$

In these expressions we use the index k instead of nlj for short.

The interaction of the electron EDM with the electromagnetic field can be written in various forms. It is better to use in calculations the form where the term which turns to zero due to the Schiff theorem [15] is excluded [12]:

$$H_d = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & \sigma \end{pmatrix}[-\nabla\phi(r)], \tag{11}$$

where ϕ is the electrostatic potential. Then for the WF (5) we have

$$W_d = C_{-1}C_1 h'_{-1,1} + C_{-2}C_2 h'_{-2,2}, \tag{12}$$

$$h'_{k',k} = 8\int_0^\infty P_{k'}Q_k \frac{d\phi}{dr}dr. \tag{13}$$

The electromagnetic interaction of the nuclear magnetic quadrupole moment M with the electron has the form [3]

$$H_M = -\frac{M}{4I(2I-1)}[I_i I_k + I_k I_i - \tfrac{2}{3}I(I+1)\delta_{ik}]$$
$$\times \frac{3}{2r^3}(\epsilon_{jli}\alpha_j n_l n_k + \epsilon_{jlk}\alpha_j n_l n_i), \tag{14}$$

where ϵ_{ikj} is the antisymmetric tensor and α_i was defined in (7). The explicit form of the electronic part of the ME is more complicated than the previous ones and we do not give it here. But two important features have to be mentioned. (i) The radial integrals involved have the form

$$h''_{k',k} = \int_0^\infty (P_{k'}Q_k + P_k Q_{k'})\frac{dr}{r^3}. \tag{15}$$

(ii) One can construct two second rank P, T-odd tensors from the vectors S' and n:

$$Q^1_{ik} = S'_i n_k + n_i S'_k - \tfrac{2}{3}(S' \cdot n)\delta_{ik} \tag{16}$$

and

$$Q^2_{ik} = (S' \cdot n)(n_i n_k + n_i n_k - \tfrac{2}{3}\delta_{ik}). \tag{17}$$

The tensor Q^2_{ik} is diagonal in the $\omega = \pm \tfrac{1}{2}$ subspace, while the tensor Q^1_{ik} is not. The electronic tensor in eq. (14) can be expressed as a sum of tensors (16) and (17) as is done in eq. (1). We have put the unsymmetrized form of these tensors there making use of the symmetry properties of the nuclear tensor. It can be shown that even for the pure $^2\Sigma_{1/2}$ state both terms in this sum are not zero.

There are two more terms in eq. (1) corresponding to the nuclear anapole moment interaction and

the P, T-odd scalar neutral currents interaction:

$$H_P = \frac{G\alpha}{\sqrt{2}} \kappa_P \mathbf{I} \cdot \boldsymbol{\alpha} n(r), \tag{18}$$

$$H_{P,T} = i \frac{G\alpha}{\sqrt{2}} Z \kappa_{P,T} \gamma_0 \gamma_5 n(r), \tag{19}$$

where G is the Fermi constant ($\sqrt{8}\, G\alpha = 3.150 \times 10^{-14}$ a.u.), γ_0 and γ_5 are the Dirac matrices and $n(r)$ is the nuclear density normalized to unity. These interactions, being nonzero only inside the nucleus, are sensitive only to the $s_{1/2}$ and $p_{1/2}$ terms in the molecular WF (5):

$$W_P = \left(\sqrt{8}\, G\alpha \right.$$

$$\left. \times \int_0^\infty (P_{-1}Q_1 + \tfrac{1}{3} P_1 Q_{-1}) n(r)\, dr \right) C_{-1} C_1, \tag{20}$$

$$W_{P,T} = \left(\sqrt{8}\, G\alpha Z \right.$$

$$\left. \times \int_0^\infty (P_{-1}Q_1 + P_1 Q_{-1}) n(r)\, dr \right) C_{-1} C_1. \tag{21}$$

These formulae as well as formulae (8)–(10), (12), (13) and (15) express the parameters of the spin-rotational Hamiltonian in terms of the coefficients C_k and the atomic radial integrals. All integrals are singular at the origin and depend on the small components of the Dirac functions.

3. Molecular SCF calculation

Today there exist well-developed methods for ab initio calculations of the heavy diatomics (see for example ref. [16]). Unfortunately, they cannot be used directly for our purpose because of the wrong behavior of the resultant WF in the vicinity of the nuclei. Here we follow a simple procedure, proposed in ref. [8], which can give the first approximate solution to the problem. The main features of this procedure are as follows.

(1) We use the minimal atomic basis set for fluorine and only five relativistic valence orbitals for lead and mercury: $5d_{3/2}$, $5d_{5/2}$, $6s_{1/2}$, $6p_{1/2}$ and

$6p_{3/2}$. Population analyses as well as the large value of the molecular dipole moment show that for both molecules the heavy metal atom is positively charged. For this reason the orbitals are calculated for the positive ions with the help of the HFD program [17].

(2) We use the shape consistent relativistic effective core potential (REP) [18] to exclude the core electrons of the metal from the calculations. The REP is divided into a spin independent part (AREP) and an effective spin–orbit potential (ESOP). The use of the REP means that we replace the valence orbitals mentioned above by pseudo-orbitals. The orbitals and the pseudo-orbitals coincide everywhere outside the core region while inside this region the pseudo-orbitals are smoothed and do not even give an approximation to the orbitals.

(3) We perform the molecular SCF calculation with the AREP in the minimal basis set to obtain the two lower molecular states $^2\Sigma$ and $^2\Pi$. For this purpose (pseudo)orbitals as well as the REP were approximated by sets of Gaussian type functions. For the fluorine orbitals this expansion was taken from ref. [19]. After that the molecular package MOLCAS [20] was used.

(4) The total molecular Hamiltonian including the AREP and the ESOP is diagonalized in the subspace of these two states giving the $^2\Sigma_{1/2}$, $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ states. In other words in this stage we find the coefficients ξ and η in eq. (2) for the $^2\Sigma_{1/2}$ and $^2\Pi_{1/2}$ states while $^2\Pi_{3/2}$ is a pure Π state.

(5) The resultant LCAO expansion for the unpaired electron has been used to calculate the singular MEs given in the previous section. To do this we substitute the pseudo-orbitals which were used in the molecular calculation by the corresponding orbitals.

A combination of points (2) and (5) is used here to restore the molecular WF in the core region. An alternative way is to use some matching of the molecular WF in the outer region with the atomic one in the inner region [9,10]. The advantage of the latter method is that one can use a much more flexible basis set of the primitive Gaussians for the molecular calculation, while in our method we are restricted to the atomic pseudo-orbitals. But a matching procedure is done inside the core and thus no REP can be used. On the other hand, the core is relativistic and cannot be treated adequately with the ex-

isting molecular programs. That can introduce a large error in the matching state. Another argument to use the REP instead of the all-electron calculation is that this method seems to be clearer from the physical point of view. Indeed, as far as molecular bonds are formed outside the core where the pseudo-orbitals coincide with the orbitals, they are almost indistinguishable from each other in the molecular calculation until the core is frozen. The use of the minimal atomic basis for the treatment of the hyperfine interaction in the diatomic radicals proved to be productive in a number of semiempirical calculations (see, for example, refs. [7,21] and references therein).

Of course, the arguments given above cannot guarantee the quality of our method. Fortunately, in the case of the HgF molecule there are experimental data on the tensors **A** and **G** [21] that give a very good test on the quality of the molecular WF. In fact, according to eqs. (3) and (4) the tensor **G** can be used to check the mixing (2) while the tensor **A** is sensitive to the behavior of the WF at the origin. For the PbF molecule the situation is not so favorable because there is only one experimental result on the ω-doubling constant Δ [14].

The method discussed above is appropriate only for the MEs of the singular operators and can provide an accuracy of about 20%. For such parameters as the rotational constant (i.e. the internuclear distance) and the molecular dipole moment, calculations in the basis set of primitive Gaussians were performed.

4. Results

In table 1 several standard spectroscopic characteristics for the two lower states of the HgF and PbF molecules are given. After the SCF calculation in the basis set of primitive Gaussians the CI study was made by means of the CASSCF program. The active space included three outer electrons. In this stage the spin-dependent part was excluded from the Hamiltonian.

For the PbF molecule there is a good agreement between the calculated and the experimentally measured internuclear distances. The calculated internuclear distance for the HgF molecule corresponds

to the rotational constant of the ground state $B = 0.222$ cm^{-1}. For the vibrational and transition frequencies the agreement with the experiment is not so good but for one exception is within 20%.

In table 2 the parameters of the spin-rotational Hamiltonian which depend on the relativistic features of the molecular WF are listed. A comparison of the calculated and experimental values for $\Delta G = G_\parallel - G_\perp$ (HgF) and $\Delta/2B$ (PbF) shows that our method leads to some overestimation of the spin-orbital mixing. This is probably due to the use of the ionic orbitals for the metal atom. The use of the atomic basis instead of the ionic one leads to the noticeably larger underestimation of this mixing.

For the HgF molecule the deviation of the calculated values from the experimental ones for $A_\parallel$ and $A_\perp$ is equal to 7%. It is also important to check the dipole constant $A_d = \frac{1}{3}(A_\parallel - A_\perp)$ where this deviation is 14%. It follows from eqs. (8) and (9) that the contribution of the s function to A_d turns to zero and the contribution of the p functions becomes dominant. As far as the s and p functions give the main contribution to the parameters W_i, we can conclude that the test on $A_\parallel$, $A_\perp$ and A_d is very important.

For the parameters W_i only theoretical results are available. Most of them differ from each other by less than 20%. The larger difference of the results [8] is caused by the overestimation of the spin–orbital mixing parameter η. For the minimal η from the interval given in that paper, the results of that work coincide with our calculation within the same 20% interval.

5. Discussion

The above treatment leads us to the conclusion that the accuracy of our calculations of the spin-rotational Hamiltonian parameters is close to 20%. This means that the results of the experiments with these molecules, proposed in refs. [5,1–3,12], can be expressed with reasonable accuracy in terms of the fundamental constants d_e, $\kappa_{P,T}$ and the parameters of the nucleus κ_P, M. As was shown in ref. [3], the nuclear physics methods allow one to calculate the latter for different models of the weak interactions. The high sensitivity of these experiments as well as the possibility of interpretation in terms of the fundamental

Table 1
Internuclear distances, vibrational constants, transition frequencies and dipole moments for HgF and PbF molecules.

			R_e (Å)	ω_e (cm^{-1})	$\|E_\Sigma - E_\Pi\|$ (cm^{-1})	D (Db)
HgF $^2\Sigma$		experiment [a]	–	491		
		this work	2.11	446		4.15
		ref. [22]	2.07	351		
HgF $^2\Pi$		experiment [14] [a]	–	488	41000	
		this work	(2.23)	333	35910	2.75
PbF $^2\Pi$		experiment [14] [a]	2.05	516		
		this work	2.06	489		4.62
		ref. [23]	2.07	553		
PbF $^2\Sigma$		experiment [14]	2.16	395	19430 [a]	
		this work	2.18	418	23380	5.5
		ref. [23]	2.16	487	19050	

[a] Averaged over the states $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$.

Table 2
Parameters of the spin-rotational Hamiltonian for the ground states of HgF and PbF. Components of the hyperfine tensor are given for the ^{199}Hg and ^{207}Pb isotopes ($I = \frac{1}{2}$), the constant W_M^i is for ^{201}Hg ($I = \frac{3}{2}$). (a) Ref. [21], experimental data. (b) Ref. [7], semiempirical calculation. W_d and W_M were calculated later with the same method. $\gamma/2B = 0.032$ (HgF). (c) This work, preliminary results [24]. $\gamma/2B = 0.036$ (HgF); $\Delta/2B = -0.347$ (PbF). (d) Ref. [14], experimental result. $\Delta/2B = -0.3033$ (PbF). (e), (f) Ref. [8], semiempirical calculation. Minimal and maximal spin–orbital mixing, respectively. In ref. [8] the parameters W_i were given with the wrong signs.

		$A_\parallel^1$ (MHz)	$A_\perp^1$ (MHz)	$G_\parallel$	$G_\perp$	W_P (kHz)	$W_{P,T}$ (kHz)	W_d (10^{25} Hz/e cm)	W_M^1 (10^{34} Hz/e cm^2)	W_M^2 (10^{34} Hz/e cm^2)
HgF	(a)	22621	21880	1.993	1.961					
	(b)					2.6	−191	−4.8	−3.6	5.2
	(c)	24150	23310	1.996	1.960	2.5	−185	−4.8	−3.8	5.4
PbF	(d)									
	(e)	8690	−7460	0.034	−0.269	−0.65	51	1.0		
	(f)	9550	−8240	0.114	−0.438	−1.25	99	1.8		
	(c)	10990	−8990	0.040	−0.326	−0.72	55	1.4		

interactions makes them very promising.

As was mentioned above the EDM of the electron is of particular interest. In the corresponding experiments the spinless isotopes of mercury and lead can be used (their natural abundances are 70% and 77%, respectively). For this case the spin-rotational structure is significantly simplified, though the fluorine hyperfine structure becomes important. The molecular enhancement factors for the EDM of the electron defined as $W_d D/2B$ are equal to 6×10^7 and 2×10^7, respectively.

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