

## Enhancement of the Electric Dipole Moment of the Electron in PbO

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The  $a(1)$  state of PbO can be used to measure the electric dipole moment of the electron  $d_e$ . We discuss a semiempirical model for this state, which yields an estimate of the effective electric field on the valence electrons in PbO. Our final result is a lower limit on the measurable energy shift, which is significantly larger than was anticipated earlier:  $2|W_d|d_e \geq 2.4 \times 10^{25} \text{ Hz}[\frac{d_e}{\text{cm}}]$ .

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In his pioneering work, Sandars pointed out that the effective electric field on a valence electron in a heavy atom is enhanced by a factor  $\sim \alpha^2 Z^3$  relative to the applied laboratory field [1]. That started a long search for the electric dipole moment (EDM) of the electron  $d_e$  in atomic experiments [2]. The most stringent limit on  $d_e$  follows from an experiment on atomic Tl ( $Z = 81$ ) [3].

Even larger enhancement is present in heavy polar diatomic molecules [2,4,5]. The heavy atom there is subjected to an internal  $E$  field of  $\sim 1 \text{ a.u.} \approx 5 \times 10^9 \text{ V/cm}$ , which is further enhanced by the relativistic factor  $\alpha^2 Z^3$ . This effective field is many orders of magnitude larger than available laboratory fields; this makes diatomic molecules very attractive systems to look for  $d_e$ .

Since  $d_e$  is linked to the electron spin, one must work either with radicals, which have an unpaired electron in the ground state, or with excited states of “normal” molecules. Diatomic radicals with the ground state  $\Sigma_{1/2}$  have large enhancement factors which can be relatively easily calculated [6,7]. The first results of an EDM measurement in such a molecule (YbF) were recently published [8]. The molecule PbO is a favorable candidate for a search for  $d_e$  in the excited state  $a(1)$  [4,9], and the group at Yale has begun EDM experiments on PbO [10]. It is therefore timely to estimate the effective internal field for the state  $a(1)$  of PbO.

The interaction of  $d_e$  with an electric field  $\mathbf{E}$  can be written in four-component Dirac notation as [11]

$$H_d = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma} \mathbf{E} \end{pmatrix}. \quad (1)$$

After averaging over the electronic wave function, this interaction can be expressed in terms of an effective spin-rotational Hamiltonian [5,6],  $H_d^{\text{eff}} = W_d d_e (\mathbf{J}_e \cdot \mathbf{n})$ , where  $\mathbf{J}_e$  is the electronic angular momentum and  $\mathbf{n}$  is the unit vector along the molecular axis. In this paper we estimate  $W_d$  for the molecular state  $a(1)$ :

$$W_d \equiv d_e^{-1} \langle a(1) | H_d | a(1) \rangle, \quad (2)$$

where we used  $\langle a(1) | \mathbf{J}_e \cdot \mathbf{n} | a(1) \rangle \equiv \Omega[a(1)] = 1$ . The  $\Omega$  doubling for states with  $\Omega = 1$  is very small, and even in a weak external electric field ( $E_0$ ), the energy eigenstates correspond to definite  $\Omega$  rather than definite parity. The energy of the molecule can be then written as

$$W(J, M, \Omega) = BJ(J+1) + W_d d_e \Omega - \frac{DE_0 \Omega M}{J(J+1)}, \quad (3)$$

where  $B$  is the rotational constant,  $D$  is the molecular dipole moment,  $J$  is the total angular momentum (including rotation), and  $M$  is the projection of  $J$  along  $E_0$ . The EDM contribution can be determined from the difference:

$$W(J, M, \Omega) - W(J, -M, -\Omega) = 2W_d d_e. \quad (4)$$

In order to estimate the matrix element in Eq. (2) we construct here a semiempirical wave function of the state  $a(1)$ . We use the MO LCAO approach, where each molecular orbital (MO) is expressed as a linear combination of atomic orbitals (LCAO), and all molecular matrix elements are reduced to the sums of atomic matrix elements. The hyperfine structure (HFS) or spin-orbit (SO) interactions as well as the EDM enhancement factor grow very rapidly with nuclear charge  $Z$ . Therefore, we are interested only in the Pb part of the MO LCAO expansion.

Analysis of the molecular observables requires knowledge of several atomic matrix elements for Pb. We calculate these in the Dirac-Fock approximation both for neutral Pb and for  $\text{Pb}^+$ . Results are given in Table I for

TABLE I. Atomic parameters  $h_{k,k'}$  (GHz),  $w_{sp}$  (a.u.), and  $\xi$  ( $\text{cm}^{-1}$ ), calculated in the Dirac-Fock approximation for Pb and  $\text{Pb}^+$ . The relativistic quantum number  $k$  is equal to  $-1, 1$ , and  $-2$  for  $s_{1/2}$ ,  $p_{1/2}$ , and  $p_{3/2}$ , correspondingly.

	$h_{-1,-1}$	$h_{1,1}$	$h_{1,-2}$	$h_{-2,-2}$	$w_{sp}$	$\frac{w_{sp}}{\sqrt{-h_{-1,-1}h_{1,1}}}$	$\xi$
$\text{Pb}^+$	45.5	-8.9	-1.1	1.8	-34.1	-1.7	9452
Pb	42.3	-7.5	-0.9	1.4	-30.0	-1.7	8077
Ratio	1.08	1.20	1.25	1.30	1.14	1.0	1.17

the orbitals  $6s$  and  $6p_j$ . For the HFS operator we calculate the parameters  $h_{k,k'}$  as defined in [5] [we use atomic units (a.u.) unless otherwise noted]:

$$h_{k,k'} = -\frac{g_n \alpha}{2m_p} \int_0^\infty (f_k g_{k'} + g_k f_{k'}) dr, \quad (5)$$

where  $g_n = 0.59$  is the nuclear  $g$  factor of  $^{207}\text{Pb}$ ,  $m_p$  is the proton mass,  $f_k$  and  $g_k$  are upper and lower components of the Dirac orbitals, and  $k = (l-j)(2j+1)$  is the relativistic quantum number. For the EDM operator (1) in our minimal basis set there is only one nonzero radial integral, between  $6s_{1/2}$  and  $6p_{1/2}$  orbitals:

$$w_{sp} = -\int_0^\infty g_{-1} g_1 \frac{d\phi}{dr} r^2 dr, \quad (6)$$

where  $\phi$  is the atomic electrostatic potential. Finally, we also need the atomic SO constant  $\xi$  for the  $6p$  shell:

$$H_{SO} = \xi \mathbf{l} \cdot \mathbf{s} \Rightarrow \xi = \frac{2}{3} (\varepsilon_{6p_{3/2}} - \varepsilon_{6p_{1/2}}). \quad (7)$$

Note that the ratio of the radial integrals for the ion and for the atom are similar for all relevant integrals (see the last row of Table I). A simple relation between  $w_{sp}$  and HFS constants holds for both cases:  $w_{sp} = -1.7\sqrt{-h_{-1,-1}h_{1,1}}$ . This relation also holds for other principal quantum numbers  $n$ , e.g., for  $7s$  and  $7p_j$ . This fact is critical for semiempirical models of the EDM enhancement: it implies that the value of  $W_d$  does not depend strongly on what set of radial integrals is used. (The particular choice of the radial integrals does enter the final result, through the normalization of the wave function.) Since the Pb atom in PbO is positively charged, we have chosen to use the ionic set of integrals from Table I.

In order to develop a semiempirical model for the state  $a(1)$ , we have found it necessary to also consider the wave functions of several low-lying states of PbO. Previous work has shown that these states correspond to the configurations and nominal  $\Lambda$ ,  $\Sigma$ -coupling terms as follows [12,13]:

$$|a(1)[^3\Sigma^+]\rangle = \frac{1}{\sqrt{2}} (|\pi_{1,\lambda=-1}\pi_{2,\lambda=1}\rangle + |\pi_{1,\lambda=1}\pi_{2,\lambda=-1}\rangle) | \uparrow \uparrow \rangle = \frac{1}{\sqrt{2}} (|\pi_{1,-1/2}\pi_{2,3/2}\rangle + |\pi_{1,3/2}\pi_{2,-1/2}\rangle); \quad (12a)$$

$$|A(0^+)[^3\Pi]\rangle = \frac{1}{\sqrt{2}} (|\sigma\pi_{2,\lambda=1}\rangle | \downarrow \downarrow \rangle - |\sigma\pi_{2,\lambda=-1}\rangle | \uparrow \uparrow \rangle) = \frac{1}{\sqrt{2}} (|\sigma_{-1/2}\pi_{2,1/2}\rangle - |\sigma_{1/2}\pi_{2,-1/2}\rangle); \text{ etc.} \quad (12b)$$

We have transformed each wave function from  $\lambda - \sigma$  to  $\omega - \omega$  representation for convenience.

The rules for calculating hole matrix elements follow from the fact that the hole in the state  $|\omega\rangle$  actually means the absence of the electron in the state  $|-\omega\rangle$ . Thus, the expectation value for an electronic operator  $\hat{P}$  over the hole state  $|\omega\rangle$  can be written as

$$\langle \omega | \hat{P} | \omega \rangle_h \equiv -\langle -\omega | \hat{P} | -\omega \rangle_e = {}^T \mp \langle \omega | \hat{P} | \omega \rangle_e, \quad (13)$$

where we applied the time-reversal operation  $T$ . Thus the final sign depends on the time-reversal symmetry of  $\hat{P}$ , with the minus sign corresponding to a  $T$ -even electronic

$$X(0^+)[^1\Sigma^+]: \sigma_1^2 \sigma_2^2 \pi_1^4, \quad (8)$$

$$a(1)[^3\Sigma^+], C'(1)[^3\Sigma^-], \text{ etc.}: \sigma_1^2 \sigma_2^2 \pi_1^3 \pi_2, \quad (9)$$

$$A(0^+)[^3\Pi], B(1)[^3\Pi], D(1)[^1\Pi]: \sigma_1^2 \sigma_2 \pi_1^4 \pi_2, \quad (10)$$

In the naive ionic model of PbO, the two  $6p$  electrons from Pb move to O and close its  $2p$  shell. This suggests that the orbitals  $\sigma_1$  and  $\pi_1$  are centered on O, and that  $\sigma_2$  is predominantly of the Pb  $6s$ -type. However, below we do not impose any constraints on the MO LCAO coefficients for these molecular orbitals, based on this expectation. Note that only the orbitals  $\sigma_2$  and  $\pi_{1,2}$  contribute to the spin density of the molecular states under consideration. Thus, we do not need to know the orbital  $\sigma_1$ , and below we omit the index for the orbital  $\sigma_2$ .

Now we specify coefficients of the MO LCAO expansion for the three valence orbitals of interest:

$$|\sigma_\omega\rangle = S_s |6s_{1/2,\omega}\rangle + S_p (-2\omega\sqrt{\frac{1}{3}} |6p_{1/2,\omega}\rangle + \sqrt{\frac{2}{3}} |6p_{3/2,\omega}\rangle), \quad (11a)$$

$$|\pi_{i,\omega}\rangle = P_i (2\omega\sqrt{\frac{2}{3}} |6p_{1/2,\omega}\rangle + \sqrt{\frac{1}{3}} |6p_{3/2,\omega}\rangle), \quad (11b)$$

$$|\pi_{i,\omega'}\rangle = P_i |6p_{3/2,\omega'}\rangle, \quad (11c)$$

where  $\omega = \pm 1/2$  and  $\omega' = \pm 3/2$ . The numerical coefficients are chosen to account for the quantum number  $\lambda$ :  $\lambda = 0(1)$  for  $\sigma(\pi)$  orbitals. In order to calculate  $W_d$  we must determine the four parameters in Eqs. (11). Below we try to constrain these parameters using experimental information about states (9) and (10). To simplify the notation, we define the ground state of the molecule as a vacuum. Then each of the excited states in Eqs. (9) and (10) is a two-particle state with one hole and one electron. We do not use any special notation for the hole states; instead, we simply write the hole orbital in front of the electron one. We construct wave functions of these states from the orbitals (11), using at the first stage the  $\Lambda$ ,  $\Sigma$ -coupling scheme classification:

operator. For example, the HFS interaction is given by the product of the  $T$ -odd electronic vector  $\hat{\mathbf{A}}\mathbf{J}_e$  and the nuclear spin  $\mathbf{I}$ . Thus, for the HFS interaction the plus sign in Eq. (13) is correct. A similar argument shows that the SO constant  $\xi$  for a hole has the opposite sign as for an electron.

From Eqs. (12), the first-order SO splitting  $\Delta_{AB}$  between states  $A(0^+)$  and  $B(1)$  is

$$\Delta_{AB} = \frac{\xi}{2} [\langle \pi_{2,3/2} | \mathbf{l} s | \pi_{2,3/2} \rangle - \langle \pi_{2,1/2} | \mathbf{l} s | \pi_{2,1/2} \rangle] = \frac{\xi P_2^2}{2}. \quad (14)$$

Using the experimental value of this splitting [14] and the ionic value for  $\xi$  from Table I, we estimate  $P_2$ :

$$P_2^2 = \frac{2\Delta_{AB}}{\xi} = \frac{2 \cdot 2420}{9450} = 0.51. \quad (15)$$

We see that the orbital  $\pi_2$  has a large contribution from the Pb orbital  $6p$ . The data on energy levels [14] show then that for all levels with one electron in the  $\pi_2$  orbital, the SO interaction is comparable to the splittings between these levels. Therefore, there must be significant SO mixing between such states.

We start with the mixing within configuration  $\sigma^2\pi_1^3\pi_2$ . The mixing angle  $\alpha$  between states  $a(1)$  and  $C'(1)$  is

$$\alpha \approx \frac{\langle {}^3\Sigma_1^- | H_{\text{so}} | {}^3\Sigma_1^+ \rangle}{|\Delta_{aC'}|} = \frac{\xi_1 + \xi_2}{2|\Delta_{aC'}|}, \quad (16)$$

where  $\Delta_{aC'}$  is the energy splitting between  $a(1)$  and  $C'(1)$ , and  $\xi_i \equiv \xi P_i^2$ . If we assume that  $P_1^2 \ll P_2^2$  (corresponding to the naive ionic model), we can estimate the value of  $\alpha$ :

$$\alpha \approx \frac{\xi_2}{2|\Delta_{aC'}|} \approx 0.3, \quad (17)$$

and write the new wave function in the form:

$$|a(1)\rangle = c_\alpha |\pi_{1,3/2}\pi_{2,-1/2}\rangle + s_\alpha |\pi_{1,-1/2}\pi_{2,3/2}\rangle, \quad (18)$$

$$c_\alpha \equiv \cos\left(\frac{\pi}{4} - \alpha\right), \quad s_\alpha \equiv \sin\left(\frac{\pi}{4} - \alpha\right). \quad (19)$$

SO interaction also mixes configuration  $\sigma^2\pi_1^3\pi_2$  with configurations  $\sigma\pi_1^3\pi_2^2$  and  $\sigma\pi_1^4\pi_2$ . These mixings can be

$$\langle a(1) | H_{\text{hfs}} | a(1) \rangle = c_\alpha^2 [\langle \pi_{1,3/2} | h_{\text{hfs}} | \pi_{1,3/2} \rangle - \langle \tilde{\pi}_{2,1/2} | h_{\text{hfs}} | \tilde{\pi}_{2,1/2} \rangle] + s_\alpha^2 [\langle \pi_{2,3/2} | h_{\text{hfs}} | \pi_{2,3/2} \rangle - \langle \tilde{\pi}_{1,1/2} | h_{\text{hfs}} | \tilde{\pi}_{1,1/2} \rangle]. \quad (25)$$

We use expressions from Ref. [5] for the one-electron matrix elements and numbers from Table I, combined with the measurement of the hyperfine constant for the state  $a(1)$ ,  $A_{||} = -4.1$  GHz [15], to find another equation relating the various coefficients of the model

$$30(c_\alpha^2 s_2^2 + s_\alpha^2 s_1^2) S_s^2 + 1.8(c_\alpha^2 s_2^2 + s_\alpha^2 s_1^2) S_p^2 + (4.6s_\alpha^2 c_1^2 - 1.4c_\alpha^2) P_1^2 + (4.6c_\alpha^2 c_2^2 - 1.4s_\alpha^2) P_2^2 - 4.7s_\alpha^2 c_1 s_1 P_1 S_p - 4.7c_\alpha^2 c_2 s_2 P_2 S_p = 4.1. \quad (26)$$

(Note that the formulas of Ref. [5] are strictly applicable only for orbitals and states with  $\omega = \Omega = 1/2$ . Equation (26) takes into account simple modifications of these formulas for the present situation.)

Finally, we introduce two additional constraints, which account for normalization and the Pauli principle:

$$S_s^2 + S_p^2 \leq N_0, \quad P_1^2 + P_2^2 \leq N_0. \quad (27)$$

We choose  $N_0 = 1.2$  here in order to account for inaccuracy of the Hartree-Fock approximation used to determine the atomic parameters in Table I.

The parameters  $\alpha$  and  $P_2$  are unambiguously fixed by Eqs. (15) and (17). We choose  $s_1$  and  $P_1$  as free parameters and solve Eqs. (21), (24), and (26) for parameters  $s_2$ ,  $S_p$ , and  $S_s$ . After that we reject solutions which do not meet the constraints (27). Only some of the parameters are well

accounted for by substitution of the original orbitals  $|\pi_{i,1/2}\rangle$  with the perturbed orbitals

$$|\tilde{\pi}_{i,1/2}\rangle = c_i |\pi_{i,1/2}\rangle + s_i |\sigma_{1/2}\rangle. \quad (20)$$

There is no experimental information about levels of the configuration  $\sigma\pi_1^3\pi_2^2$ , so we cannot reliably estimate the mixing parameter  $s_2$ . In contrast, both levels with  $\Omega = 1$  of the configuration  $\sigma\pi_1^4\pi_2$  are known [i.e.,  $B(1)$  and  $D(1)$ ]. That allows us to write for  $s_1$  the estimate

$$s_1 = 2.8s_\alpha^2 P_1 S_p. \quad (21)$$

These SO mixings then lead to the final form of the wave function of the state  $a(1)$ ,

$$|a(1)\rangle = c_\alpha |\pi_{1,3/2}\tilde{\pi}_{2,-1/2}\rangle + s_\alpha |\tilde{\pi}_{1,-1/2}\pi_{2,3/2}\rangle. \quad (22)$$

The  $G$  factor for the state (22) is given by

$$G_{||} = \langle a(1) | L_0 + 2S_0 | a(1) \rangle = 2 - s_\alpha^2 s_1^2 - c_\alpha^2 s_2^2. \quad (23)$$

The measured value  $G_{||} = 1.84(3)$  [15] corresponds to the following equation for mixing parameters:

$$s_\alpha^2 s_1^2 + c_\alpha^2 s_2^2 = 0.16(3). \quad (24)$$

The signs of the parameters  $s_{1,2}$  should be chosen so that the contribution of atomic orbital  $6p_{1/2}$  to the molecular orbital  $\sigma$  is increased: in this case relativistic corrections to the binding energy of the  $\sigma$  orbital are positive.

The matrix element of the HFS interaction for the state  $a(1)$  (22) has the form

constrained. The variation ranges are

$$\begin{cases} s_1 \leq 0.2; & 0.4 \leq s_2 \leq 0.5; \\ S_p^2 \leq 0.5; & S_s^2 \geq 0.5. \end{cases} \quad (28)$$

The parameter  $P_1$  appears to be restricted only by the normalization condition (27).

It may be possible to add some restrictions to reduce the ranges of variation in Eq. (28). For example, the relatively large value of  $s_2$  should require a large value of  $S_p$ . However, such additional restrictions would add arbitrariness to the model and may affect its reliability. We use only the minimal set of constraints to determine the range of possible values of  $W_d$ .

For the wave function (22), there are two contributions to the EDM parameter  $W_d$  from each of the one-electron orbitals with  $|\omega| = 1/2$ :

TABLE II. Dependence of the EDM constant  $W_d$  (in a.u.) on the parameters of the model.

$A_{\parallel}$ (GHz)	$G_{\parallel}$	$\alpha$	$P_2^2$	$ W_d $	
				max	min
-4.1	1.84	0.30	0.51	19.6	13.7
-4.1	1.81	0.30	0.51	19.1	12.0
-4.1	1.87	0.30	0.51	20.3	15.4
-4.1	1.84	0.24	0.51	19.8	13.2
-4.1	1.84	0.36	0.51	20.3	15.5
-4.1	1.84	0.30	0.41	18.2	12.1
-4.1	1.84	0.30	0.61	20.3	15.1
-3.3	1.84	0.30	0.51	17.0	11.2
-4.9	1.84	0.30	0.51	22.0	16.4

$$W_d = -c_{\alpha}^2 W_d^{\tilde{\pi}^2} - s_{\alpha}^2 W_d^{\tilde{\pi}^1} \quad (29a)$$

$$= \frac{4w_{sp}}{\sqrt{3}} S_s (\sqrt{2} c_{\alpha}^2 c_2 s_2 P_2 - c_{\alpha}^2 s_2^2 S_p + \sqrt{2} s_{\alpha}^2 c_1 s_1 P_1 - s_{\alpha}^2 s_1^2 S_p) \quad (29b)$$

We find that the first term in (29b) always dominates the sum. The second term is not negligible, but the final two terms contribute  $\leq 10\%$ . It is important that the leading contribution to  $W_d$  is similar to the first term in Eq. (26), which dominates the HFS. This implies that the parameter  $W_d$  is well constrained even though some of the parameters of the wave function are not. We obtain

$$|W_d| = 16.6 \pm 3.0 \text{ a.u.}, \quad (30)$$

where the uncertainty reflects the range of values found within the model just described.

It is also important to check how  $W_d$  depends on the “fixed” parameters  $\alpha$  and  $P_2$ , as well as on the input data for  $A_{\parallel}$  and  $G_{\parallel}$ , since our model relating the MO LCAO coefficients to these parameters is rather crude. In Table II we solve the model equations for values of these quantities varying from the best values by  $\pm 20\%$ . We find that this variation of the input parameters widens the range for  $W_d$  substantially (to  $\pm 5.4$  a.u.), but still does not allow dramatically smaller values of  $W_d$ .

It is known from previous calculations of  $W_d$  for other diatomic molecules, that correlation corrections tend to decrease the result by 10%–20% from the Hartree-Fock level. Therefore, we state our final result as a conservative lower limit on  $W_d$ ,

$$|W_d| \geq 10 \text{ a.u.} = 12 \times 10^{24} \frac{\text{Hz}}{e \text{ cm}}. \quad (31)$$

This lower bound is several times larger than earlier, naive estimates which did not consider the effect of SO mixing on the (nominally)  $\pi$ -type orbitals of the  $a(1)$  state [5]. Our model shows significant similarity between the orbital  $\tilde{\pi}_{2,1/2}$  in PbO and the single valence orbital in the ground state of the free radical PbF. It is thus natural that our bound is close to the value calculated for PbF [16]. (Coincidentally, our bound is also similar to the calculated value for YbF [17–20].) However, we stress that this first semiempirical estimate of the effective field in PbO has very limited accuracy. Thus, more elaborate calculations of the  $a(1)$  state are highly desirable.

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