In search of the electron dipole moment: *Ab initio* calculations on $^{207}$PbO excited states

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Abstract

We report *ab initio* correlated relativistic calculations of the effective electric field $W_d$ acting on the electron in two excited electronic states of PbO, required for extracting the electric dipole moment of the electron from an ongoing experiment at Yale, which has the potential of improving accuracy for this elusive property by several orders of magnitude. The generalized relativistic effective core potential and relativistic coupled cluster methods are used, followed by nonvariational one-center restoration of the four-component wavefunction in the heavy atom core. $W_d$ is $-3.2 \times 10^{24}\text{Hz/(e\cdot cm)}$ for the $a(1)$ state and $-9.7 \times 10^{24}\text{Hz/(e\cdot cm)}$ for the $B(1)$ state. Comparison of calculated and experimental values of the hyperfine constant $A_\parallel$ provides an accuracy check for the calculation.
**Introduction.** Following the discovery of the combined CP-parity violation in $K_0$-meson decay [1], the search for the electric dipole moment (EDM) of the electron, $d_e$, has become one of the most fundamental problems in physics [2]. Considerable experimental effort has been invested in measuring atomic EDMs induced by the electron EDM. The best available results for the electron EDM were obtained in the atomic Tl experiment [3], which established an upper limit of $|d_e| < 1.6 \cdot 10^{-27}$ e·cm. It is expected that diatomic molecules containing a heavy atom can yield more definite results. Modern experiments searching for $d_e$ in these molecules exploit the fact that the effective electric field seen by an unpaired electron, $W_d$, is greatly enhanced by the relativistic effects relative to the external field [4, 5] reachable in a laboratory. The value of $W_d$ is necessary to extract $d_e$ from experimental measurements. For diatomic molecules with one unpaired electron, such as YbF and BaF, semiempirical estimates or *ab initio* calculations with approximate accounting for correlation and relativity provide reasonably reliable $W_d$ values (see Refs. [6, 7, 8]). These molecules are, however, chemical radicals, posing experimental problems. It was pointed out recently that the excited $a(1)$ or $B(1)$ states of PbO can be used effectively in the search for $d_e$. A novel experiment, using a vapor cell to study excited PbO, has been started at Yale University. The unique suitability of PbO for searching the elusive $d_e$ is demonstrated by the very high statistical sensitivity of the Yale experiment to the electron EDM, allowing detection of $d_e$ of order $10^{-31}$ e·cm [5], four orders of magnitude lower than the current limit quoted above. While semiempirical calculations [10] may be valuable, the authors of [10] stressed that “more elaborate calculations were highly desirable”. High-order *ab initio* correlated relativistic calculations of the type developed recently [11] are required to give accurate values of $W_d$ acting on the unpaired PbO electrons. An accuracy check is provided by calculating experimentally known properties which also depend on the electron spin density near the heavy nucleus, such as hyperfine constants.

The terms of interest for PbO in the effective spin-rotational Hamiltonian may be written following Ref. [12]. The P,T-odd interaction of $d_e$ with $W_d$ is

$$H_{\text{edm}} = W_d \ d_e (\mathbf{J} \cdot \mathbf{n}),$$

(1)

where $\mathbf{J}$ is the total electron moment and $\mathbf{n}$ is the unit vector along the axis from Pb to O. The hyperfine interaction of the electrons with the $^{207}$Pb nucleus is

$$H_{\text{hfs}} = \mathbf{J} \cdot \hat{A} \cdot \mathbf{I},$$

(2)
where $\hat{A}$ is the hyperfine tensor, characterized for a linear molecule by the constants $A_\parallel$ and $A_\perp$, and $I$ is the spin of the $^{207}\text{Pb}$ nucleus ($I = 1/2$).

In practice, the effective operator

$$H_d = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & \sigma E \end{pmatrix}$$  \hspace{1cm} (3)$$

is used to express the interaction of $d_e$ with the inner molecular electric field $E$ ($\sigma$ are the Pauli matrices), to avoid the large terms which cancel each other [13] because of Schiff’s theorem. After averaging over the electronic coordinates in the molecular wavefunction, one obtains

$$W_d = \frac{1}{2d_e} \langle \Psi_\Omega | \sum_i H_d(i) | \Psi_\Omega \rangle ,$$  \hspace{1cm} (4)$$

where $\Psi_\Omega$ is the wavefunction for either $a(1)$ or $B(1)$, and $\Omega = \langle \Psi_\Omega | \mathbf{J} \cdot \mathbf{n} | \Psi_\Omega \rangle$. The hyperfine constant $A_\parallel$ is determined by the expression [14]

$$A_\parallel = \frac{1}{\Omega \mu_{\text{Pb}}} \langle \Psi_\Omega | \sum_i (\alpha_i \times \mathbf{r}_i \mathbf{r}_i^3)Z | \Psi_\Omega \rangle ,$$  \hspace{1cm} (5)$$

where $\mu_{\text{Pb}}$ is the magnetic moment of $^{207}\text{Pb}$, $\alpha_i$ are the Dirac matrices for the $i$th electron, and $\mathbf{r}_i$ is its radius-vector in a coordinate system centered on the Pb atom.

Both $A_\parallel$ and $W_d$ depend strongly on the electronic spin density near the heavy nucleus, while the molecular bonds are formed in the valence region. As shown previously [6, 11, 15] and references therein), it is possible to evaluate the electronic wavefunction near the heavy nucleus in two steps. Using this strategy here, a high-accuracy relativistic coupled cluster (RCC) calculation [16] of the molecular electronic structure with the generalized relativistic effective core potential (GRECP) is carried out, providing proper electronic density in the valence and outer core regions. This is followed by restoration of the proper shape of the four-component molecular spinors in the inner core region of the heavy atom.

Methods and calculations. A 22-electron GRECP for Pb [17] is used in the first stage of the two-step calculations of PbO: the inner shells of the Pb atom ($1s$ to $4f$) are absorbed into the GRECP, and the $5s5p5d6s6p$ electrons and all the oxygen electrons are treated explicitly. Two series of calculations are carried out, denoted as (a) and (b): calculation (a) correlates 10 electrons, freezing the $5s5p5d$ shells of Pb and the $1s$ shell of O; (b) correlates all 30 electrons treated explicitly. States with the leading configurations $\sigma_1^2\sigma_2^2\pi_1^4$, $\sigma_1^2\sigma_2^2\pi_1^3\pi_2^1$, and $\sigma_1^2\sigma_2^1\pi_1^1\pi_2^1$ are calculated. Here $\sigma_{1,2}$ and $\pi_{1,2}$ are molecular valence orbitals, with the subscript
enumerating them in order of increasing energy. For each series of calculations, correlation
spin-orbital basis sets are optimized in atomic two-component GRECP/RCC calculations
of Pb. The four 6s and 6p electrons are correlated in the basis set optimization stage of
calculation (a), and 22 electrons (5s to 6p) are correlated in the optimization of the basis
set used in series (b). Correlation is taken into account at this stage by the RCC method
with single and double excitations (RCC-SD) \[18\]; the average energy of the five lowest
states of Pb is minimized. The detailed description of the basis set generation procedure
may be found in Refs. \[19, 20\]. A \([4s3p2d]\) basis, obtained by omitting the \(f\) function from
Dunning’s correlation-consistent \((10s5p2d1f)/[4s3p2d1f]\) basis listed in the MOLCAS 4.1
library \[21\], is used for oxygen. We found that the \(f\) orbital has little effect on the core
properties calculated here. Previous calculations show that these basis sets are adequate for
our purpose.

PbO calculations start with a one-component self consistent field (SCF) computation
of the molecular ground state, using the spin-averaged GRECP (AGREP). The Pb spinors
5s5p5d are frozen in the (a) series, using the level-shift technique \[22\]. An AGREP/RASSCF
(restricted active space SCF) calculation \[21, 23\] of the lowest \(\Sigma^+\) state of PbO is then
performed. In the RASSCF method, orbitals are divided into three active subspaces: RAS1,
with a restricted number of holes allowed; RAS2, where all possible occupations are included;
and RAS3, with an upper limit on the number of electrons.

Different distributions of electrons in these active subspaces are used (details may be
found in \[24\]) to estimate the different correlation contributions to the RASSCF values of
\(A_\parallel\) and \(W_d\). Two-component RCC-SD molecular calculations are then performed. The
AGREP/RASSCF calculations include only the most important correlation and scalar-
relativistic effects, while the GRECP/RCC-SD calculations also account for spin-orbit in-
teraction. The Fock-space RCC calculations start from the ground state of PbO and use
the scheme

\[
\begin{align*}
PbO^+ & \leftarrow PbO \rightarrow PbO^- \\
& \uparrow \downarrow \\
& PbO^* \\
\end{align*}
\]
(6)

Details on the model spaces used may be found in \[24\].

Only valence and outer core electrons have been treated so far. Since we are interested in
properties near the Pb nucleus, the shape of the four-component molecular spinors has to be
restored in the inner core region. All molecular spinors are restored using the nonvariational one-center restoration scheme (see [6, 11, 22, 25] and references therein). This is done in two steps:

First, equivalent numerical one-center basis sets of four-component spinors and two-component pseudospinors are generated by the finite-difference all-electron Dirac-Hartree-Fock (DHF) and GRECP/SCF calculations, respectively, of the same valence configurations of Pb and its ions. In the DHF calculations the inner core spinors (1s to 4f) are frozen after the calculation of Pb\(^{2+}\), and the nucleus is modeled by a uniform charge distribution within a sphere of radius \(r_{\text{nucl}} = 7.12\text{fm} = 1.35 \times 10^{-4}\text{a.u.}\). The root mean square radius of the nucleus is 5.52 fm, in accord with the parametrization of Johnson and Soff [26], and agrees with the \(^{207}\text{Pb}\) nucleus experimental value of 5.497 fm [27]. Taking the experimental value for the root mean square radius and a Fermi distribution for the nuclear charge changes \(A_{\parallel}\) and \(W_{d}\) by 0.1\% or less. The all-electron four-component HFD [28] and two-component GRECP/HFJ [17, 29] codes are employed for the basis generation, using the procedure developed in Refs. [19, 20]. The basis sets generated are [9s14p7d] for series (a) and [6s7p5d] for series (b), with the latter carefully optimized. These sets are orthogonal to the inner core (see above). They describe mainly the core region, and are generated independently of the basis set for the molecular GRECP calculations discussed earlier.

In the second step, the basis of one-center two-component atomic pseudospinors is used to expand the molecular pseudospinorbitals; these two-component pseudospinors are then replaced by the equivalent four-component spinors, retaining the expansion coefficients. A very good description of the wave function in the core region is obtained.

The RCC-SD calculation of \(W_{d}\) and \(A_{\parallel}\) employs the finite field method [30, 31]. The operator corresponding to the desired property [Eq. (1) or (2)] is multiplied by a parameter \(\lambda\) and added to the Hamiltonian. The first derivative of the calculated energy with respect to \(\lambda\) gives the evaluated property. This is strictly correct only at the limit of vanishing \(\lambda\), but it is usually possible to find a range of \(\lambda\) where the energy is linear in \(\lambda\) and the energy changes are large enough to attain the required precision. The quadratic dependence of the energy on \(\lambda\) is eliminated here by averaging the components of a given term, \(a(1)\) or \(B(1)\), with opposite signs of \(\lambda\).

Results and discussion. Calculated results for the (a) and (b) series are presented in Table [I]. The internuclear distance is 2.0 Å. The RASSCF calculations use the 22-electron
TABLE I: Calculated parameters $A_\parallel$ (in MHz) and $W_d$ (in $10^{24}$ Hz/(e·cm)) for the a(1) and B(1) states of $^{207}$PbO. The experimental value of $A_\parallel$ in a(1) is $-4113$ MHz. The preliminary value of $A_\parallel$ in B(1) is $5000 \pm 200$ MHz$^1$

| State  | Parameters | Expansion | $A_\parallel$ | $W_d$ | $A_\parallel$ | $W_d$ |
|--------|------------|-----------|---------------|-------|---------------|-------|
|        | a(1)       |           |               |       |               |       |
|        | $\sigma_1^2\sigma_2^2\pi_1^3\pi_2^1$ | $3\Sigma_1$ |               |       |               |       |
| 10e-RASSCF | s, s,p, s,p,d | s, s,p, s,p,d | -759, -1705, -1699 | 0.96, 0.91 | 1900, 0.0, 0.0 |
| 10e-RCC-SD | s, s,p, s,p,d | s, s,p, s,p,d | -2635, -2.93 | 3878, -11.1 |
| 30e-RCC-SD | s, s,p, s,p,d | s, s,p, s,p,d | -359, -3062, -3012 | -3.08, -3.18, 195, 4510, 4568 | -10.4, -9.7 |

$^1$ private communication, D.DeMille, 2003.

GRECP for Pb. Twenty of the 30 electrons treated were in the inactive space, and only 10 were correlated. Using the $C_{2v}$ classification scheme, 2 $A_1$ orbitals are in RAS1, 6 orbitals (2 $A_1$, 2 $B_1$, and 2 $B_2$) in RAS2, and 41 (16 $A_1$, 5 $A_2$, 10 $B_1$, and 10 $B_2$) in RAS3. No more than two holes in RAS1 and two particles in RAS3 are allowed. The basis sets on Pb are $(14s18p16d8f)/(4s7p5d3f)$ for the RASSCF and 30-electron RCC-SD calculations and $(15s16p12d9f)/(5s7p4d2f)$ for 10-electron RCC-SD. A $(10s5p2d)/(4s3p2d)$ basis is put on O in all calculations.

We discuss mainly the results for the a(1) state (leading configuration $\sigma_1^2\sigma_2^2\pi_1^3\pi_2^1$), for which the reliable experimental value of $A_\parallel$ is available ($-4113$ MHz) and a semiempirical estimate of $|W_d| \geq 12 \times 10^{24}$ Hz/(e·cm) was made recently. There are several points to note: (1) Inclusion of the spin-orbit interaction changes $A_\parallel$ and $W_d$ dramatically, as may be seen from the difference between the 10-electron RASSCF and RCC-SD results. (2) The ab initio value of $W_d$ is four times smaller than the semiempirical estimate. (3) Accounting for outer core–valence correlation by 30-electron RCC-SD changes $W_d$ by 5% and $A_\parallel$ by 15%, yet the error in the calculated $A_\parallel$ is 25%; calculations on BaF and YbF gave 10% accuracy. (4) $A_\parallel$ is mainly determined by the $p$ wave, whereas $W_d$ mostly comes from s-p mixing.

The need for including correlation in the PbO molecule for the properties discussed here can be seen already in the semiempirical model. The leading contribution to the highest occupied $\sigma_2$ orbital in this model comes from the Pb 6s atomic orbital, with a weight of $\sim 0.5$
(the corresponding coefficient in the molecular orbital expanded as a linear combination of atomic orbitals is $\sim 0.7$). This contradicts the qualitative analysis of the chemical bond formation, which predicts that the $\sigma_2$ orbital is mainly formed from the oxygen $2p_{\sigma}$ and lead $6p_{\sigma}$ orbitals. The RASSCF calculations of the lowest $3\Sigma^+$ state confirm this point, with the weight of the Pb $6s$ orbital varying between 0.04 for 10 active electrons and 0.1 for 30 active electrons. The weight of the oxygen $2p_{\sigma}$ is $\sim 0.5$ and that of the lead $6p_{\sigma}$ is $\sim 0.1$, whereas $\sigma_1$ consists mainly of the lead $6s$ orbital, with negligible contribution from lead $6p_{\sigma}$. Note that the oxygen $2p_{\sigma}$ and lead $6p_{\sigma}$ orbitals are not orthogonal to each other; after one-center reexpansion of the oxygen basis functions on lead (see [15] and Eq. (6) in [11]), the weight of the $6p_{\sigma}$ orbital goes up to 0.3. We expect that such strong admixture of the $s$-wave to the $\sigma_2$ orbital would not appear in the semiempirical model if configurations describing the correlation of the $\sigma_2$ electrons were included in the model space. It is important to add that the lowest virtual $\sigma_3$ orbital gets the main contribution from the lead $6p_{\sigma}$ (with a weight of about 0.5), and the configurations containing this orbital are first admixed into the leading configuration of the $a(1)$ state due to the spin-orbit interaction on Pb.

If the spin-orbit interaction is neglected, the $s$-wave contribution to $A_\parallel$ and the $s, p$-wave contributions to $W_d$ are due primarily to correlation of the $\sigma$ electrons. The RASSCF calculation indicates (see Table II) that such contributions increase $A_\parallel$ but decrease $W_d$, resulting in a sign change for $W_d$, in agreement with the final RCC-SD result (details may be found in Ref. [33]). Besides, as correlation is expected to have a strong influence on the values of $A_\parallel$ and $W_d$, introducing the SO interaction with the $3\Pi$ and $1\Pi$ states by just mixing the corresponding $\sigma$ and $\pi$ orbitals may not be satisfactory. All these conclusions could be reached only after extensive molecular calculations, and the estimates made in Ref. [10] were important at the first stage of the experimental effort.

As may be expected, the accuracy of the calculated $A_\parallel$ and $W_d$ values is lower for such a complicated system as the excited states of the PbO molecule than for the ground states of BaF and YbF. The valence electron in the latter molecules is in a $\sigma$ orbital, with much higher density near the heavy nucleus than the valence $\pi$ electrons in PbO. Thus, the $s, p, d$-waves on the Pb nucleus are affected more strongly by correlation, and higher-order inclusion of correlation (triple and quadruple amplitudes in the RCC method) as well as larger basis sets may be necessary. As pointed out above, $W_d$ is more stable than $A_\parallel$ with respect to changing the number of correlated electrons, and we expect the accuracy of the calculated
$W_d$ to be better than for $A_{∥}$. Our estimated error bounds put the real $W_d$ between 75\% and 150\% of the calculated value, which is quite satisfactory for the first stage of the EDM experiment on PbO. It should be noted that the estimate of statistical sensitivity to the electron EDM made in [5] is based on a $W_d$ value close to that obtained here.

A detailed analysis of correlation and spin-orbital effects on $A_{∥}$ and $W_d$ in PbO will be published elsewhere [33]. Unfortunately, the experimentally available $A_{∥}$ of the $a(1)$ and $B(1)$ states provides a check on the $p$ wave only. It would be desirable to measure $A_{∥}$ in some state with an excited $σ_1$-electron, with the main contribution coming from the $s$-wave. Another accuracy check, using $\sqrt{A_{∥}A_{⊥}}$, is not applicable here, because of experimental difficulties in measuring the very small $A_{⊥}$ for diatomic molecules with total electronic momentum $J \geq 1$. Our estimate of the accuracy of the calculated $W_d$ is therefore not as straightforward as for YbF and BaF [7, 8].

Finally, we would like to note that we identified the lowest $^3Π_1$ state as $B(1)$ according to the $ΛS$ classification given in [34]. Conclusive identification requires more extensive $ab\ initio$ correlation calculations.

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