Electric dipole moments of actinide atoms and RaO molecule

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We have calculated the atomic electric dipole moments (EDMs) induced in ^{229}Pa and ^{225}Ac by their respective nuclear Schiff moments S. The results are $d(^{229}\mathrm{Pa})=-9.5\times10^{-17}$ $[S/(e\ \mathrm{fm})]e$ cm $=-1.1\times10^{-20}\eta$ e cm and $d(^{225}\mathrm{Ac})=-8.6\times10^{-17}$ $[S/(e\ \mathrm{fm})]e$ cm$=-0.8\times10^{-21}\eta$ e cm. EDM of ^{229}Pa is 3×10^4 times larger than ^{199}Hg EDM and 40 times larger than ^{225}Ra EDM. Possible use of actinides in solid state experiments is also discussed. The (T,P)-odd spin-axis interaction in RaO molecule is 500 times larger than in TlF.

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Measurements of atomic electric dipole moments (EDMs) allow one to test CP violation theories beyond the standard model (see, e.g., [1,2]). The best limits on atomic EDM have been obtained for diamagnetic atoms Hg [3] and Xe [4]; there is also a limit on (T,P)-odd spin-axis interaction in TlF molecule [5]. EDM of diamagnetic atoms and molecules is induced by the interaction of atomic electrons with the nuclear Schiff moment. Schiff moments produced by the nuclear (T,P)-odd interactions have been calculated in Refs. [7–13]. Two to three orders of magnitude enhancement can exist in nuclei with octupole deformation [14] or soft octupole vibrations [15]. This motivated new generation of atomic experiments with ^{225}Ra and ^{223}Rn. Current status of EDM experiments and theory can be found on the website of the INT workshop [16]. Most accurate calculations of atomic EDM produced by the nuclear Schiff moments have been performed for Hg, Xe, Rn, Ra, Pu [17], Yb, and He [18] atoms and TlF molecule [6,17]. In this work we would like to note that several orders of magnitude larger effects appear in different systems.

Due to the octupole enhancement [14] the Schiff moments of ^{225,223}Ra exceed that of ^{205,203}Tl [7,8] ~200 times. There is an additional enhancement due to the higher nuclear charge of Ra since the effect produced by the Schiff moment increases faster than Z^2. Therefore, one hopes that experiments with RaO may be up to three orders of magnitude more sensitive to the nuclear (T,P)-violating interactions than the experiments with TlF. The results of molecular calculations are usually expressed in terms of the following matrix element:

$$X=-\frac{2\pi}{3}\langle\Psi_0|[\boldsymbol{\nabla}\cdot\mathbf{n},\delta(\mathbf{R})]|\Psi_0\rangle, \tag{1}$$

where Ψ_0 is the ground state wave function and $\mathbf{n}$ is the unit vector along the molecular axis. The (T,P)-odd spin-axis interaction constant can be expressed in terms of the Schiff moment S (see, e.g., [17]):

$$\langle\Psi_0|H_W|\Psi_0\rangle=6X\mathbf{S}\cdot\mathbf{n}. \tag{2}$$

Here $\mathbf{S}$ is the Schiff moment vector. For TlF molecule $X=7475$ atomic units (a.u.) [6,17]. We use this result to estimate X for RaO. One can view TlF molecule as an ion compound Tl^+F^-. The electronic configuration of Tl^+ is $\ldots6s^2$. The electric field of F^- produces s-p hybridization of Tl^+ orbitals and nonzero matrix element X in Eq. (1). The electronic configuration of Ra, $\ldots7s^2$, is similar to Tl^+, and the (T,P)-odd spin-axis interaction in RaO is also due to the s-p hybridization. The simplest way to estimate X for RaO is to use known Z dependence of the Schiff moment effect: $Z^2R(Z\alpha)$, where $R(Z\alpha)$ is the relativistic factor [7]. This gives $X(\mathrm{RaO})/X(\mathrm{TlF})\approx1.6S(\mathrm{Ra})/S(\mathrm{Tl})$. A slightly more accurate result may be obtained using existing atomic EDM calculations [atomic EDM and molecular (T,P)-odd spin-axis interaction depend on the same matrix elements of the Schiff moment field]. Hg atom has the same electronic configuration as Tl^+. The ratio of Ra and Hg EDM was calculated in [17] $d(\mathrm{Ra})/d(\mathrm{Hg})=3.04S(\mathrm{Ra})/S(\mathrm{Hg})$. The larger value for Ra is due to higher nuclear charge: $Z=88$ for Ra, $Z=80$ for Hg, and $Z=81$ for Tl. Using $d(\mathrm{Ra})/d(\mathrm{Hg})=3.04S(\mathrm{Ra})/S(\mathrm{Hg})$ we obtain an estimate $X(\mathrm{RaO})/X(\mathrm{TlF})\approx2.8S(\mathrm{Ra})/S(\mathrm{Tl})$. As a final value we will use an intermediate result $X(\mathrm{RaO})/X(\mathrm{TlF})\approx2.2S(\mathrm{Ra})/S(\mathrm{Tl})$, which is between the EDM estimate and the relativistic factor estimate. This gives the (T,P)-odd spin-axis interaction in RaO

$$\langle\Psi_0|H_W|\Psi_0\rangle=1.\times10^5(\mathbf{S}\cdot\mathbf{n})\ \text{a.u.} \tag{3}$$

The Ra Schiff moment S is 200 times larger than the Tl Schiff moment; altogether we obtain 500 times enhancement in RaO in comparison with TlF. Note that the error of this number is probably dominated by the nuclear calculations of the Schiff moments.

The largest Schiff moment was found for ^{229}Pa [14] where the atomic calculation of EDM is absent. Below we obtain the result for this EDM. The enhancement of (P,T)-violation in ^{229}Pa nucleus was found by Haxton and Henley in Ref. [19]. This nucleus contains a very close excited level (220 eV) which has the same spin as the ground state level $(I=5/2)$ and opposite parity. These ground and excited states, $5/2^+$ and $5/2^-$, can be mixed by the nucleon (P,T)-odd interaction. Haxton and Henley performed calculations in the Nilsson model (using single-particle orbitals for the quadrupole nuclear deformation) and found that nuclear EDM and magnetic quadrupole moment are signifi-

cantly enhanced. Unfortunately, they did not calculate Schiff moment. Calculation of the Schiff moment was performed in Ref. [14] assuming a different model (octupole nuclear deformation) which gives an additional enhancement due to the collective nature of the Schiff moment in nuclei with octupole deformation. A similar mechanism produces enhancement of the (T,P)-odd electric octupole moment [20]. It is interesting that in ^{229}Pa all four (T,P)-odd nuclear moments (Schiff, EDM, magnetic quadrupole, and octupole) contribute to atomic EDM. Let us start from the Schiff moment which gives a dominating contribution in ^{229}Pa.

The electron configuration of Pa is $\ldots 7s^2 5f^2 6d$. The Schiff moment field is confined inside the nucleus. The high-wave $6d$ and $5f$ electrons practically do not penetrate inside the nucleus and have very small matrix elements for the Schiff moment field. If we neglect these small matrix elements, the atomic EDM comes from the Ra-like core $\ldots 7s^2$. In this approximation we may use the result for Ra, $d=-8.23\times 10^{-17}$ $[S/(e\ \mathrm{fm})]e$ cm from Ref. [17], to calculate Pa EDM. The coefficient actually should be slightly larger since the Pa charge $Z=91$ is larger than the Ra charge $Z=88$. Another reference point is Pu, Z=98, where $d=-10.9\times 10^{-17}$ $[S/(e\ \mathrm{fm})]e$ cm from Ref. [17]. Pu has the electron configuration $\ldots 7s^2 5f^6$ where the contribution of $5f$ electrons is not very important (as explained above). The Pa atom, $Z=91$, is exactly in between Ra, $Z=88$, and Pu, Z=94. Therefore, we take the average value as Pa EDM, $d=-9.5\times 10^{-17}$ $[S/(e\ \mathrm{fm})]e$ cm. The accuracy of this result is about 20% (see Ref. [17]).

Now we discuss the contributions of other (T,P)-odd moments. Nuclear EDM contributes in combination with magnetic hyperfine interaction between nucleus and atomic electrons [21]. However, this contribution has relatively slow increase with nuclear charge, $\sim Z$, and may be neglected. The contributions of magnetic quadrupole, electric octupole, and Schiff moments increase faster than Z^2. Electric octupole and magnetic quadrupole induce atomic EDM only if electron angular momentum J is not zero (since the EDM vector d_i can only be produced from nuclear magnetic quadrupole tensor M_{ik} as $d_i \sim M_{ik}J_k$ or octupole third rank tensor as $d_i \sim O_{ikj}J_kJ_j$). The electron angular momentum $J=11/2$ is actually carried out by $6d$ and $5f$ electrons. The matrix elements of very singular magnetic quadrupole and electric octupole fields for these orbitals are small since these matrix elements come from small distances where the high-wave electrons do not penetrate. If we neglect these small matrix elements, the atomic EDM comes from the Ra-like core $\ldots 7s^2$ which has zero electron angular momentum and no contributions from the magnetic quadrupole and electric octupole. Atomic EDM in this approximation comes entirely from the Schiff moment field which mixes s-p orbitals. There are additional arguments why we do not need to include the electric octupole and magnetic quadrupole contributions into our approximate calculations. Without any enhancement (e.g., for spherical nuclei), the electric octupole contribution to atomic EDM is substantially smaller than the magnetic quadrupole and Schiff contributions (see comparison of the corresponding matrix elements in Ref. [20]). The octupole deformation (or the soft octupole mode) gives the collective enhancement of the Schiff and octupole moments, however, it does not enhance the magnetic quadrupole (the small nuclear energy denominator is a common factor for all three contributions, so it does not influence the ratio of them). These arguments stress again importance of the Schiff moment contribution.

The Schiff moment of ^{229}Pa was calculated in Ref. [14]: $S=1.2\times 10^{-4}$ e fm^3 η, where η is the dimensionless strength of the nucleon (P,T)-odd interaction in units of the Fermi constant. Substituting this value we obtain the EDM of the ^{229}Pa atom:

$$d=-1.1\times 10^{-20}\eta\ e\ \mathrm{cm}. \tag{4}$$

This value is 3×10^4 times larger than ^{199}Hg atomic EDM, $4\times 10^{-25}\eta$ e cm, and 40 times larger than ^{225}Ra EDM, $2.6\times 10^{-22}\eta$ e cm (this comparison is based on the Schiff moments from Refs. [8,14] and the atomic calculations for Hg and Ra from Ref. [17]).

A similar calculation for ^{225}Ac ($Z=89$, atomic configuration $\ldots 7s^2 6d$, $J=3/2$) gives

$$d=-8.6\times 10^{-17}\ [S/(e\ \mathrm{fm})]e\ \mathrm{cm}=-0.8\times 10^{-21}\eta\ e\ \mathrm{cm}. \tag{5}$$

We would like to suggest another possible application of actinides. Recently, the measurements of electron EDM and nuclear Schiff moments in the solid compounds contaning rare-earth atoms (e.g., gadolinium) have been proposed [22,23,25] (corresponding calculations have been performed in [24,25]). The actinides are electronic analogs of rare-earth atoms. Because of rapid increase of atomic EDM with nuclear charge it may be worth considering similar compounds with actinides. For example, uranium and thorium have isotopes which are practically stable. Atomic EDM induced by the electron EDM increases with Z as [26]

$$d\sim \frac{Z^3}{(j+1)(4\gamma^2-1)\gamma}, \tag{6}$$

where $\gamma=[(j+1/2)^2-Z\alpha^2]^{1/2}$ and j is the electron angular momentum (maximal contribution comes from $j=1/2$). Comparing uranium ($Z=92$) with gadolinium ($Z=64$) we see that in uranium compounds the effect is ~ 5 times larger. A similar enhancement happens for the effects induced by the nuclear (T,P)-odd moments.

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