Multiconfiguration Dirac-Hartree-Fock calculations of atomic electric dipole moments of $^{225}\text{Ra}$, $^{199}\text{Hg}$, and $^{171}\text{Yb}$

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The multiconfiguration Dirac-Hartree-Fock (MCDHF) method has been employed to calculate atomic electric dipole moments (EDM) of $^{225}\text{Ra}$, $^{199}\text{Hg}$, and $^{171}\text{Yb}$. For the calculations of the matrix elements we extended the relativistic atomic structure package GRASP2K [1]. The extension includes programs to evaluate matrix elements of $(P,T)$-odd e-N tensor-pseudotensor and pseudoscalar-scalar interactions, the atomic electric dipole interaction, the nuclear Schiff moment, and the interaction of the electron electric dipole moment with nuclear magnetic moments. The interelectronic interactions were accounted for through valence and core-valence electron correlation effects. The electron shell relaxation was included with separately optimised wave functions of opposite parities.

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I. INTRODUCTION

The existence of a non-zero permanent electric dipole moment (EDM) of an elementary particle or a composite system of particles would violate time reversal symmetry (T), as well as the combined charge conjugation and parity symmetry (CP), due to the CPT theorem [2]. One of the principal motivations behind the experimental searches of EDMs is to shed light on the observed matter-antimatter asymmetry in the Universe, which in turn is linked to an asymmetry in the Big Bang baryon-antibaryon production. The standard model (SM) of elementary particles cannot explain the matter-antimatter asymmetry in the Universe, as SM predicts sources of CP violation (and of EDMs) several orders of magnitude weaker than those needed to account for the observed baryon numbers. This leads to proliferation of the extensions to the standard model. Some of these extensions predict larger EDMs, sometimes within the reach of current experiments. The experimental searches have not yet detected a non-zero EDM, but they continue to improve the limits on EDMs of individual elementary particles, as well as limits on CP-violating interactions, usually parametrized by the interaction constants $C_T$ and $C_P$ (see section II for details and the Table II in the reference [3] for a summary). These limits constrain the theoretical extensions of the standard model of elementary particles. In recent years these constraints have been set by the measurements of EDMs of neutrons [4], electrons in a paramagnetic atom (a thallium atom experiment [5]), electrons in a diamagnetic atom (mercury atom [6]), and in TlF and YbF molecules [8]. The search for EDMs is not restricted to the above species, though — see e.g. [7].

The search for a permanent electric dipole moment of an elementary particle, or a composite system of particles (see [2], or a recent reference [8] for a review), is a challenge, not only for experiments, but also for theories of composite systems. Heavy atoms are excellent examples of composite systems with large EDMs, due to the existence of mechanisms which may induce atomic EDMs several orders of magnitude larger than an intrinsic particle EDM. In the present paper we computed the EDMs of three diamagnetic atoms, $^{225}\text{Ra}$, $^{199}\text{Hg}$, and $^{171}\text{Yb}$. The purpose of the present paper is fourfold. Firstly, we tested the newly developed programs to evaluate matrix elements of $(P,T)$-odd e-N tensor-pseudotensor and pseudoscalar-scalar interactions, the atomic electric dipole interaction, the nuclear Schiff moment, and the interaction of the electron electric dipole moment with nuclear magnetic moments. Secondly, we generated the atomic wave functions in several different approaches, in order to test the dependence of the calculated atomic EDMs on options available in the GRASP2K [1] implementation of the MCDHF method. The approaches depended on the choice of variational energy functional (Average Level versus Optimal Level, with different numbers of optimised levels), the choice of wave functions built on a common orbital set or several separately optimised orbital sets, in the latter case biorthogonal transformations of wave functions had to be applied, as well as on specific methods of one-electron orbital generation. All these approaches are discussed in more detail in section II B, III C, III D and III E and presented in Tables II B, III C and III E. Thirdly, we sequentially generated several layers of virtual (correlation) orbitals for each of the three elements and observed the effects of electron correlation on atomic EDMs. All valence and core-valence electron correlation effects were included through single and restricted double electron substitutions from core-valence to virtual orbitals. And finally, we provide independently calculated atomic EDMs in $^{225}\text{Ra}$, $^{199}\text{Hg}$, and $^{171}\text{Yb}$, and...
compare our results with those of other authors. Our results, presented in the Tables, were obtained within the multiconfiguration Dirac-Hartree-Fock (MCDF) method, using the relativistic atomic structure package GRASP2K, which, to the best of our knowledge, and with the exception of one paper on the Schiff moment in radium, has been employed for the first time in the calculations of matrix elements of $(P,T)$-odd e-N tensor-pseudotensor and pseudoscalar-scalar interactions, nuclear Schiff moment, and interaction of electron dipole moment with nuclear magnetic moments.

The three atoms, $^{225}\text{Ra}$, $^{199}\text{Hg}$, and $^{171}\text{Yb}$, have been chosen on the grounds that they have similar valence shell structure. All these elements are diamagnetic, with closed outer $s$ shell ($^{225}\text{Ra}$ 6$p^67$s$^2$, $^{199}\text{Hg}$ 5$d^{10}6$s$^2$, and $^{171}\text{Yb}$ 4$f^{14}6$s$^2$). In the future we will be able to perform these calculations to closed-$p$-valence-shell atoms, as well as to any other, closed- or open-shell system. Our current MCDHF machinery is robust enough to deal with electron correlation effects in arbitrary atomic systems, including the lanthanides and actinides.

II. EDM THEORY

The interactions which mix atomic states of different parities and induce a static electric dipole moment of an atom are quite weak. Therefore an atomic wave function can be expressed as

$$\bar{\Psi}(JM_J) = a\Psi(\gamma PJM_J) + \sum_i b_i \Psi(\gamma_i(-P)JM_J).$$  \hspace{1cm} (1)

where the coefficient $a$ of the dominant contribution can be set to 1. The expansion coefficients of opposite parity $(-P)$ admixtures, $b_i$, can be found using first order perturbation theory:

$$b_i = \frac{\langle \Psi(\gamma_i(-P)JM_J) | \hat{H}_{\text{int}} | \Psi(\gamma PJM_J) \rangle}{E(\gamma P) - E(\gamma_i(-P)JM_J)}.$$  \hspace{1cm} (2)

$\hat{H}_{\text{int}}$ represents the Hamiltonian of the $(P,T)$-odd interaction, which mixes states of opposite parities. The mixed-parity state of a particular atomic level $^{2S+1}L_J$ induces a static EDM of an atom:

$$d_{ab}^{\text{int}} = \langle \bar{\Psi}(\gamma PJM_J) | \hat{D}_z | \Psi(\gamma_i(-P)JM_J) \rangle = 2\sum_i b_i \langle \Psi(\gamma PJM_J) | \hat{D}_z | \Psi(\gamma_i(-P)JM_J) \rangle,$$  \hspace{1cm} (3)

where $\hat{D}_z$ represents the $z$ projection of the electric dipole moment operator. Eventually an atomic EDM can be written as a sum:

$$d_{ab}^{\text{int}} = 2\sum_i \frac{\langle 0 | \hat{D}_z | i \rangle \langle i | \hat{H}_{\text{int}} | 0 \rangle}{E_0 - E_i},$$  \hspace{1cm} (4)

where $|0\rangle$ represents the ground state $|\Psi(\gamma PJM_J)\rangle$, with $J = 0$ and even parity, and the summation runs over excited states $|\Psi(\gamma_i(-P)JM_J)\rangle$, with $J_i = 1$ and odd parity. $E_0$ and $E_i$ are energies of ground and excited states, respectively. In practice this sum needs to be truncated at some level.

Calculations of atomic EDM require evaluation of the matrix element of the static EDM $(|0\rangle \hat{D}_z | i \rangle)$ and the matrix element of the interactions which induced EDM in an atom $\langle i | \hat{H}_{\text{int}} | 0 \rangle$. The operators associated with the above matrix elements are all one-particle operators.

For the general tensor operator $\hat{T}^k_q$, the matrix element between states of different parity can be expressed by Wigner-Eckart theorem as:

$$\langle \Psi(\gamma PJM_J) | \hat{T}^k_q | \Psi(\gamma_i(-P)JM_J) \rangle = (-1)^{J-M_J} \sqrt{2J+1} \begin{pmatrix} J & k & J_i \\ -M_J & 0 & M_i \end{pmatrix} \times \left| \Psi(\gamma PJM_J) \right|^2 \left| \Psi(\gamma_i(-P)JM_J) \right|^2.$$  \hspace{1cm} (5)

Expanding the wave functions in configuration state functions (CSFs), $\Phi(\gamma P)$, that are built from one-electron Dirac orbitals, see section the reduced matrix elements of $\hat{T}^k_q$ can be written

$$\left| \Psi(\gamma PJM_J) \right|^2 \left| \Psi(\gamma_i(-P)JM_J) \right|^2 = \sum_{r,s} c_r c_s \left| \Phi(\gamma_r P) \right|^2 \left| \Phi(\gamma_s(-P)JM_J) \right|^2$$  \hspace{1cm} (6)

where $c_r$ and $c_s$ are mixing coefficients of CSFs (even and odd parity, respectively). The matrix elements between the CSFs, in turn, can be written as sums of single-particle matrix elements

$$\left| \Phi(\gamma_r P) \right|^2 \left| \Phi(\gamma_s(-P)JM_J) \right|^2 = \sum_{n,a,b} d^k_{ab}(rs) [n_a \kappa_a | i^k | n_b \kappa_b].$$  \hspace{1cm} (7)

In the latter expansion, the $d^k_{ab}(rs)$ are known as ‘spin-angular coefficients’ that arise from using Racah’s algebra in the decomposition of the many-electron matrix elements. The expressions (5), (6) and (7) are general and can be used for any one-particle operator.

We consider the following four mechanisms which may induce atomic EDM: tensor-pseudotensor $(\hat{H}_{TTPT})$, pseudoscalar-scalar $(\hat{H}_{SSPS})$, Schiff moment $(\hat{H}_{SM})$, and electron EDM interaction with nuclear magnetic field $(\hat{H}_B)$. The interactions, which are all of rank $k = 1$, are discussed in more detail in the next sections. In addition the expression for the electric dipole interaction is given.
A. The electric dipole operator

The electric-dipole moment operator has the rank $k=1$ in $[6], [7]$, and $[11]$, and the single-particle reduced matrix element $[n_a \kappa_a \| t^k \| n_b \kappa_b]$ in equation (7) can be written as

$$[n_a \kappa_a \| t^k \| n_b \kappa_b] =$$

$$- [\kappa_a \| C^1 \| \kappa_b] \int_0^\infty (P_a P_b + Q_a Q_b) \, r \, dr,$$  

where $P$ and $Q$ are large and small components of the relativistic radial wave functions, respectively. The single-particle angular reduced matrix elements can be expressed as:

$$[\kappa_a \| C^1 \| \kappa_b] =$$

$$(-1)^{j_a + 1/2} \sqrt{2j_b + 1} \left( \begin{array}{ccc} j_a & k & j_b \\ 1/2 & 0 & -1/2 \end{array} \right) \pi (l_a, l_b, k),$$  

where $\pi (l_a, l_b, k)$ is defined as:

$$\pi (l_a, l_b, k) = \begin{cases} 1; & \text{if } l_a + k + l_b \text{ even}, \\ 0; & \text{otherwise}. \end{cases}$$  

B. Tensor-pseudotensor interaction

One of the possible sources of the EDM in diamagnetic atoms is the tensor-pseudotensor (TPT) interaction between electrons and nucleons, violating both parity (P) and time (T)-reversal invariance. It can be expressed as

$$\hat{H}_{TPT} = i \sqrt{2} G_F C_T \sum_{j=1}^N (\langle \sigma_A \rangle \cdot \gamma_j) \rho (r_j).$$  

$G_F$ is the Fermi coupling constant, $A$ is the number of nucleons, $\gamma_j$ is the Dirac matrix, and $C_T$ is a dimensionless coupling constant of the TPT interaction. $C_T$ is equal to zero within the standard model, but it is finite in some theories beyond the standard model of elementary particle physics. According to Dzuba et al [12]

$$C_T \langle \sigma_A \rangle = \left\{ C_T^p \sum_p \sigma_p + C_T^n \sum_n \sigma_n \right\},$$

where $\langle \ldots \rangle$ represents averaging over the nuclear state with the nuclear spin $I$. The nuclear charge density distribution $\rho (r)$ is the normalized to unity two-component Fermi function [13]

$$\rho(r) = \frac{\rho_0}{1 + e^{(r-b)/a}}$$

where $a$ and $b$ depend on the mass of the isotope.

The single-particle reduced matrix elements $[n_a \kappa_a \| t^k \| n_b \kappa_b]$ in equation (7) for the tensor-pseudotensor interaction has the form

$$[n_a \kappa_a \| t^k \| n_b \kappa_b] = \sqrt{2} G_F C_T \langle \sigma_A \rangle \left[ n_a \kappa_a \| i \gamma^1 \rho (r) \| n_b \kappa_b \right] =$$

$$- \sqrt{2} G_F C_T < \sigma_A > \left\{ [-\kappa_a \| \sigma^1 \| \kappa_b] \int_0^\infty P_a Q_a \rho \, dr + [\kappa_a \| \sigma^1 \| - \kappa_b] \int_0^\infty P_a Q_b \rho \, dr \right\},$$

where the single-particle angular reduced matrix elements can be expressed as:

$$[-\kappa_a \| \sigma^1 \| \kappa_b] =$$

$$\left\langle l_a \frac{1}{2} 0 \frac{1}{2} \| j_a \frac{1}{2} \right\rangle \left\langle l_b \frac{1}{2} 0 \frac{1}{2} \| j_b \frac{1}{2} \right\rangle - \left\langle l_b \frac{1}{2} 1 \frac{1}{2} \| j_a \frac{1}{2} \right\rangle \left\langle l_a \frac{1}{2} 1 \frac{1}{2} \| j_b \frac{1}{2} \right\rangle,$$

$$\left\langle j_b \frac{1}{2} 0 \frac{1}{2} \| j_a \frac{1}{2} \right\rangle,$$

$$[\kappa_a \| \sigma^1 \| \kappa_b] =$$

$$\left\langle l_a \frac{1}{2} 0 \frac{1}{2} \| j_a \frac{1}{2} \right\rangle \left\langle l_a \frac{1}{2} 0 \frac{1}{2} \| j_b \frac{1}{2} \right\rangle = \left\langle l_a \frac{1}{2} \frac{1}{2} \| j_a \frac{1}{2} \right\rangle \left\langle l_a \frac{1}{2} \frac{1}{2} \| j_b \frac{1}{2} \right\rangle.$$  

C. Pseudoscalar-scalar interaction

The interaction Hamiltonian for the pseudoscalar-scalar (PSS) interaction between the electrons and the nucleus reads

$$\hat{H}_{PSS} = -\frac{G_F C_F}{2 \sqrt{2} m_P c} \sum_{j=1}^N \gamma_0 \left( \nabla \cdot \rho (r_j) \right) \langle \sigma_A \rangle.$$  


$C_P$ is dimensionless coupling constant of the $PSS$ interaction. Analogously to the TPT interaction, $C_P$ constant is zero within the standard model. According to Dzuba et al. [12]

$$C_P \langle \sigma_A \rangle = \left< C_P^p \sum_p \sigma_p + C_P^n \sum_n \sigma_n \right>.$$  

(18)

$$\left[ n_a \kappa_a \| \hat{h}_{PSS} \| n_b \kappa_b \right] = -\frac{G_F C_P}{2\sqrt{2}m_e c} \langle \sigma_A \rangle \left[ n_a \kappa_a \| \gamma_0 \nabla_1 \rho \| n_b \kappa_b \right] =$$

$$-\frac{G_F C_P}{2\sqrt{2}m_e c} \langle \sigma_A \rangle \left[ \kappa_a \| C^1 \| \kappa_b \right] \int_0^\infty (P_a P_b + Q_a Q_b) \frac{d\rho}{dr} dr.$$  

(19)

### D. Schiff moment

The Hamiltonian of this interaction ($H_{SM}$) can be expressed as:

$$\hat{H}_{SM} = \frac{3}{B} \sum_{j=1}^N (S \cdot r_j) \rho(r_j).$$  

(20)

The Schiff moment $S$ is directed along the nuclear spin $I$ and $S = SI/I$, with $S$ being the coupling constant, and $B = \int_0^\infty \rho(r)r^4 dr$. The single-particle reduced matrix element $\left[ n_a \kappa_a \| \hat{h}_3^M \| n_b \kappa_b \right]$ in expansion (7) for SM can be factorized into reduced angular matrix element and radial integral

$$\left[ n_a \kappa_a \| \hat{h}_3^M \| n_b \kappa_b \right] = \frac{3}{B} S \left[ n_a \kappa_a \| \gamma_1 \rho \| n_b \kappa_b \right] =$$

$$\frac{3}{B} S \left[ \kappa_a \| C^1 \| \kappa_b \right] \int_0^\infty (P_a P_b + Q_a Q_b) \rho(r) dr.$$  

(21)

$$\left[ n_a \kappa_a \| \hat{h}_{PSS} \| n_b \kappa_b \right] =$$

$$\frac{d_e \mu}{2m_e c} \left\{ -3 \left[ -\kappa_a \| C^1 \| - \kappa_b \right] \int_R^{\infty} \frac{Q_a P_b}{r^3} dr - 3 \left[ \kappa_a \| C^1 \| \kappa_b \right] \int_R^{\infty} \frac{P_a Q_b}{r^3} dr - \left[ -\kappa_a \| \sigma^1 \| \kappa_b \right] \int_R^{\infty} \frac{Q_a P_b}{r^3} dr \right\},$$  

(23)

where $R$ and $\mu$ represent the nuclear radius and nuclear magnetic moment, respectively.

We extended the GRASP2K [1] package for the calculation of the matrix elements [7] and for the calculation of single-particle reduced matrix elements [8, 14, 19, 21, and 23]. The extension, presented in this work, includes subroutines for calculation of matrix elements of type $\langle i | H_{int} | 0 \rangle$ for tensor-pseudotensor $H_{TPT}$,
pseudoscalar-scalar \( \hat{H}_{PSS} \), Schiff moment \( \hat{H}_{SM} \), electron EDM interaction with nuclear magnetic field \( \hat{H}_B \), and electric dipole moment \( \hat{D}_z \).

III. MCDHF CALCULATIONS

A. MCDHF theory

We used the MCDHF approach to generate numerical representations of atomic wave functions. An atomic state function (ASF) \( \Psi(\gamma P J M_j) \) is obtained as a linear combination of configuration state functions \( \Phi(\gamma P J M_j) \), eigenfunctions of the parity \( P \), and total angular momentum operators \( J^2 \) and \( M_j \):

\[
\Psi(\gamma P J M_j) = \sum_r c_r \Phi(\gamma P J M_j),
\]

where \( c_r \) are configuration mixing coefficients. The multiconfiguration energy functional was based on the Dirac-Coulomb Hamiltonian, given (in a.u.) by

\[
\hat{H}_{DC} = \sum_{j=1}^{N} \left( c \alpha_j \cdot \mathbf{p}_j + (\beta_j - 1)c^2 + V(r_j) \right) + \sum_{j<k} \frac{1}{r_{jk}},
\]

where \( \alpha \) and \( \beta \) are the Dirac matrices, and \( p \) is the momentum operator. The electrostatic electron-nucleus interaction, \( V(r_j) \), has been generated from a 2-parameter Fermi nuclear charge distribution [13]. The effects of the Breit interaction, as well as QED effects, were neglected, since they are expected to be small at the level of accuracy attainable in the present calculations.

B. Energy functionals

Several different methods of wave function generation were employed, in order to test the dependence of the calculated atomic EDMs on options available in the GRASP2K [1] implementation of the MCDHF method. One option is related to the variational energy functional in the wave function optimisation procedure. Two general forms of the energy functional are implemented in the GRASP2K [1] package:

1. Extended Optimal Level

One-electron orbitals based on the Extended Optimal Level (EOL) form are optimised to minimise the energy functional, which is defined through the equation (39) in reference [13], where generalised weights (equation (40) in ref. [13]) determine a specific atomic state ASF (or a set of ASFs). Consequently, the orbitals in the EOL approach are optimal for a specific atomic state ASF or a set of ASFs.

2. Extended Average Level

One-electron orbitals based on the Extended Average Level (EAL) form are optimised to minimise the (optionally weighted) sum of energies of all ASFs which may be constructed from a given set of CSFs, so eventually it yields an (optionally weighted) average energy of a set of atomic states. This approach is computationally much cheaper, but usually less accurate than the approach based on the EOL functional.

C. Virtual orbital sets

The numerical wave functions were obtained independently for the two parities. The calculations proceeded in two phases. Spectroscopic (occupied) orbitals were obtained in the Dirac-Hartree-Fock approximation. They were kept frozen in all subsequent calculations. Then virtual (correlation) orbitals were generated in several consecutive steps. At each step the virtual set has been extended by one layer of virtual orbitals. A layer is defined as a subset of virtual orbitals, usually with different angular symmetries, optimized simultaneously in one step, and usually frozen in all subsequent steps. In the present paper three or four layers of virtual orbitals of each of the \( s, p, d, f, g \) symmetries were generated. At each stage only the outermost layer is optimized and the remaining orbitals (spectroscopic as well as other virtual layers) are kept frozen. Virtual orbitals were generated in an approximation in which all single and restricted double substitutions from valence orbitals and a subset of core orbitals to subsequent layers of virtual orbitals were included. The restriction was applied to double substitutions in such a way that only one electron was substituted from core shells, the other one had to be substituted from the valence shells (i.e. from \( 7s \) shell in the case of even parity ground state of radium atom; \( 7s \) and \( 7p \) shells in the case of odd parity excited states of radium; \( 6s \) and \( 6p \) in the cases of mercury and ytterbium). Four layers of virtual orbitals were generated for each of the three elements – Ra, Hg, Yb. The combined contribution of the \( n = 3 \) shells to the hyperfine constants of the \( 7s7p^1P \) state was evaluated in a previous paper [14] and found to be negligible, while the combined contribution of the \( n = 4 \) shells was below 1 percent level. Therefore in the present calculations the innermost core orbitals \( 1s, 2s, 2p, 3s, 3p, 3d \) of the radium atom were kept closed for electron substitutions. All other core orbitals, as well as valence orbitals, were subject to electron substitutions. By similar argument, the innermost core orbitals \( 1s, 2s, 2p \) of Hg and Yb were kept closed for electron substitutions. The reader is referred to the papers [14, 15] for further details of wave function generation.
D. Non-orthogonal orbital sets

The matrix elements of all interactions were calculated between the ground state $ns^2$ ($J = 0$) and excited states with total angular momentum $J = 1$ and opposite parity for $^{225}$Ra, $^{199}$Hg, and $^{171}$Yb. In principle, the optimal wave functions for calculations of EDM matrix elements are obtained in the Extended Optimal Level form (see section III B 1 above) separately for each parity. The wave functions optimised separately for the ground and excited states are built from independent sets of one-electron orbitals. The two sets are mutually non-orthogonal and they automatically account for relaxation effects involved in calculations of matrix elements between different atomic states $|3, 12|$. On the other hand, the transition energies obtained from wave functions based separately optimised orbital sets may be less accurate than transition energies obtained from calculations based on a common set of mutually orthogonal one-electron orbitals. The above situation often arises when multiconfiguration expansions are tailored specifically to include only those electron correlation effects that are important for the one-electron expectation values. For one-electron matrix elements involved in the present calculations the dominant contributions arise from single and restricted double substitutions. We have not included the unrestricted double substitutions i.e. the electron correlation effects with dominant contributions to the total energy, as well as higher order substitutions, since their impact on EDMs is indirect and usually small $|15|$. We evaluated the effect of the relaxation of the wave functions by performing two parallel sets of calculations based on a common orbital set (orthogonal) and on two separately optimised orbital sets (non-orthogonal), respectively. Table II lists the atomic EDM for $^{225}$Ra, calculated in several approximations. The first line (denoted 0(DF) in the first column) lists the results obtained with uncorrelated Dirac-Fock wave functions. The following lines provide the results obtained with different numbers (1-4) of virtual orbital layers included in the Virtual Orbital Set (VOS). The number of virtual orbital layers in a given VOS is quoted in the first column. We skipped the ‘orthogonal’ calculation with four virtual orbital layers, since the preceding lines show clearly that the effects of non-orthogonality (i.e. the relaxation of wave functions) are of the order of a few percent, up to 11% for the interaction of the electron electric dipole moment with the nuclear magnetic field (eEDM entry in Table II).

The calculation of matrix elements in the non-orthogonal case requires a transformation of one-electron orbitals from which the wave functions of ground and excited states are built. The program BIOTRA2 $|13|$ was applied to transform both wave functions to a biorthonormal form $|13, 16|$ which then permits to use standard Racah algebra in evaluation of matrix elements.

| TABLE I: Contributions to the atomic EDM from TPT, PSS, SM, and electron EDM interactions, calculated for $^{225}$Ra, using orthogonal (Orth) and non-orthogonal (Non-O) orbital sets. The number VOS in the first column is the number of virtual orbital layers. Transition energies are experimental. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| VOS             | Orth Non-O Orth Non-O Orth Non-O Orth Non-O Orth Non-O Orth Non-O Orth Non-O | | | |
| 0(DF)           | -16.3 -15.81 -59.7 -57.87 -6.53 -6.32 | -55.6 | -46.67 |
| 1               | -14.5 -15.51 -53.3 -57.09 -6.28 -7.01 | -48.1 | -43.69 |
| 2               | -18.8 -19.90 -69.0 -72.95 -7.79 -8.16 | -63.5 | -58.07 |
| 3               | -19.9 -20.68 -70.3 -75.83 -8.27 -8.59 | -66.9 | -60.13 |
| 4               | -20.28 -74.42 | -8.63 | -58.45 |

E. Extended Optimal Level calculations

The final values of atomic EDMs, presented in the Tables II, III, IV, V, VI, and VII were obtained with the Extended Optimal Level optimisation procedure described in section III B 1 above. At each stage of generation of virtual orbital sets, a decision had to be made with respect to the number of atomic levels included in the variational energy functional. Table III presents the contributions $d_{at,TPT}$ to the atomic EDM of $^{225}$Ra from the tensor-pseudotensor interaction $|11|$. The contributions from particular atomic states are listed in subsequent lines. The radial wave functions were optimised within the EOL procedure, with different numbers of EOL levels: 4, 6, 8, 10, or 12 levels, as indicated in the first line of the Table II. These data were obtained with experimental transition energies quoted from the the NIST Atomic Spectra Database (NIST ASD) $|20|$. An inspection of the Table IV (the last line, denoted ‘Sum All’) indicates that the $d_{at,TPT}$ expectation value becomes stable when eight or more levels are included in the Extended Optimal Level energy functional. Analogous decisions were made for all virtual orbital sets, as well as for the other two elements. The final calculations were made with varying numbers of EOL levels, between 2 levels for uncorrelated Dirac-Fock wave functions, with 6-8 levels in most correlated calculations, and up to 13 levels in one case.

F. Orbital contributions

Another interesting conclusion arises from the analysis of contributions of particular one-electron orbitals generated in the EOL optimisation procedure. The analysis presented in the Table II was made with only one virtual orbital layer, because the Extended Optimal Level optimisation procedure described in section III B 1 above becomes unstable with the increasing numbers of virtual layers and of EOL levels. However, already at this level of approximation the dominant contributions come from the singlet $7s7p\ 3P$ and triplet $7s7p\ 3P$ excited states. The states $7s8p\ 3P$ and $7s8p\ 3P$, involving $8p$ orbital,
multiconfiguration expansions designed for valence and virtual orbitals generated in our calculations were optimised with orbitals are not meaningful. All excited and virtual or-particles are not from individual one-electron orbitals which are not variationally stable, and in particular the small contributions may vary significantly, but the partial sums are more stable, and the total sum ('Sum All') is strongly stabilized by the contributions from the dominant states.

It is interesting to make a comparison of Table II with Table VI from the reference [21]. In reference [21], the contributions from $7s_{1/2}$-$7p_{1/2}$ and $7s_{1/2}$-$8p_{1/2}$ single-particle matrix elements (pairings in their language) are of comparable sizes, -324.468 and -306.133, respectively, while in our calculations the relative sizes of the contributions from $7s_{1/2}$-$8p_{1/2}$, with respect to the contribution from $7s_{1/2}$-$7p_{1/2}$ pairing, are 9% and 3% for singlet and triplet states, respectively. Also, there are differences with respect to the contributions of higher symmetry orbitals. For instance, the contribution from $d_{5/2}$ orbitals is of the order of 4% (see TABLE VII in reference [21]), while in our calculations the contributions from $d_{5/2}$ orbitals are below 1%.

It is difficult to explain these differences, but one possible explanation is due to differences in optimisation procedures and radial shapes of one-electron orbitals which resulted from these procedures, as discussed in the section III B 2. Different compositions of particular atomic states are likely consequences of differences in radial bases. The authors of the reference [21] used Gaussian basis sets, while in our calculations we use numerical orbitals defined on a grid. We do not have insight into the details of the calculations presented in the reference [21], but their Gaussians are likely to be evenly distributed over the entire configurational space.

Different theories use different methods of construction for atomic states. A consequence of these differences is the fact that comparisons of contributions from particular atomic states or from individual one-electron orbitals are not meaningful. All excited and virtual orbitals generated in our calculations were optimised with multiconfiguration expansions designed for valence and core-valence electron correlation effects, resulting in virtual orbital shapes with maximal overlaps with valence and outer core spectroscopic orbitals. Consequently, the correlation corrections to the wave function are likely to be larger for the lower states included in the Extended Optimal Level procedure. We performed comparison calculations with virtual orbitals generated with three different methods: the Extended Average Level procedure, as described in the section III B 2, with virtual orbitals generated within the screened hydrogenic approximation; and virtual orbitals from Thomas-Fermi potential. As described in the section III B 2, one-electron virtual orbitals generated with the EAL functional are optimised to minimise the sum of energies of all states. Hydrogenic and Thomas-Fermi virtual orbitals are not variationally optimized, they just form orthogonal bases. Our comparison calculations indicate, that calculations based on Extended Average Level, hydrogenic, and Thomas-Fermi virtual orbitals converge slower than Extended Optimal Level calculations, and the contributions of higher lying levels are larger, compared to EOL results.

TABLE II: $d_{5/2}^{PT}$ contribution to atomic EDM, calculated with the EOL method for 1st VOS, using different numbers of optimized levels and experimental transition energies, in units $(10^{-20} \text{C} \tau \sigma_A |e| \text{cm})$, for $^{225}$Ra. Numbers in brackets represent powers of 10.

| Levels | 4 | 6 | 8 | 10 | 12 |
|--------|---|---|---|----|----|
| $7s_{1/2} 2P$ | -5.00 | -4.46 | -4.63 | -4.59 | -4.63 |
| $7s_{1/2} 1P$ | -1.03$^{[1]}$ | -8.80 | -8.70 | -8.69 | -8.57 |
| $7s_{8/2} 2P$ | 0.39 | 0.30 | 0.33 | 0.44 | |
| $7s_{8/2} 1P$ | -1.12 | -0.96 | -1.01 | -1.24 | |
| $7s_{p+s} 1P$ | -1.58$^{[1]}$ | -1.40$^{[1]}$ | -1.40$^{[1]}$ | -1.40$^{[1]}$ | |
| $6d_{p} 2P$ | 2.53$^{[-3]}$ | -7.72$^{[-2]}$ | 2.96$^{[-2]}$ | -9.30$^{[-2]}$ | -6.91$^{[-2]}$ |
| $6d_{p} 1P$ | 1.98$^{[-1]}$ | -3.08$^{[-2]}$ | 3.55$^{[-2]}$ | 7.34$^{[-2]}$ | |
| $7s_{p+s} 1P$ | 2.00$^{[-1]}$ | -3.16$^{[-2]}$ | -8.33$^{[-2]}$ | -7.85$^{[-2]}$ | 4.25$^{[-3]}$ |
| $s_{p+s} 1P$ | -1.51$^{[-1]}$ | -1.40$^{[-1]}$ | -1.34$^{[-1]}$ | -1.41$^{[-1]}$ | -1.40$^{[-1]}$ |
| $6d_{p} 2P$ | -4.79$^{[-2]}$ | -9.44$^{[-3]}$ | -3.63$^{[-3]}$ | |
| $6d_{p} 1P$ | -1.15$^{[-1]}$ | -4.90$^{[-2]}$ | 8.36$^{[-2]}$ | |
| $7p_{8/2} 2P$ | -1.96$^{[-2]}$ | 2.20$^{[-2]}$ | |
| $7p_{8/2} 1P$ | -6.02$^{[-3]}$ | -6.31$^{[-3]}$ | |
| $6d_{p} 1P$ | -5.12$^{[-3]}$ | |
| $8s_{p} 1P$ | 1.50$^{[3]}$ | |
| $s_{p+s} 1P$ | -1.63$^{[-1]}$ | -8.41$^{[-2]}$ | -1.40$^{[-1]}$ | |
| $s_{p+s} 1P$ | -1.51$^{[-1]}$ | -1.40$^{[-1]}$ | -1.41$^{[-1]}$ | -1.41$^{[-1]}$ | |

G. Transition energies

The summation in equation (11) runs over all excited states of appropriate parity and symmetry. The contributions of higher lying levels are gradually decreasing, since they are suppressed both by the energy denominators, as well as by decreasing overlaps of one-electron radial orbitals, entering integrals in the equations: (14), (19), (21) and (23). In numerical calculations they have to be cut off at certain level of accuracy. Except where indicated otherwise, the results presented in the present paper were computed with experimental transition energies in the denominators of the matrix elements in equa-
tion [4]. The transition energies were calculated from the NIST ASD database [20] and we include levels up to $6d7p \, ^3P$ for $^{225}$Ra, $6s8p \, ^1P$ for $^{171}$Yb, and $6s9p \, ^1P$ for $^{199}$Hg. However, several levels are missing in [20], so we employed an approach, where those transition energies which were not available, were replaced by the energies calculated with one of the three different methods: (1) using theoretical energies obtained from MCDHF approach; (2) with the energy of the upper level replaced by the energy of the lowest excited state; (3) with the energy of the upper level replaced by the experimental ionisation limit. The choice was made between the above three options in case of each missing level, based on availability of a reliable theoretical energy, or alternatively on the proximity of the lowest excited state or the experimental ionisation limit. To verify this approach we performed test calculations, where all three choices were used together. Table III presents the contributions from the tensor-pseudotensor interaction to the atomic EDM of radium isotope $^{225}$Ra. Transition energies in Table III were taken from: MCDHF RSCF calculation (RSCF), MCDHF RCI calculation (RCI), experimental data (Expt), experimental ionisation limit (ExIL), experimental energy of the lowest excited level (Exp1). The MCDHF RSCF case was a self-consistent-field Extended Optimal Level calculation, with 2, 6, 8 and 6 EOL levels for DF, 1, 2, 3 and 4 VOS, respectively. The MCDHF RCI case was a configuration-interaction calculation with 100 levels included. Their differences indicate the deviation incurred when the number of EOL levels is varied. It should be noted that experimental values of the energies of the $7s7p$ levels were used in all cases in columns 'Expt', 'ExIL', and 'Exp1'. The lowest $nsnp$ levels yield the largest contributions to all EDM matrix elements in the present calculations, and their energies are available for all elements in question, therefore replacements were made only for higher lying levels. The number VOS in the first column of Table III represents the number of virtual orbital layers. These data indicate the sizes of errors, which may arise from replacing experimental transition energies with experimental ionisation limit (ExIL) or experimental energy of the lowest excited level (Exp1). As can be seen, the deviation is less than 10% in case of radium. The deviations of the data obtained with calculated transition energies are larger, due to the nature of the wavefunctions built from nonorthogonal orbital sets, as explained in the section IIIID above.

**H. Uncertainty estimates**

Estimates of uncertainty in *ab initio* calculations are far more difficult than the calculations themselves, particularly in situations, where an atomic property is evaluated, which has not been calculated before within the same approach for any other element. We can indicate possible sources of uncertainties, but their sizes are difficult to estimate. The possible sources of uncertainties are the following.

| **VOS** | **225Ra** | **199Hg** | **171Yb** |
|---------|-----------|-----------|-----------|
|         | RSCF | RCI | Expt | ExIL | Expt | ExIL | Expt | ExIL |
| 0(DF)   | -18.31 | -18.31 | -15.81 | -15.81 | -15.81 | -15.81 | -15.81 | -15.81 |
| 1       | -10.37 | -11.81 | -15.51 | -14.70 | -13.92 | -13.92 | -13.92 | -13.92 |
| 2       | -12.04 | -12.58 | -19.90 | -20.08 | -20.45 | -20.45 | -20.45 | -20.45 |
| 3       | -20.68 | -21.22 | -22.52 | -22.52 | -22.52 | -22.52 | -22.52 | -22.52 |
| 4       | -20.28 | -21.16 | -22.32 | -22.32 | -22.32 | -22.32 | -22.32 | -22.32 |
| Ref. [12](DHF) | -3.5  |          |         |         |         |         |         |         |
| Ref. [12](CI+MBPT) | -17.6 |          |         |         |         |         |         |         |
| Ref. [12](RPA) | -16.7  |          |         |         |         |         |         |         |
| Ref. [21](CPHF) | -16.585 |          |         |         |         |         |         |         |

1. **Electron correlation effects**

In extensive, large-scale calculations the relative accuracy can reach 1-5 percent, depending on the expectation value in question (see eg. [14, 15]). An estimate of uncertainty associated with the electron correlation effects can be obtained in several ways. In the limit of very large number of virtual orbital layers an estimate of uncertainty may be related to oscillations of the calculated expectation value plotted as a function of the size of the multiconfiguration expansion [15]. In the present paper an estimate of the uncertainty was based on the differences between the data obtained with the largest two multiconfiguration expansions, represented by 3 and 4 layers of virtual orbitals in Tables IV, V, VI, and VII. We abstained from extending the virtual sets beyond fourth
layer, because there are several other possible sources of uncertainty in the present calculations. An inspection of the Tables indicates that the differences between the last two lines range between 0.47% for the Schiff moment of Ra, and 15.77% for the Schiff moment of Hg (Table VI). We may assume the latter as an estimate of uncertainty associated with the neglected electron correlation effects.

**TABLE VI: Schiff moment contributions to atomic EDM, calculated with the EOL method in different virtual sets, in units \(10^{-23} C_P \langle \sigma_{\alpha} \rangle |e| \text{cm}\) for \(^{225}\text{Ra}, \(^{199}\text{Hg},\) and \(^{171}\text{Yb},\) compared with data from other methods.**

| VOS       | \(^{225}\text{Ra}\)  | \(^{199}\text{Hg}\)  | \(^{171}\text{Yb}\) |
|-----------|----------------------|----------------------|----------------------|
| 0(DF)     | -57.87 -21.49 -10.84 |                      |                      |
| 1         | -57.09 -17.16 -6.31  |                      |                      |
| 2         | -72.95 -19.94 -12.20 |                      |                      |
| 3         | -75.83 -21.53 -13.26 |                      |                      |
| 4         | -74.42 -19.45 -13.94 |                      |                      |
| Ref. [12](DHF) | -13.0 -8.7 -2.4 |                      |                      |
| Ref. [12](CI+MBPT) | -64.2 -18.4 -12.4 |                      |                      |
| Ref. [12](RPA) | -61.0 -20.7 -10.9 |                      |                      |

2. Wave function relaxation

As explained in the section III D, the effects of wave function relaxation were partially accounted for in the present calculations, by using non-orthogonal orbital sets for the opposite parities. An inspection of Table II indicates that the uncertainty which may arise from wave function relaxation effects is of the order of 10%, although this estimate is based on relaxing only the ASF wave function of the ground state on one hand, and the ASF wave functions of all excited states taken together, on the other hand. A more general, albeit far more expensive approach would be to generate separate atomic state functions for the ground state, as well as for each excited state, implying non-orthogonality between all ASFs of both parities.

**TABLE VII: Contributions of electron EDM interaction with magnetic field of nucleus, to atomic EDM are calculated with the EOL method in different virtual sets, in units \((d_e \times 10^{-4})\), for \(^{225}\text{Ra}, \(^{199}\text{Hg},\) and \(^{171}\text{Yb},\) compared with data from other methods.**

| VOS       | \(^{225}\text{Ra}\)  | \(^{199}\text{Hg}\)  | \(^{171}\text{Yb}\) |
|-----------|----------------------|----------------------|----------------------|
| 0(DF)     | -46.07 13.41 5.37    |                      |                      |
| 1         | -43.69 9.58 3.17     |                      |                      |
| 2         | -58.07 12.22 5.72    |                      |                      |
| 3         | -60.13 12.80 6.09    |                      |                      |
| 4         | -58.45 11.45 6.44    |                      |                      |
| Ref. [27](DHF) | -11 4.9 1.0 |                      |                      |
| Ref. [27](DHF) | 5.1 |                      |                      |
| Ref. [12](CI+MBPT) | -55.7 10.7 5.45 |                      |                      |
| Ref. [12](RPA) | -53.3 12.3 5.05 |                      |                      |
| Ref. [27](RPA) | 13 |                      |                      |

3. Energy denominators

As discussed in the section III C the summation in equation (4) runs over all excited states of appropriate parity and symmetry. The NIST Atomic Spectra Database [20] is of course finite, therefore several levels with unknown energies had to be included in the present calculations. The uncertainty which may arise due to replacements described in the section III C should not exceed 10% in case of radium atom, and we expect the same order of magnitude in case of ytterbium and mercury.

**TABLE VI: Schiff moment contributions to atomic EDM, calculated with the EOL method in different virtual sets, in units \(10^{-17} [S/(|e| \text{fm}^3)] |e| \text{cm}\) for \(^{225}\text{Ra}, \(^{199}\text{Hg},\) and \(^{171}\text{Yb},\) compared with data from other methods.**

| VOS       | \(^{225}\text{Ra}\)  | \(^{199}\text{Hg}\)  | \(^{171}\text{Yb}\) |
|-----------|----------------------|----------------------|----------------------|
| 0(DF)     | -6.32 -2.46 -1.54    |                      |                      |
| 1         | -7.01 -2.45 -0.88    |                      |                      |
| 2         | -8.16 -2.23 -1.83    |                      |                      |
| 3         | -8.59 -2.98 -2.05    |                      |                      |
| 4         | -8.63 -2.51 -2.15    |                      |                      |
| Ref. [12](DHF) | -1.8 -1.2 -0.42 |                      |                      |
| Ref. [12](CI+MBPT) | -8.84 -2.63 -2.12 |                      |                      |
| Ref. [12](RPA) | -8.27 -2.99 -1.95 |                      |                      |
| Ref. [24](RPA) | -8.5 -2.8 |                      |                      |
| Ref. [24](RPA) | -1.9 |                      |                      |
| Ref. [25](CCSD) | -5.07 |                      |                      |

4. Systematic errors

The possible sources of systematic errors include: omission of double, triple, and higher order substitutions; the effects of Breit interaction; and QED effects. The calculations of EDMs involve radial integrals of atomic one-electron orbitals, but all these integrals include factors in the integrands, which effectively cut off the integrals outside the nucleus, so the contribution to the integral comes from within or in the vicinity of the nucleus. Therefore an estimate of systematic errors can be made by comparing the EDM calculations with hyperfine structure calculations, where integrand in the form \(r^{-2}\) appears in a one-electron integral, which in turn renders the dominant contribution from the first half of the radial orbital oscillation, i.e. near the nucleus. In certain cases in the hyperfine structure calculations the effects of double and triple substitutions can be quite sizeable, of the order of 10-20%, but they often partly cancel and the net deviation is often smaller than 10% [28, 29]. The effects of quadruple and higher order substitutions are negligible. The effects of Breit and QED are usually of the order of 1-2 percent or less for neutral systems.
IV. FINAL RESULTS, DISCUSSION, AND OUTLOOK

A. Summary

Atomic EDMs arising from \((P, T)\)-odd tensor-pseudotensor and pseudoscalar-scalar electron-nucleon interactions, nuclear Schiff moment, and interaction of electron electric dipole moment with nuclear magnetic field, are presented in Tables [V], [VI] and [VII] for \(^{225}\)Ra, \(^{199}\)Hg, and \(^{171}\)Yb. The matrix elements and atomic EDMs were calculated using recently developed programs in the framework of the GRASP2K code [1]. One of the objectives of the present calculations was to test these programs. Therefore the results are compared with the data obtained by other methods: random phase approximations (RPA), many-body perturbation theory and configuration interaction technique (CI+MBPT), coupled-cluster single-double (CCSD), and coupled-perturbed Hartree-Fock (CPHF) theory. These methods are usually more accurate in calculations of properties of closed-shell atoms. An inspection of the Tables indicates that the differences between our results and the data obtained with the RPA methods [12, 22–25, 27] range between 1.5\% for the Schiff moment of Ra (Table [VI]), and 22.1\% for the tensor-pseudotensor of Hg (Table [V]), all of them within the error bounds estimated in the section III H 5 above.

Despite the reasonable agreement at the level of the correlated calculations, very large differences should be noted at the uncorrelated levels, DF (Dirac-Fock) in our calculations, and DHF (Dirac-Hartree-Fock) in references [12] and [23]. We used the different symbols to visually differentiate the results obtained with different numerical codes, but the DF and DHF approximations are formally identical within the Dirac-Fock theory, and they should yield similar values, within numerical accuracies of the Dirac-Fock codes. A possible explanation of these large differences may be the fact that in our (DF) calculations the summation in equation (1) runs over only the two lowest excited states, singlet \(nsnp \: 1P\) and triplet \(nsnp \: 3P\), which are generated at the Dirac-Fock level of the GRASP2K code [1]. On the other hand, in references [12] and [27] the summation was probably carried over all excited states, which can be constructed from a suitable set of virtual orbitals. Otherwise we do not have an explanation.

Large differences at the level of the correlated calculations should be noted between our results and the data obtained with the CPHF theory [21]. The differences are: 18\% for TPT of Ra and 39\% for TPT of Hg (see Table [V]). The largest disagreement appears to be between the result of the present calculations and the value obtained with the CCSD theory [26] for the Schiff moment of Hg (see Table [VI]). The difference amounts to 102\%. It is difficult to explain some of the abovementioned differences. They may be due to different orbital shapes, orbital contributions, and relaxation effects, discussed in the sections III F and III D, respectively.

Another objective of the present calculations was to test the methods of wave function generation, as described in more detail in the section III A, and of multiconfiguration expansions designed to account for valence and core-valence electron correlation effects. A reasonably good agreement of our results with the data obtained within the RPA and CI+MBPT methods [12, 22–25, 27] seems to indicate that the multiconfigurational model employed in the present calculations accounts for the bulk of the electron correlation effects. With adequate computer resources, these calculations may be extended in the future and include also core-core effects. Based on the experiences with other atomic properties, as well as on the present EDM calculations, we expect that the accuracy of the EDM calculations may be improved by a factor of ten, with respect to the current relative root-mean-square deviation of the order of 25\%.

B. Outlook

Several refinements are possible with respect to the methods used in the present paper. To account more accurately for the electron relaxation, separate wave functions for the leading contributors to EDM may be generated. A more general, albeit far more expensive approach would be to generate separate ASFs for the ground state, as well as for each excited state, relaxing orthogonality of the orbital sets between all ASFs of both parities.

The expectation values \(d_{\alpha\beta}^{\text{int}}\) were calculated with theoretical (if reliable), and experimental (if available) transition energies, as explained in the section III C. In fully correlated calculations theoretical transition energies would have to be evaluated with all single and unrestricted double substitutions. They would be computationally much more expensive than those presented in the present paper, but possible with the currently available massively-parallel computers. Electron correlation effects can also be accounted for using the partitioned correlation function interaction (PCFI) method [30], that allows contributions from single and unrestricted double substitutions deep down in the atomic core to be summed up in a very efficient way. In the near future we will be able to perform fully \(ab\) \(\text{initio}\) calculations for atoms with arbitrary shell structures. We are currently testing the latest version of the GRASP package [1], with angular programs providing full support for arbitrary numbers of electrons in open \(spdf\) shells.

5. Error budget

Based on the above estimates, the relative root-mean-square deviation of the present calculations yields \(\sigma = 25\%\).
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[1] P. Jönsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, and I. Grant, Comput. Phys. Commun. 184, 2197 (2013).
[2] I. B. Khriplovich and S. K. Lamoreaux, CP Violation Without Strangeness (Springer, Berlin, 1997).
[3] W. C. Griffith, M. D. Swallows, T. H. Loftus, M. V. Romalis, B. R. Heckel, and E. N. Fortson, Phys. Rev. Lett. 102, 101601 (2009).
[4] C. A. Baker, D. D. Doyle, P. Geltenbort, K. Green, M. G. D. van der Grinten, P. G. Harris, P. Iaydjiev, S. N. Ivanov, D. J. R. May, J. M. Pendlebury, et al., Phys. Rev. Lett. 97, 131801 (2006).
[5] B. C. Regan, E. D. Commins, C. J. Schmidt, and D. DeMille, Phys. Rev. Lett. 88, 071805 (2002).
[6] J. J. Hudson, D. M. Kara, I. J. Smallman, B. E. Sauer, M. R. Tarbutt, and E. A. Hinds, Nature 473, 493 (2011).
[7] B. L. Roberts and W. J. Marciano, eds., Advanced Series on Directions in High Energy Physics, vol. 20 (World Scientific, Singapore, 2009).
[8] V. A. Dzuba and V. V. Flambaum (2012), 1209.2200v1.
[9] J. Bieroń, G. Gaigalas, E. Gaidamauskas, P. Indelicato, S. Fritzsche, and P. Jönsson, Phys. Rev. A 80, 012513 (2009).
[10] I. P. Grant, Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation (Springer, New York, 2007).
[11] G. Gaigalas, Z. Rudzikas, and C. Froese Fischer, J. Phys. B 30, 3747 (1997).
[12] V. A. Dzuba, V. V. Flambaum, and S. G. Porseev, Phys. Rev. A 80, 032120 (2009).
[13] K. G. Dyall, I. P. Grant, C. T. Johnson, F. A. Parpia, and E. P. Plummer, Comput. Phys. Commun. 55, 425 (1989).
[14] J. Bieroń and P. Pyykö, Phys. Rev. A 71, 032502 (2005).
[15] J. Bieroń, C. Froese Fischer, P. Indelicato, P. Jönsson, and P. Pyykö, Phys. Rev. A 79, 052502 (2009).
[16] J. Bieroń, C. Froese Fischer, S. Fritzsche, and K. Pachucki, J. Phys. B 37, L305 (2004).
[17] B. M. Roberts, V. A. Dzuba, and V. V. Flambaum (2013), 1309.3371v1.
[18] P. A. Malmqvist, Int. J. Quantum Chem. 30, 479 (1986).
[19] J. Olsen, M. R. Godefroid, P. Jönsson, P. A. Malmqvist, and C. Froese Fischer, Phys. Rev. E 52, 4499 (1995).
[20] URL http://www.nist.gov/pml/data/asd.cfm
[21] K. V. P. Latha and P. R. Amjith, Phys. Rev. A 87, 022509 (2013).
[22] A.-M. Mårtensson-Pendrill, Phys. Rev. Lett. 54, 1153 (1985).
[23] K. V. P. Latha, D. Angom, R. J. Chaudhuri, B. P. Das, and D. Mukherjee, J. Phys. B 41, 035005 (2008).
[24] V. A. Dzuba, V. V. Flambaum, J. S. M. Ginges, and M. G. Kozlov, Phys. Rev. A 66, 012111 (2002).
[25] V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. A 76, 034501 (2007).
[26] K. V. P. Latha, D. Angom, B. P. Das, and D. Mukherjee, Phys. Rev. Lett. 103, 083001 (2009).
[27] A.-M. Mårtensson-Pendrill and P. Öster, Phys. Scr. 36, 444 (1987).
[28] B. Engels, Theor. Chim. Acta 86, 429 (1993).
[29] J. Bieroń, C. Froese Fischer, P. Jönsson, and P. Pyykö, J. Phys. B 41, 115002 (2008).
[30] S. Verdebout, P. Rynkun, P. Jönsson, G. Gaigalas, C. Froese Fischer, and M. Godefroid, J. Phys. B 46, 085003 (2013).