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All-order calculations of the spectra of Ba II, Ra II, Fr I, and superheavy elements E119 I and E120 II

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A technique based on summation of dominating classes of correlation diagrams to all orders in Coulomb interaction is used to calculate the energies of the lowest s,p, and d states of Ba II, Ra II, Fr I, E119 I, and E120 II. Breit and quantum electrodynamic corrections are also included. Comparison with experiment for Ba II, Ra II, and Fr I demonstrates that the accuracy of the calculations is on the level of 0.1%. The technique has been applied to predict the spectra of superheavy elements E119 and E120$^+$. The role of the ladder diagrams [Dzuba, Phys. Rev. A **78**, 042502 (2008)], which is the most recent addition to the method, has been emphasized. Their inclusion significantly improves the accuracy of the calculations and expands the applicability of the method.

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I. INTRODUCTION

Accurate atomic calculations are very important for a number of applications, such as the search for new physics beyond the standard model in the measurements of the parity and time-invariance violation in atoms [1,2], the search for space-time variation of fundamental constants [3], prediction of the properties of atoms and ions where experimental data are poor or absent, etc. The latter include in particular highly charge ions [4] and superheavy elements ($Z > 100$) [5,6].

Atoms with one valence electron above closed shells play a special role in these studies. Their relatively simple electron structure allows high accuracy of the calculations, leading to a very accurate interpretation of experimental data. For example, the current best low-energy test of the standard model is based on the measurements of parity nonconservation (PNC) in cesium [7], which has one valence electron above closed shells of a Xe-like core. Interpretation of the measurements is based on accurate calculations of Ref. [8]. Further progress for the PNC measurements is considered for atoms and ions which have an electron structure similar to that of cesium. This includes Rb [9], Ba$^+$ [10], Ra$^+$ [11], Fr [12], and Fr-like ions [13]. Accurate predictions of the spectra and other properties of the superheavy elements were done for E119, and E120$^+$ [14–18], which are also analogous to cesium.

The most popular method currently used for accurate calculations for atoms with one valence electron is the coupled-cluster (CC) method. Its accuracy depends on the number of terms included in the expansion of the wave function. Its simplest version, which includes only terms with single and double excitations (SD) from the reference ground-state configuration, gives good accuracy for only a limited number of systems. In particular, the accuracy is poor for cesium, and missing third-order diagrams need to be included for better accuracy [19]. The accuracy is significantly better if valence triple excitations are also included (the CCSDvT approximation) [20]. However, the method becomes very demanding for computer power.

An alternative approach was developed in our group about 25 years ago. It is based on summations of selected classes of higher-order correlation diagrams to all orders in Coulomb interactions [21]. Later in the paper we will call it the correlation potential method (CPM) for convenience. The following classes of correlations were included in CPM in all orders: (a) screening of Coulomb interaction of the valence electron with electrons in the core by other core electrons, (b) interaction between an electron excited from the atomic core with the hole in the core caused by this excitation, and (c) iterations of the correlation operator $\hat{\Sigma}$. This turned out to be a very powerful method which gives a fraction of a percent accuracy for the energies of s and p states of alkali-metal atoms. The computer power needed for the calculations is small even compared to the simple SD approximation. On the other hand, accuracy for d states and accuracy for atoms other than alkali metals was not high. For example, the accuracy for Ba$^+$ is almost the same as for Cs. This is contrary to what is expected since the relative values of the correlation corrections are smaller for Ba$^+$ than for Cs due to a two times stronger central potential. The reason for lower accuracy was explained in Ref. [22] for the cases of cesium and thallium. The high accuracy for s and p states of alkali-metal atoms and lower accuracy for other atomic systems is related to a particular choice of higher-order diagrams included in the CPM method. The three classes of higher-order diagrams listed above dominate in systems where the valence electron is a large distance from the core. When the valence electron is closer to the core, another class of higher-order diagrams becomes important. These diagrams describe the residual Coulomb interaction of the valence electron with the core. When the valence electron is close to the core, this interaction becomes strong and needs to be included in all orders. In the CPM method this interaction is included in the second order only. This limits the accuracy of the calculations for systems where the external electron is close to the core. The most pronounced example is probably the thallium atom, where the external $6p$ electron is very close to the $6s$ electrons and strongly interacts with them [22].

A method to include the core-valence residual interaction in all orders was developed in Ref. [22]. It is based on iterations of equations similar to the CCSD equations. The terms arising from the iterations of theses equations were described by diagrams which are called *ladder diagrams*. When the contribution of the ladder diagrams was added to the result of the CPM calculations, it led to significant improvement of the accuracy of the calculations for the s, p, and d states of Cs and Tl.

In present paper we further extend the application of the method by performing calculations for Ba^+ and Ra^+ ions and demonstrating that inclusion of ladder diagrams leads to very accurate results. Then we apply the method to calculate the spectra of superheavy elements E119 and $\mathrm{E120}^+$. Calculations for francium are also included as another test of the method, which helps to estimate the accuracy for the E119 superheavy element. Breit and QED corrections are included for higher accuracy. The spectra of E119 and $\mathrm{E120}^+$ were considered before [15,16]. However, the present paper presents more complete and accurate results.

II. METHOD OF CALCULATIONS

Accurate calculations for heavy and superheavy many-electron atoms need accurate treatment of correlations and relativistic effects. We use the all-order correlation potential method [21] supplemented by inclusion of ladder diagrams [22] to include dominating correlation effects to all orders in residual Coulomb interaction. For accurate treatment of relativistic effects we start the calculations with the relativistic Hartree-Fock (RHF) method based on solving Dirac-like equations, and then we include Breit interaction and quantum electrodynamic (QED) corrections.

A. Correlations

Calculations start from the RHF in the V^{N-1} approximation. States of the valence electron are calculated with the use of the correlation potential $\hat{\Sigma}$:

$$(\hat{H}_0 + \hat{\Sigma} - \epsilon_v)\psi_v = 0. \tag{1}$$

Here $\hat{H}_0$ is the RHF Hamiltonian, and ψ_v and ϵ_v are the wave function and removal energy of the valence electron. The correlation potential $\hat{\Sigma}$ is defined in such a way that its average value over the wave function of the valence electron in state v is the correlation correction to the energy of this state:

$$\delta\epsilon_v = \int \psi_v(r_1)\Sigma(r_1,r_2)\psi_v(r_2)dr_1dr_2. \tag{2}$$

$\hat{\Sigma}$ is a nonlocal operator similar to the Hartree-Fock exchange potential. Many-body perturbation theory expansion for $\hat{\Sigma}$ starts from second order. The second-order correlation operator $\hat{\Sigma}^{(2)}$ has been described in our previous works [22,23]. For most atomic systems inclusion of just second-order $\hat{\Sigma}$ leads to significant improvements of the accuracy of the calculations. Further improvement is achieved when higher-order correlations are also included. Beyond second order we include four dominating classes of higher-order correlations: (a) screening of Coulomb interaction, (b) hole-particle interaction, (c) iterations of $\hat{\Sigma}$, and (d) ladder diagrams. All these higher-order correlations are included in all orders of residual Coulomb interaction.

Two of these classes of higher-order correlations are included in the calculations of $\hat{\Sigma}$ [21], the screening of Coulomb interaction between valence and core electrons by other core electrons and hole-particle interaction between a hole left in the core by electron excitation and the excited electron. The third chain of all-order diagrams, the iteration of the correlation potential, is included by iterating Eq. (1). Note that the single-electron wave functions for the states of the valence electron found by solving Eq. (1) are often called Brueckner orbitals (BO).

Another chain of all-order diagrams describes the residual Coulomb interaction of the external electron with the core. It is included by solving coupled-cluster-like equations for ladder diagrams [22]. The equations are obtained by taking the SD approximation for the CC method and removing terms which otherwise would lead to double counting of the effects which are already included in the correlation potential $\hat{\Sigma}$. We stress once more that the most important all-order effect, the screening of Coulomb interaction, is better treated in the calculation of the all-order correlation potential $\hat{\Sigma}$ than in solving the CC equations. This is because of the use of the relativistic Feynman diagram technique while calculating $\hat{\Sigma}$. The relativistic technique includes all possible time ordering of the hole-particle loops, which, in terms of the CC expansion, means inclusion of selected triple and higher excitations.

The equations for ladder diagrams can be written as two sets of equations [22]. The first is for the atomic core:

$$\begin{aligned}(\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n)\rho_{mnab} \\ = g_{mnab} + \sum_{rs} g_{mnrs}\rho_{rsab} + \sum_{rc}(g_{cnbr}\rho_{mrca} + g_{cmar}\rho_{nrcb}).\end{aligned} \tag{3}$$

Another is for a specific state v of an external electron:

$$\begin{aligned}(\epsilon_v + \epsilon_b - \epsilon_m - \epsilon_n)\rho_{mnvb} \\ = g_{mnvb} + \sum_{rs} g_{mnrs}\rho_{rsvb} + \sum_{rc}(g_{cnbr}\rho_{mrcv} + g_{cmvr}\rho_{nrcb}).\end{aligned} \tag{4}$$

Here parameters g are Coulomb integrals,

$$g_{mnab} = \iint \psi_m^\dagger(r_1)\psi_n^\dagger(r_2)e^2/r_{12}\psi_a(r_1)\psi_b(r_2)d\mathbf{r}_1d\mathbf{r}_2,$$

variables ρ are the coefficients representing the expansion of the atomic wave function over double excitations from the zero-order Hartree-Fock reference wave function, and parameters ϵ are the single-electron Hartree-Fock energies. Coefficients ρ are found by solving the equations iteratively, starting from

$$\rho_{mnij} = \frac{g_{mnij}}{\epsilon_i + \epsilon_j - \epsilon_m - \epsilon_n}.$$

Indices a,b,c numerate states in the atomic core, indices m,n,r,s numerate states above the core, and indices i,j numerate any states.

The equations for the core (3) do not depend on the valence state v and are iterated first. The convergence is controlled by the correction to the core energy,

$$\delta E_C = \frac{1}{2}\sum_{abmn} g_{abmn}\tilde{\rho}_{mnab}, \tag{5}$$

where

$$\tilde{\rho}_{mnab} = \rho_{mnab} - \rho_{mnba}.$$

When iterations for the core are finished, Eq. (4) is iterated for as many valence states v as needed.

The correction to the energy of the valence state v arising from the iterations of Eqs. (3) and (4) is given by

$$\delta\epsilon_v = \sum_{mab} g_{abvm}\tilde{\rho}_{mvab} + \sum_{mnb} g_{vbmn}\tilde{\rho}_{mnvb}. \tag{6}$$

Since Brueckner energy ϵ_v, in Eq. (1), and the correction $\delta\epsilon_v$, in Eq. (6), both include the second-order correlation correction, it is convenient to define the correction associated with the ladder diagrams as a difference:

$$\delta\epsilon_v^{(l)} = \delta\epsilon_v - \langle v|\hat{\Sigma}^{(2)}|v\rangle. \tag{7}$$

Here $\hat{\Sigma}^{(2)}$ is the second-order correlation potential.

B. Breit interaction

We treat Breit interaction in the zero-energy transfer approximation. The Breit Hamiltonian includes magnetic interaction between moving electrons and retardation:

$$\hat{H}^B = -\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2 + (\boldsymbol{\alpha}_1\cdot\mathbf{n})(\boldsymbol{\alpha}_2\cdot\mathbf{n})}{2r}. \tag{8}$$

Here $\mathbf{r} = \mathbf{n}r$, r is the distance between electrons, and $\boldsymbol{\alpha}$ is the Dirac matrix.

Similar to the way the Coulomb interaction is used to form the self-consistent Coulomb potential, the Breit interaction is used to form the self-consistent Breit potential. In other words, Breit interaction is included in the self-consistent Hartree-Fock procedure. Thus the important relaxation effect is included. The resulting interelectron potential in (1) consists of two terms,

$$\hat{V} = V^C + V^B, \tag{9}$$

where V^C is the Coulomb potential and V^B is the Breit potential. Coulomb interaction in the second-order correlation potential $\hat{\Sigma}^{(2)}$ is also modified to include the Breit operator (8). The Breit correction to the energy of the external electron is found by comparing the second-order Brueckner energies [Eq. (1)] calculated with and without the Breit interaction.

C. QED corrections

We use the radiative potential method developed in Ref. [24] to include quantum radiative corrections. This potential has the form

$$V_{\mathrm{rad}}(r) = V_U(r) + V_g(r) + V_e(r), \tag{10}$$

where V_U is the Uehling potential, V_g is the potential arising from the magnetic form factor, and V_e is the potential arising from the electric form factor. The V_U and V_e terms can be considered additions to the nuclear potential, while the inclusion of V_g leads to some modification of the Dirac equation (see Ref. [24] for details). As for the case of the Breit interaction, the QED corrections to the energies of the

TABLE I. Removal energies (cm^{-1}) of the lowest s, p, and d states of Ba$^+$, Ra$^+$, E120$^+$, Fr, and E119 in different approximations together with ladder diagram, Breit, and QED corrections and experimental data. $\Delta = 100(E_{\mathrm{final}} - E_{\mathrm{expt}})/E_{\mathrm{expt}}$.

Ion/atom	State	RHF	$\Sigma^{(2)}$	Σ^{∞}	Ladder	Breit	QED	Final	Δ (%)	Expt.[a]
Ba$^+$	$6s_{1/2}$	75339	82379	80780	−156	−4	−45	80575	−0.14	80687
	$6p_{1/2}$	57265	61216	60571	−128	−27	3	60419	−0.01	60425
	$6p_{3/2}$	55873	59424	58847	−118	−7	0	58722	−0.02	58735
	$5d_{3/2}$	68138	77444	76377	−763	58	22	75694	−0.16	75813
	$5d_{5/2}$	67664	76500	75536	−765	84	18	74873	−0.19	75012
Ra$^+$	$7s_{1/2}$	75898	83864	82035	−219	−12	−90	81714	0.16	81842
	$7p_{1/2}$	56878	61432	60744	−182	−51	0	60511	0.03	60491
	$7p_{3/2}$	52905	56278	55776	−140	−11	−3	55625	−0.01	55633
	$6d_{3/2}$	62355	71364	70294	−620	72	42	69788	0.04	69758
	$6d_{5/2}$	61592	69313	68563	−643	92	33	68045	−0.08	68099
E120$^+$	$8s_{1/2}$	83262	92195	90241	−518	−68	−132	89523		
	$8p_{1/2}$	60040	66792	65448	−378	−125	−16	64929		
	$8p_{3/2}$	49290	52744	52006	−178	−12	−11	51805		
	$7d_{3/2}$	56610	66765	64815	−590	68	61	64354		
	$7d_{5/2}$	56408	63526	62678	−623	82	46	62183		
Fr	$7s_{1/2}$	28767	34136	32924	−136	5	−47	32746	−0.3	32849
	$7p_{1/2}$	18855	21004	20707	−76	−14	0	20617	0	20612
	$7p_{3/2}$	17655	19179	18971	−57	0	−1	18913	−0.06	18925
	$6d_{3/2}$	13825	17190	16724	−139	34	11	16630	0.07	16619
	$6d_{5/2}$	13924	16849	16512	−153	37	9	16405	−0.09	16419
E119	$8s_{1/2}$	33608	40489	39040	−403	−24	−77	38536		
	$8p_{1/2}$	20130	23905	23473	−184	−47	−6	23236		
	$8p_{3/2}$	16672	18335	18114	−74	−1	−3	18036		
	$7d_{3/2}$	13477	17495	16807	−149	34	19	16711		
	$7d_{5/2}$	13827	16899	16567	−181	34	15	16435		

[a] Ba$^+$ and Ra$^+$ data are from Ref. [25]; Fr data are from Ref. [26].

external electron are found by solving Eq. (1) with and without the radiative potential.

III. RESULTS AND DISCUSSION

The results of the calculations of the energies of the lowest s, p, and d states of Ba$^+$, Ra$^+$, E120$^+$, Fr, and E119 in different approximations are presented in Table I. The RHF column presents Hartree-Fock energies obtained by solving Eq. (1) without $\hat{\Sigma}$, and the $\hat{\Sigma}^{(2)}$ column presents Brueckner energies obtained by solving Eq. (1) with the second-order correlation potential $\hat{\Sigma}^{(2)}$. Note that since these energies are obtained by solving the Eq. (1) rather than by calculating the average value of the correlation potential $\hat{\Sigma}^{(2)}$ as in (2), they already include one all-order effect, the iterations of $\hat{\Sigma}^{(2)}$. The $\hat{\Sigma}^{\infty}$ column presents Brueckner energies obtained by solving Eq. (1) with all-order $\hat{\Sigma}^{\infty}$. The difference between this and previous columns illustrates the importance of higher-order correlation effects in $\hat{\Sigma}$, screening the Coulomb interaction, and hole-particle interaction.

The ladder column presents contributions from ladder diagrams given by (7). We present these contributions separately for the convenience of the discussion. We would like to emphasize the role of ladder diagrams since it is the latest addition to our all-order technique, which has been tested before only for cesium and thallium atoms [22]. If ladder diagrams are not included, the all-order correlation potential method developed in Ref. [21] gives good accuracy for s and p states of alkali-metal atoms and their isoelectronic sequences. As demonstrated in Ref. [22], adding ladder diagrams widens the range of atomic systems for which the technique gives good accuracy. The ladder diagram contributions do not affect the s and p states of alkali-metal atoms much while significantly improving the accuracy for d states. They also significantly improve the accuracy for such complicated systems as the thallium atom [22]. As one can see from Table I, ladder diagrams are important for all systems considered in the present paper, leading to significant improvements of the results. Breit and QED corrections are relatively small. However, adding them generally leads to better agreement with experiment. The data for Breit and QED corrections for Fr and E119 are in good agreement with recent calculations by Thierfelder and Schwerdtfeger [27]. A detailed discussion of the QED corrections and a comparison with other calculations

TABLE II. Removal energies (cm^{-1}) of Cs, Fr, E119, and E120$^+$ and comparison with experiment [25,26], our earlier calculations [16,22], and the CCSD calculations of Eliav *et al.* [15].

Atom	State	This work[a]	CCSD [15]	Expt.[b]	Atom/ion	State	This work	Ref. [16]	CCSD [15]
Cs	$6s_{1/2}$	31384	31485	31407	E119	$8s_{1/2}$	38536	38852	38577
	$6p_{1/2}$	20185	20233	20229		$8p_{1/2}$	23236	23272	22979
	$6p_{3/2}$	19632	19681	19675		$8p_{3/2}$	18036	18053	18007
	$5d_{3/2}$	16932	19909	16908		$7d_{3/2}$	16711		16505
	$5d_{5/2}$	16849	16809	16810		$7d_{5/2}$	16435		16297
	$7s_{1/2}$		12886	12872		$9s_{1/2}$	14061	14079	14050
	$7p_{1/2}$		9642	9641		$9p_{1/2}$	10439	10415	10365
	$7p_{3/2}$		9462	9459		$9p_{3/2}$	8882	8866	8855
	$6d_{3/2}$		8815	8818		$8d_{3/2}$	8513		8455
	$6d_{5/2}$		8772	8775		$8d_{5/2}$	8399		8338
	$8s_{1/2}$		7082	7090		$10s_{1/2}$	7521	7536	7519
	$8p_{1/2}$		5689	5698		$10p_{1/2}$	6024	6018	5997
	$8p_{3/2}$		5606	5615		$10p_{3/2}$	5334	5328	5320
	$7d_{3/2}$		5354	5359		$9d_{3/2}$	5177		5154
	$7d_{5/2}$		5333	5338		$9d_{5/2}$	5118		5092
Fr	$7s_{1/2}$	32746	32930	32849	E120$^+$	$8s_{1/2}$	89523	89931	
	$7p_{1/2}$	20617	20597	20612		$8p_{1/2}$	64929	65080	
	$7p_{3/2}$	18913	18918	18925		$8p_{3/2}$	51805	51874	
	$6d_{3/2}$	16630	16527	16619		$7d_{3/2}$	64354		
	$6d_{5/2}$	16405	16339	16419		$7d_{5/2}$	62183		
	$8s_{1/2}$	13075	13131	13116		$9s_{1/2}$	40085	40110	
	$8p_{1/2}$	9730	9732	9736		$9p_{1/2}$	32618	32604	
	$8p_{3/2}$	9184	9190	9191		$9p_{3/2}$	27978	27951	
	$7d_{3/2}$	8584	8597	8604		$8d_{3/2}$	31489		
	$7d_{5/2}$	8490	8507	8516		$8d_{5/2}$	30727		
	$9s_{1/2}$	7160	7184	7178		$10s_{1/2}$	23307	23357	
	$9p_{1/2}$	5726	5738			$10p_{1/2}$	19887	19926	
	$9p_{3/2}$	5477	5493			$10p_{3/2}$	17664	17678	
	$8d_{3/2}$	5209	5243	5248		$9d_{3/2}$	19293		
	$8d_{5/2}$	5162	5198	5203		$9d_{5/2}$	18921		

[a] Results for Cs are taken from Ref. [22].

[b] Cs data are from Ref. [25]; Fr data are from Ref. [26].

are presented in our previous work [16]. Our final results for Ba^+, Ra^+, and Fr (see Table I) differ from the experimental data by a small fraction of a percent only.

Final results for Fr and superheavy elements E119 and $\mathrm{E}120^+$ are presented in Table II together with the results of our previous calculations for Cs [22], E119, and $\mathrm{E}120^+$ [16]; the results of the coupled-cluster calculations by Eliav *et al.* [15] for Cs, Fr, and E119; and experimental data for Cs and Fr. Judging by the data in Table II, we believe that the accuracy of the calculated energies is at the level of 0.2%.

There are two important differences between the present calculations and those of Ref. [16]. Ladder diagrams were not included in [16]. On the other hand, the *ab initio* results for superheavy elements were corrected in [16] by extrapolating the theoretical error from lighter elements. This extrapolation assumes a similar electron structure of the elements. In contrast, the present calculations are pure *ab initio* calculations with no fitting or extrapolating. The calculation of the ladder diagrams reveals some small differences in the electron structure of superheavy elements and their lighter analogs. Indeed, the contribution of the ladder diagrams tends to be larger for superheavy elements. This is consistent with larger removal energies. Larger removal energies mean that the valence electron is closer to the core; therefore its residual Coulomb interaction with the core described by ladder diagrams should be larger as well. Note that the difference between our present and previous [16] results is sometimes larger than 0.2% (the accuracy of the present calculations). This is particularly true for the ground-state energies. We believe that the accuracy of the present calculations is better than in Ref. [16] since they are pure *ab initio* calculations with no fitting and no extrapolation and they do take into account small differences in the electron structure between superheavy elements and their lighter analogs.

Table II shows very good agreement between the present results and the results of the coupled-cluster calculations of Ref. [15]. The agreement is better than with our previous calculation [16]. In the end, both methods, the method of the present work and the CCSD method used in Ref. [15], demonstrate very similar levels of accuracy.

Table II also presents the energies of the d states of E119 and $\mathrm{E}120^+$. Correlations for d states are usually larger than for s and p states, and the accuracy of the calculations is lower. That was part of the reason why these states were not considered before. However, as is evident from the data in Table I, the inclusion of ladder diagrams leads to practically the same accuracy for d states as for s and p states. Therefore we include the results for the energies of the d states of superheavy elements in Table II.

IV. CONCLUSION

The results of this paper are twofold. First, we demonstrate that supplementing the previously developed all-order correlation potential method with ladder diagrams leads to a significant improvement in the accuracy of calculations not only for alkali atoms but also for their isoelectronic ions. Second, we apply the developed technique to perform very accurate calculations of the spectra of superheavy elements E119 and $\mathrm{E}120^+$.

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[1] J. S. M. Ginges and V. V. Flambaum, Phys. Rep. **397**, 63 (2004).

[2] V. A. Dzuba and V. V. Flambaum, Int. J. Mod. Phys. E **21**, 1230010 (2012).

[3] V. A. Dzuba and V. V. Flambaum, Can. J. Phys. **87**, 15 (2009); **87**, 25 (2009).

[4] J. C. Berengut, V. A. Dzuba, V. V. Flambaum, and A. Ong, Phys. Rev. A **86**, 022517 (2012).

[5] V. Pershina, Radiochim. Acta **99**, 459 (2011).

[6] A. Türler and V. Pershina, Chem. Rev. **113**, 1237 (2013).

[7] C. S. Wood, S. C. Bennett, D. Cho, B. P. Masterson, J. L. Roberst, C. E. Tanner, and C. E. Wieman, Science **275**, 1759 (1997).

[8] V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. D **66**, 076013 (2002); S. G. Porsev, K. Beloy, and A. Derevianko, Phys. Rev. Lett. **102**, 181601 (2009); V. A. Dzuba, J. C. Berengut, V. V. Flambaum, and B. Roberts, *ibid.* **109**, 203003 (2012).

[9] V. A. Dzuba, V. V. Flambaum, and B. Roberts, Phys. Rev. A **86**, 062512 (2012).

[10] N. Fortson, Phys. Rev. Lett. **70**, 2383 (1993); V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. A **63**, 062101 (2001).

[11] L. W. Wansbeek, B. K. Sahoo, R. G. E. Timmermans, K. Jungmann, B. P. Das, and D. Mukherjee, Phys. Rev. A **78**, 050501 (2008).

[12] E. Gomez, L. A. Orozco, and G. D. Sprouse, Rep. Prog. Phys. **69**, 79 (2006); D. Sheng, J. Zhang, and L. A. Orozco, Rev. Sci. Instrum. **83**, 043106 (2012).

[13] B. M. Roberts, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **88**, 012510 (2013).

[14] I. S. Lim, M. Pernpointner, M. Seth, J. K. Laerdahl, P. Schwerdtfeger, P. Neogrady, and M. Urban, Phys. Rev. A **60**, 2822 (1999).

[15] E. Eliav, M. J. Vilkas, Y. Ishikawa, and U. Kaldor, Chem. Phys. **311**, 163 (2005).

[16] T. H. Dinh, V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. A **78**, 022507 (2008).

[17] T. H. Dinh, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **80**, 044502 (2009).

[18] A. Borschevsky, V. Pershina, E. Eliav, and U. Kaldor, J. Chem. Phys. **138**, 124302 (2013).

[19] S. A. Blundell, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **38**, 4961 (1988); **42**, 3751 (1990).

[20] A. Derevianko and S. G. Porsev, Eur. Phys. J. A **32**, 517 (2007).

[21] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, Phys. Lett. A **140**, 493 (1989).

[22] V. A. Dzuba, Phys. Rev. A **78**, 042502 (2008).

[23] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, J. Phys. B **20**, 1399 (1987).

[24] V. V. Flambaum and J. S. M. Ginges, Phys. Rev. A **72**, 052115 (2005).

[25] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U.S.), Circ. No. 467 (U.S. GPO, Washington, DC, 1958), Vol. III.

[26] J. E. Sansonetti, J. Phys. Chem. Ref. Data **36**, 497 (2007).

[27] C. Thierfelder and P. Schwerdtfeger, Phys. Rev. A **82**, 062503 (2010).