The Landé g Factors for the $6S_{1/2}$ and $5D_{3/2,5/2}$ States of Ba^+ Ions

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The Landé g factors of Ba^+ are very important in high-precision measurement physics. The wave functions, energy levels, and Landé g factors for the 6s $^2S_{1/2}$ and 5d $^2D_{3/2,5/2}$ states of Ba^+ ions were calculated using the multi-configuration Dirac–Hartree–Fock method and the model-quantum electrodynamics (QED) method. The contributions of the electron correlation effects and QED effects were discussed in detail. The transition energies are in excellent agreement with the experimental results, with differences of approximately 5 cm^{-1}. The presently calculated g factor of 2.0024905(16) for the $6S_{1/2}$ agrees very well with the available experimental and theoretical results, with a difference at a level of 10^{-6}. For the $5D_{3/2,5/2}$ states, the present results of 0.7993961(126) and 1.2003942(190) agree with the experimental results of 0.7993278(3) [*Phys. Rev. A* **54** 1199 (1996)] and 1.20036739(14) [*Phys. Rev. Lett.* **124** 193001 (2020)] very well, with differences at the level of 10^{-5}.

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1. Introduction. The Landé g factors are very important in high-precision measurement physics, including applications in atomic clocks,[1,2] quantum computation,[3,4] and quantum information.[5–7] They also play a significant role in exploring high-order quantum electrodynamics (QED)[8] and electron correlation effects,[8,9] as well as in testing the accuracy of theoretical methods. For few-electron systems, such as H-like[10–12] and Li-like[13–15] systems, both theoretical and experimental results have achieved remarkable agreement.[10,16–19] The two-loop QED effects,[12,14,20–22] screened QED effects,[23] higher-order electron correlation effects,[17,24] and higher-order nuclear recoil effects[25–27] have been identified as crucial. However, for many-electron systems, high-precision theoretical calculations remain challenging due to the complexity of electron correlations.

Ba^+ is a promising candidate for quantum computing, quantum information, and atomic clock research.[28,29] Its ground state is 6s, and the metastable excited 5d states have lifetimes of 48 and 32 s for the $5D_{3/2}$ and $5D_{5/2}$ states, respectively.[30,31] The $6S_{1/2}$–$5D_{5/2}$ transition is a clock transition with a high quality factor of 5.4×10^{15}. The g factor of the ground state $6s_{1/2}$ has been measured with an uncertainty at the level of 10^{-7}.[32–34] Recently, Arnold *et al.*[29] and Hoffman *et al.*[35] have measured the g factor of the $5D_{5/2}$ state in Paul traps, achieving uncertainties at the levels of 10^{-7} and 10^{-6}, respectively.

Theoretically, Lindroth *et al.* have calculated the g factor of the ground state $6S_{1/2}$ of Ba^+,[32] and their theoretical results are in agreement with the most accurate experimental results at the level of 10^{-6}. However, for the excited state of $5D_{3/2}$, there is only one theoretical result available from Ref. [36], which agrees with the most accurate experimental results at a level of 10^{-4}. To our knowledge, there are no theoretical results for the $5D_{5/2}$ state available for comparison with recent experimental data. Therefore, highly accurate theoretical calculations of the g factors for these excited states are required.

In this work, the wave functions, energy levels, and g factors of the $6S_{1/2}$ and $5D_{3/2,5/2}$ states of Ba^+ were calculated using the multi-configuration Dirac–Hartree–Fock (MCDHF) method and the Model-QED method. The electron correlation effects, Breit interactions, and QED effects were discussed in detail.

2. Theoretical Methods. The MCDHF method is described in detail in Refs. [37–39]; here, we only provide a brief overview. In this method, the atomic state wave function for a given parity P, total angular momentum J and its projection on the Z-axis M_J is expressed as a linear combination of symmetry-adapted configuration state wave functions (CSFs),[38] i.e.,

$$\Psi(\gamma PJM_J) = \sum_{j=1}^{N_{\rm CSFs}} c_j \Phi(\gamma_j PJM_J), \tag{1}$$

where c_j is the mixing coefficient and γ represents other quantum numbers of the corresponding states. The single electron orbitals are optimized through the relativistic self-consistent field (SCF) method. Subsequently, the mixing coefficients are obtained by performing relativistic configuration interaction (RCI) calculations, i.e., by diagonalising the Hamiltonian matrix of the configuration state space.

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In this step, the Breit interaction, QED effects, and nuclear recoil corrections can be added in the Hamiltonian matrix.

The Breit interaction is written as [37,38,40]

$$H_{\rm Breit} = -\sum_{i<j}^{N}\Big[\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j\frac{\cos(\omega_{ij}r_{ij}/c)}{r_{ij}} + (\boldsymbol{\alpha}_i\cdot\nabla_i)(\boldsymbol{\alpha}_j\cdot\nabla_j)\frac{\cos(\omega_{ij}r_{ij}/c)-1}{\omega_{ij}^2 r_{ij}/c^2}\Big], \quad (2)$$

where $\boldsymbol{\alpha}_i$ is the Dirac matrix consisting of three 4×4 matrices, ∇ is the momentum operator, c is the speed of light, and r_{ij} is the distance between electron i and electron j. The frequency ω_{ij} corresponds to the virtual photon exchanged between the electrons. The value of ω_{ij} can be the difference of single electron energies. If $\omega_{ij}\to0$, the operator reduces to the frequency-independent Breit interaction.

The contribution of QED was calculated using the Model-QED method. [41–43] This method has been successfully applied to studies of various atomic systems. [44–54] The QED effect is represented by the sum of the self-energy and the vacuum polarization. [41–43] The vacuum polarization was calculated by the sum of the Uehling potential [55] and the Wichmann–Kroll potential. [56] The self-energy operator is written as [41,43]

$$h^{\rm SE} = h^{\rm SE}_{\rm loc} + h^{\rm SE}_{\rm nloc}, \quad (3)$$

where $h^{\rm SE}_{\rm loc}$ is the quasi-local operator, while $h^{\rm SE}_{\rm nloc}$ denotes the nonlocal operator, these two operators are depicted in detail in Refs. [41,43].

The g factor can be written as [57]

$$g = \frac{1}{2\mu_{\rm B}}\frac{\langle\Psi(\gamma PJ)\|\boldsymbol{N}^{(1)}\|\Psi(\gamma PJ)\rangle}{\sqrt{J(J+1)(2J+1)}}, \quad (4)$$

where the operator

$$\boldsymbol{N}^{(1)} = -{\rm i}\sum_j\sum_{q=0,\pm1}\sqrt{\frac{8\pi}{3}}r_j\alpha_j\cdot\boldsymbol{Y}^{(0)}_{1q}(\hat{\boldsymbol{r}}_j), \quad (5)$$

and $\boldsymbol{Y}^{(0)}_{1q}$ is the vector spherical harmonic. [58] The QED correction due to the anomalous magnetic moment of the electron can be written as [57,58]

$$\Delta g_{\rm QED} = \frac{(g_s-2)\langle\Psi(\gamma PJ)\|\sum_j\Delta\boldsymbol{N}^{(1)}_j\|\Psi(\gamma PJ)\rangle}{2\sqrt{J(J+1)(2J+1)}}, \quad (6)$$

where $g_s = 2.0023193$. [59] The operator $\Delta\boldsymbol{N}^{(1)}_j = \beta_j\boldsymbol{\Sigma}_j$ and $\boldsymbol{\Sigma}_j$ is the relativistic spin matrix.

3. Energy Level. In order to accurately deal with the effects of electron correlation, three different correlation models, designated as Model A, Model B, and Model C, were employed. In Model A, the calculations were performed using the single-reference configurations $5s^25p^66s$ and $5s^25p^65d$, with the 5p, 5d, and 6s electrons set as active electrons. The configuration space was subsequently generated through single and double (SD) excitations from the occupied orbitals of the reference configurations to unoccupied (virtual) orbitals. The virtual orbitals were constrained to principal quantum numbers $n_{\rm max}\le9$ and orbital quantum numbers $l\le5$ (i.e., the angular symmetries are s, p, d, f, g). In this model, the core-valence (CV) electron correlation effects between the 5p core electrons and the 6s or 5d valence electrons were considered. Model B was based on Model A, and included the 5s core electrons as active electrons. This model extended Model A by incorporating the CV electron correlations between the 5s core electrons and the 6s and 5d valence electrons, as well as the core-core (CC) electron correlations between the 5s and 5p electrons. The third model, Model C, incorporated higher-order electron correlations through SD excitations from multi-reference configurations.

The reference configurations included $5s^2_25p^6_26s_1$, $5s^2_25p^6_25d_1$, $5s^2_15p^4_25d_16s_16d_1$, $5s^25p^5_25d_16p_1$, $5s^25p^4_15d^2_26s_1$, and $4d^95s^25p^66s_16d_1$. The subscript denotes the maximum number of electrons that can be excited. These configurations contribute significantly to the wave functions for $6S_{1/2}$ and $5D_{3/2}$, and $5D_{3/2}$ states. For example, the contributions of the $5s^25p^5_25d_16p_1$ and $5s^25p^4_15d^2_26s_1$ to the wavefunction of the $6S_{1/2}$ state are 0.48% and 0.2%, respectively. The contribution of the $5s^25p^4_15d^1_16s_16d_1$ to the wave function of the $5D_{3/2}$ state is 0.39%. The contribution of $4d^95s^25p^66s_16d_1$ to the wave function of the $5D_{5/2}$ state is 0.43%. Table 1 lists the numbers of CSFs that expand with the principal quantum number n. It should be noted that in Model C, the configurations that do not interact with $6S_{1/2}$ and $5D_{3/2,5/2}$ were eliminated by using the program "rcsfinteract" in the GRASP2018. [60] In this model, the 4d orbital was open, allowing the calculation to include the CC and CV correlations of the 4d electrons.

Table 2 shows the convergence of the transition energies with the expansion of the configuration space. It can be seen that the transition energies calculated in each model converged very well when $n_{\rm max}$ was increased to 9. To illustrate the convergence of the different correlation models, figure 1 shows the difference in the transition energies between the calculated results for

Table 1. The number of CSFs for the $6S_{1/2}$ and $5D_{3/2,5/2}$ states of Ba^+ ions in Model A, B, and C.

$n_{\rm max}$	$6S_{1/2}$	$5D_{3/2}$	$5D_{5/2}$
		Model A	
6	3 409	6 160	7 820
7	7 976	14 397	18 219
8	14 525	26 188	33 058
9	23 056	41 533	52 337
		Model B	
6	6 331	11 447	14 550
7	14 889	26 877	34 016
8	27 125	48 893	61 690
9	43 039	77 495	97 572
		Model C	
6	194 770	370 667	482 445
7	442 030	876 772	1 170 127
8	780 002	1 591 337	2 153 107
9	1 208 686	2 514 362	3 431 385

Table 2. The convergence of transition energies of the $6S_{1/2}$ and $5D_{3/2,5/2}$ states of Ba^+ ions calculated using Model A, B, and C, respectively (in cm^{-1}).

n_{max}	$5D_{3/2}$–$6S_{1/2}$	$5D_{5/2}$–$6S_{1/2}$	$5D_{5/2}$–$5D_{3/2}$
		Model A	
6	4887	5659	771
7	5316	6081	766
8	5360	6124	764
9	5367	6131	763
		Model B	
6	4528	5308	780
7	4970	5743	773
8	5036	5807	770
9	5048	5818	770
		Model C	
6	4683	5497	813
7	4945	5758	813
8	4945	5762	817
9	4925	5742	818

Table 3. Transition energy (in cm^{-1}) of the $6D_{1/2}$ and $5D_{3/2,5/2}$ states of Ba^+. "Breit($\omega \to 0$)" and "Breit" represent the contributions from the frequency-independent and frequency-dependent interactions, respectively. "Total" is the sum of CI, Breit, and QED contributions. "SD" represents the SD all-order method. "CP+CI" and "SDCC+CI" represents correlation-potential (CP) method and linearized single-double-coupled-cluster (SDCC) method combine configuration-interaction (CI) techniques, respectively.

Contribution	$5D_{3/2}$–$6S_{1/2}$	$5D_{5/2}$–$6S_{1/2}$	$5D_{5/2}$–$5D_{3/2}$
CI	4924.7	5742.3	817.6
Breit($\omega \longrightarrow 0$)	−55.4	−80.8	−25.5
Breit	−55.6	−81.6	−25.9
CI+Breit	4869.0	5660.7	791.7
QED	9.4	9.3	−0.1
Total	4878.4(24.5)	5670.0(24.8)	791.6(25.2)
SD [61]	4762	5521	759
SDCC+CI [62]	4869	5736	867
CP+CI [62]	4750	5611	861
Exp. [63]	4873.852	5674.807	800.955

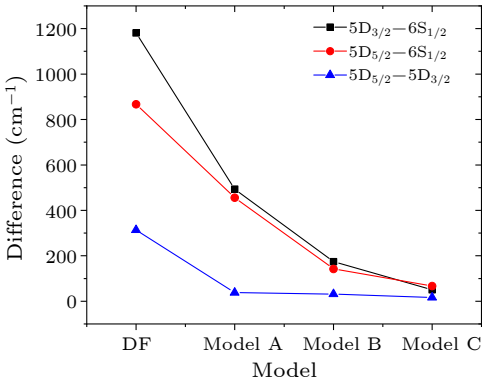

Fig. 1. Difference of the transition energies between the calculated results for each correlation model with $n_{max} = 9$ and the NIST standard values. DF is the results calculated using Dirac–Fock energies.

each correlation model with $n_{max} = 9$ and the NIST standard values,[63] which are 4874, 5675, and 801 cm^{-1} for the $5D_{3/2}$–$6S_{1/2}$, $5D_{5/2}$–$6S_{1/2}$, and $5D_{5/2}$–$5D_{3/2}$ transitions, respectively. It is evident that Model C provides very good results. The difference between Dirac–Fock (DF) and Model A indicates the CV and CC correlations for the 5p orbitals, which account for −10% of the transition energy. The contributions of CV and CC correlations involving the 5s orbital are about −6%, which were obtained by the difference between Model A and Model B. Similarly, the contribution of CV and CC correlations involving the 4d orbital, along with partial triple- and quadruple-excitations, is −2% which was derived from the difference between Model B and Model C.

Then, we further calculated the Breit interactions, QED effects, and nuclear recoil by re-diagonalizing the Hamiltonian matrix on the basis of Model C with $n_{max} = 9$. The matrix elements of self-energy and vacuum polarization were calculated using the Model-QED program.[41,42] It should be noted that the Breit interactions and QED effects are included in the RCI calculations but are not included in the SCF calculations. These matrix elements were then added to the Hamiltonian matrix, and the QED contributions to the energy levels and wave functions were obtained through diagonalization. Table 3 presents the individual contributions of the Breit interaction, QED effects and total transition energies for the $5D_{3/2}$–$6S_{1/2}$, $5D_{5/2}$–$6S_{1/2}$, and $5D_{5/2}$–$5D_{3/2}$ states, along with a comparison to some available results. Two types of Breit interactions, namely frequency-independent ($\omega \to 0$) and frequency-dependent Breit interactions, were calculated in the present work. For the frequency-dependent Breit interactions calculations, the frequencies were still set to zero for virtual orbitals. It can be seen that the contribution of the Breit interaction comes mainly from the frequency-independent term, while the correction for $\omega \neq 0$ is negligible. Additionally, the contributions of nuclear recoil were also assessed and found to be negligible, with a magnitude of less than 0.1 cm^{-1}. The final energy levels labeled "Total", which included the contributions from the electronic correlation effects, Breit interactions, and QED effects, show excellent agreement with the experimental results of the NIST tabulation.[63] The main sources of uncertainty are convergence (≈24 cm^{-1}) and higher-order QED contributions.

4. Landé g Factor. Ignoring the electron correlation effects, QED effects and nuclear recoil, the g factor is reduced to the analytical Dirac value[64]

$$g_D = \frac{\kappa}{2J(J+1)}(2\kappa\varepsilon_{n\kappa} - 1), \tag{7}$$

where $\varepsilon_{n\kappa}$ is the Dirac energy of the orbital and κ is the relativistic quantum number. For the states $6S_{1/2}$, $5D_{3/2}$, and $5D_{5/2}$ of the Ba^+, the g_D are 1.9968281, 0.7963948, and 1.1965435, respectively.

Table 4 shows the convergence of our calculated g factors using Eq. (4) as the maximum principal quantum number n_{max} increased in Model C. The contributions of electron correlation effects were obtained from the difference between the calculated g factor and the g_D values. When the configuration space reached $n_{max} = 9$, this contribution converged to a level of 10^{-6}.

Table 4. The convergence of positive-energy states to the g factor of the $6S_{1/2}$, $5D_{3/2}$, and $5D_{5/2}$ states for Ba^+ ions calculated using Model C. Δg_{PS} represents the contribution of positive-energy states. g_D is the Dirac value.

n_{max}	$6S_{1/2}$		$5D_{3/2}$		$5D_{5/2}$	
	$g_D = 1.9968281$		$g_D = 0.7963948$		$g_D = 1.1965435$	
	g	$\Delta g_{PS} = g - g_D$	g	$\Delta g_{PS} = g - g_D$	g	$\Delta g_{PS} = g - g_D$
6	2.0001674	0.0033393	0.7998653	0.0034705	1.1999431	0.0033996
7	2.0001617	0.0033336	0.7998623	0.0034674	1.1999382	0.0033948
8	2.0001680	0.0033399	0.7998610	0.0034662	1.1999364	0.0033930
9	2.0001678	0.0033397	0.7998604	0.0034656	1.1999355	0.0033921

We also evaluated the contributions of the negative-energy states. The estimation method is similar to our previous calculations of the g factor for Ar^{13+} and Li-like Sn^{47+} and Bi^{80+} ions.[65,66] The negative-energy orbitals were calculated by the relativistic configuration interaction plus core polarization method.[67] Then we performed the RCI calculations again, in which the positive-energy orbitals of $n \geq 7$ are replaced by the negative-energy orbitals and the orbitals of $n \leq 6$ remain unchanged. In addition, the Breit interaction is also included. For the $6S_{1/2}$, $5D_{3/2}$, and $5D_{5/2}$ states, the contributions converged to 0.0000021, −0.0000002, and −0.0000054, respectively.

Table 5 lists the individual contributions to the g factors from different effects and compares them with existing theoretical and experimental results. The contributions of QED effects, denoted as "Δg_{QED}", were calculated using Eq. (6). For the $6S_{1/2}$ ground state, the accuracy of the total g factors for all theoretical and experimental results reaches 10^{-6}, demonstrating excellent consistency within their respective uncertainty ranges. Our calculated results show a difference of 6×10^{-7} from the theoretical result reported by Lindroth *et al.*[32] Notably, our results are in excellent agreement with the experimental results,[34] with a difference of less than 10^{-7}.

For the excited state $5D_{3/2}$, three experimental results[32,36,68] and one theoretical result[36] are available. The difference between the two most accurate experiments[36,68] is 1.6×10^{-5}. The discrepancy between our result and the result of the most accurate experiment[36] is 6.6×10^{-5}, representing approximately an order of magnitude improvement in the accuracy of the theoretical result reported in Ref. [36]. The details of the theoretical calculations are not provided in Ref. [36], the difference between the current results and results from Ref. [36] should mainly be from multi-reference configurations and higher-order effects. For the $5D_{5/2}$ state, three sets of experimental results are available for comparison. The difference between the two most accurate experiments[29,35] is 5×10^{-6}. The difference between our theoretical results and the most recent experimental results[29] is 2.7×10^{-5}. The primary sources of this discrepancy are the higher-order electron correlation effects and higher-order QED effects. Based on the contribution of the few-electron system,[20,21] the contribution to the two-loop QED effect for the multi-electronic system should also be approximated as 0.2% of the total QED contribution. The contribution of higher-order electron correlation is about 2% of the total electron correlations.

Table 5. The g factor of the states $6S_{1/2}$, $5D_{3/2}$, and $5D_{5/2}$ for Ba^+ ions. "Total" represent the sum of g_D, Δg_{PS}, Δg_{NS}, and Δg_{QED}. Δg_{NS} represents the contribution of the negative-energy states. The results of Δg_{QED} are calculated using Eq. (6).

	$6S_{1/2}$	$5D_{3/2}$	$5D_{5/2}$
g_D	1.9968281	0.7963948	1.1965435
Δg_{PS}	0.0033397	0.0034656	0.0033921
Δg_{NS}	0.0000021	−0.0000002	−0.0000054
Δg_{QED}	0.0023205	−0.0004641	0.0004641
Total	2.0024905(16)	0.7993961(126)	1.2003942(190)
Exp.	2.0024922(10) [36]	0.800(9) [32]	1.20036739(24) [29]
	2.00249192(3) [33]	0.7993278(3) [36]	1.200372(4)stat(7)sys [35]
	2.0024906(12) [34]	0.799311(4) [68]	1.2020(5) [69]
Theory	2.0024911(30) [32]	0.79946 [36]	

5. Conclusions. The wave function, energy levels, and g factors for the $6S_{1/2}$ and $5D_{3/2,5/2}$ states of Ba^+ ions were calculated using the MCDHF method and Model-QED method. The electron correlation effects were investigated in detail using three different correlation models. The contribution of CV and CC correlation effects of 5p, 5s, and 4d electrons (along with partial triple- and quadruple-excitations) to the transition energies, reaches −10%, −6%, and −2%, respectively. By including Breit interactions and QED effects, the differences between the currently calculated transition energies and the NIST standard values are reduced to approximately $5\,cm^{-1}$. In the calculation of the Landé g factors, the contributions from both positive and negative energy states and QED effects were analyzed. The present results show good agreement with the experimental results, with differences at the level of 10^{-6} and 10^{-5} for the $6S_{1/2}$ and $5D_{3/2,5/2}$ states, respectively.

The current calculations demonstrate significantly improved accuracy compared to existing theoretical calcula-

tions and show good agreement with the most precise experimental results. However, discrepancies persist between theoretical and experimental values for the excited states $5D_{3/2}$ and $5D_{5/2}$, where the theoretical results lie outside the experimental error bars. The difference, on the order of 10^{-5}, is two orders of magnitude larger than the experimental precision of 10^{-7}. Therefore, further advanced theoretical work is still needed, particularly regarding the higher-order electron correlation effects, two-loop QED effects, and relativistic nuclear recoil effects. These effects have been proven critical in few-electron systems but remain challenging to address in many-electron systems due to computational complexity.

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References

[1] Han J, Yu Y, Sahoo B, Zhang J, and Wang L 2019 *Phys. Rev. A* **100** 042508
[2] Ma Z X, Zhang B L, Huang Y, Hu R M, Zeng M Y, Gao K L, and Guan H 2024 *Phys. Rev. A* **110** 063102
[3] Dietrich M R, Kurz N, Noel T, Shu G, and Blinov B B 2010 *Phys. Rev. A* **81** 052328
[4] Hanson R and Awschalom D D 2008 *Nature* **453** 1043
[5] Hucul D, Christensen J E, Hudson E R, and Campbell W C 2017 *Phys. Rev. Lett.* **119** 100501
[6] Inlek I V, Crocker C, Lichtman M, Sosnova K, and Monroe C 2017 *Phys. Rev. Lett.* **118** 250502
[7] Leibfried D, Barrett M D, Schaetz T, Britton J, Chiaverini J, Itano W M, Jost J D, Langer C, and Wineland D J 2004 *Science* **304** 1476
[8] Yerokhin V A, Pachucki K, Puchalski M, Harman Z, and Keitel C H 2017 *Phys. Rev. A* **95** 062511
[9] Zinenko D, Glazov D, Kosheleva V, Volotka A, and Fritzsche S 2023 *Phys. Rev. A* **107** 032815
[10] Häffner H, Beier T, Hermanspahn N, Kluge H J, Quint W, Stahl S, Verdú J, and Werth G 2000 *Phys. Rev. Lett.* **85** 5308
[11] Hannen V, Vollbrecht J, Andelkovic Z, Brandau C, Dax A, Geithner W, Geppert C, Gorges C, Hammen M, Kaufmann S *et al.* 2019 *J. Phys. B* **52** 085003
[12] Morgner J, Tu B, König C M, Sailer T, Heiße F, Bekker H, Sikora B, Lyu C, Yerokhin V A, Harman Z, Crespo López-Urrutia J R, Keitel C H, Sturm S, and Blaum K 2023 *Nature* **622** 53
[13] Glazov D A, Köhler-Langes F, Volotka A V, Blaum K, Heiße F, Plunien G, Quint W, Rau S, Shabaev V M, Sturm S, and Werth G 2019 *Phys. Rev. Lett.* **123** 173001
[14] Glazov D, Shabaev V, Tupitsyn I, Volotka A, Yerokhin V, Indelicato P, Plunien G, and Soff G 2005 *Nucl. INstrum. Meth. B* **235** 55
[15] Kosheleva V, Volotka A, Glazov D, Zinenko D, and Fritzsche S 2022 *Phys. Rev. Lett.* **128** 103001
[16] Verdú J, Djekiá S, Stahl S, Valenzuela T, Vogel M, Werth G, Beier T, Kluge H J, and Quint W 2004 *Phys. Rev. Lett.* **92** 093002
[17] Sturm S, Wagner A, Schabinger B, Zatorski J, Harman Z, Quint W, Werth G, Keitel C H, and Blaum K 2011 *Phys. Rev. Lett.* **107** 023002
[18] Sturm S, Wagner A, Kretzschmar M, Quint W, Werth G, and Blaum K 2013 *Phys. Rev. A* **8** 030501
[19] Wagner A, Sturm S, Köhler F, Glazov D A, Volotka A V, Plunien G, Quint W, Werth G, Shabaev V M, and Blaum K 2013 *Phys. Rev. Lett.* **110** 033003
[20] Cakir H, Yerokhin V A, Oreshkina N S, Sikora B, Tupitsyn I I, Keitel C H, and Harman Z 2020 *Phys. Rev. A* **101** 062513
[21] Arapoglou I, Egl A, Höcker M *et al.* 2019 *Phys. Rev. Lett.* **122** 253001
[22] Jentschura U D 2009 *Phys. Rev. A* **79** 044501
[23] Glazov D A, Shabaev V M, Tupitsyn I I, Volotka A V, Yerokhin V A, Plunien G, and Soff G 2004 *Phys. Rev. A* **70** 062104
[24] Aleksandrov I A, Glazov D A, Malyshev A V, Shabaev V M, and Tupitsyn I I 2018 *Phys. Rev. A* **98** 062521
[25] Sailer T, Debierre V, Harman Z, Heiße F, König C, Morgner J, Tu B, Volotka A V, Keitel C H, Blaum K *et al.* 2022 *Nature* **606** 479
[26] Glazov D A, Malyshev A V, Shabaev V M, and Tupitsyn I I 2020 *Phys. Rev. A* **101** 012515
[27] Malyshev A, Anisimova I, Mironova D, Shabaev V, and Plunien G 2019 *Phys. Rev. A* **100** 012510
[28] Sherman J A, Trimble W, Metz S, Nagourney W, and Fortson N 2005 *Digest of the LEOS Summer Topical Meetings* p. 99
[29] Arnold K J, Kaewuam R, Chanu S R, Tan T R, Zhang Z, and Barrett M D 2020 *Phys. Rev. Lett.* **124** 193001
[30] Gurell J, Biémont E, Blagoev K *et al.* 2007 *Phys. Rev. A* **75** 052506
[31] Nagourney W, Sandberg J, and Dehmelt H 1986 *Phys. Rev. Lett.* **56** 2797
[32] Lindroth E and Ynnerman A 1993 *Phys. Rev. A* **47** 961
[33] Marx G, Tommaseo G, and Werth G 1998 *Eur. Phys. J. D.* **4** 279
[34] Knab H, Knöll K H, Scheerer F, and Werth G 1993 *Zeitschrift für Physik D Atoms, Molecules and Clusters* **25** 205
[35] Hoffman M R, Noel T W, Auchter C, Jayakumar A, Williams S R, Blinov B B, and Fortson E N 2013 *Phys. Rev. A* **88** 025401
[36] Knöll K H, Marx G, Hübner K, Schweikert F, Stahl S, Weber C, and Werth G 1996 *Phys. Rev. A* **54** 1199
[37] Froese Fischer C, Godefroid M, Brage T, Jönsson P, and Gaigalas G 2016 *J. Phys. B* **49** 182004
[38] Jönsson P, Gaigalas G, Rynkun P, Radžiūtė L, Ekman J, Gustafsson S, Hartman H, Wang K, Godefroid M, Froese Fischer C *et al.* 2017 *Atoms* **5** 16
[39] Grant I 2007 *Relativistic Quantum Theory of Atoms and Molecules* **40** p. 173
[40] Rodrigues G C, Ourdane M A, Bieroń J, Indelicato P, and Lindroth E 2000 *Phys. Rev. A* **63** 012510
[41] Shabaev V, Tupitsyn I, and Yerokhin V 2015 *Comput. Phys. Commun.* **189** 175
[42] Shabaev V M, Tupitsyn I I, and Yerokhin V A 2013 *Phys. Rev. A* **88** 012513
[43] Shabaev V, Tupitsyn I, and Yerokhin V 2018 *Comput. Phys. Commun.* **223** 69
[44] Malyshev A V, Glazov D A, Shabaev V M, Tupitsyn I I, Yerokhin V A, and Zaytsev V A 2022 *Phys. Rev. A* **106** 012806
[45] Anisimova I S, Malyshev A V, Glazov D A, Kaygorodov M Y, Kozhedub Y S, Plunien G, and Shabaev V M 2022 *Phys. Rev. A* **106** 062823
[46] Tupitsyn I I, Malyshev A V, Glazov D A, Kaygorodov M Y, Kozhedub Y S, Savelyev I M, and Shabaev V M 2021 *Opt. Spectrosc.* **129** 1038
[47] Shabaev V M, Tupitsyn I I, Kaygorodov M Y, Kozhedub Y S, Malyshev A V, and Mironova D V 2020 *Phys. Rev. A* **101** 052502

[48] Volotka A V, Bilal M, Beerwerth R, Ma X, Stöhlker T, and Fritzsche S 2019 *Phys. Rev. A* **100** 010502
[49] Si R, Guo X L, Brage T, Chen C Y, Hutton R, and Fischer C F 2018 *Phys. Rev. A* **98** 012504
[50] Machado J, Szabo C I, Santos J P, Amaro P, Guerra M, Gumberidze A, Bian G, Isac J M, and Indelicato P 2018 *Phys. Rev. A* **97** 032517
[51] Yerokhin V A, Surzhykov A, and Müller A 2017 *Phys. Rev. A* **96** 042505
[52] Tupitsyn I I, Mironova D V, Malyshev A V, and Shabaev V M 2017 *Nucl. Instrum. Meth. B* **408** 76
[53] Tupitsyn I I, Kozlov M G, Safronova M S, Shabaev V M, and Dzuba V A 2016 *Phys. Rev. Lett.* **117** 253001
[54] Li B B, Jiang J, Wu L, Zhang R K, Li X J, and Dong C Z 2024 *J. Phys. B* **57** 115003
[55] Fullerton L W and Rinker J 1976 *Phys. Rev. A* **13** 1283
[56] Fainshtein A G, Manakov N L, and Nekipelov A A 1991 *J. Phys. B* **24** 559
[57] Cheng K T and Childs W J 1985 *Phys. Rev. A* **31** 2775
[58] Akhiezer A I 1965 *Quantum electrodynamics* (Interscience Publishers)
[59] Shabaev V M, Glazov D A, Shabaeva M B, Yerokhin V A, Plunien G, and Soff G 2002 *Phys. Rev. A* **65** 062104
[60] Froese Fischer C, Gaigalas G, Jönsson P, and Bieroń J 2019 *Comput. Phys. Commun.* **237** 184
[61] Safronova U 2010 *Phys. Rev. A* **81** 052506
[62] Dzuba V 2014 *Phys. Rev. A* **90** 012517
[63] Kramida A, Ralchenko YU, Reader J, and NIST ASD Team 2025 *NIST Atomic Spectra Database* (ver. 5.12)
[64] Zapryagaev S A 1979 *Opt. Spectrosc.* **47** 9
[65] Wu L, Jiang J, Wu Z W, Cheng Y J, Gaigalas G, and Dong C Z 2022 *Phys. Rev. A* **106** 012810
[66] Liu M, Li B B, Wu L, and Jiang J 2024 *Phys. Scr.* **99** 055406
[67] Jiang J, Mitroy J, Cheng Y, and Bromley M W J 2016 *Phys. Rev. A* **94** 062514
[68] Werth G 1995 *Phys. Scr.* **1995** 206
[69] Kurz N, Dietrich M R, Shu G, Noel T, and Blinov B B 2010 *Phys. Rev. A* **82** 030501