Polarizabilities of Si^{2+}: A benchmark test of theory and experiment

M. S. Safronova,[1] S. G. Porsev,[1,2] M. G. Kozlov,[2,3] and Charles W. Clark[4]

[1]*Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, USA*

[2]*Petersburg Nuclear Physics Institute, Gatchina, Leningrad District 188300, Russia*

[3]*St. Petersburg Electrotechnical University "LETI", Prof. Popov Str. 5, St. Petersburg, 197376, Russia*

[4]*Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, Gaithersburg, Maryland, 20899-8410, USA*

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We have calculated electric dipole polarizabilities of the $3s^2\,{}^1S_0$, $3s3p\,{}^3P_0$, and $3s3p\,{}^1P_1$ states of the Si^{2+} ion using the recently developed configuration interaction + all-order method. A detailed evaluation of the uncertainties of the final results is carried out. Our value for the ground-state electric dipole polarizability 11.670(13) a.u. is in excellent agreement with the resonant excitation Stark ionization spectroscopy value 11.669(9) a.u. [Komara *et al.*, J. Phys. B **38**, 87 (2005); Mitroy, Phys. Rev. A **78**, 052515 (2008)]. This paper represents a benchmark test of theory and experiment in divalent atoms. The near cancellation of the $ns^2\,{}^1S_0$ ground state and the lowest $nsnp\,{}^3P_0$ polarizabilities previously observed in B^+, Al^+, In^+, Tl^+, and Pb^{2+} is also found in the Si^{2+} ion.

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I. INTRODUCTION

The atomic dipole polarizability describes the first-order response of an atom to an applied electric field. Atomic polarizabilities have been the subject of considerable interest and heightened importance in recent years due to a number of applications, including the development of next-generation optical atomic clocks, optical cooling and trapping schemes, quantum information with atoms and ions, tests of fundamental symmetries, studies of cold degenerate gases, thermometry and other macroscopic standards, study of long-range interactions, and atomic transition rate determinations [1]. An imperfect knowledge of atomic polarizabilities is one of the largest sources of uncertainty in the new generation of optical frequency standards [1,2].

Most of the applications listed above involve monovalent or divalent atoms and ions. There are a number of high-precision benchmark tests of experimental and theoretical values for the polarizabilities of monovalent systems [1,3–12]. However, there are few high-precision experimental data for the polarizabilities of divalent systems, which are of particular interest to optical clock development [13–16] and quantum information [17]. The most recent data for polarizability and Stark shifts of divalent systems are compiled in Tables 11, 13, and 14 of Ref. [1].

For the first row monovalent systems, such as Li and Be^+, the highest-precision determination of the polarizabilities by theoretical and experimental methods are found to be in good agreement (see recent reviews [1,18] and references therein). Here, we provide such a comparison for a second row divalent species Si^{2+}. We believe that the experimental data for this ion provide the most precise value of the polarizability of any atomic system with two valence electrons.

A. Experimental determination of polarizabilities from Rydberg spectra

The polarizability of an ion can be extracted from the energies of the nonpenetrating Rydberg series of the corresponding parent system (see Ref. [19] and references therein). The polarization interaction between the ionic core and the Rydberg electron shifts the energy levels away from their hydrogenic values. If the Rydberg electron is in a high angular momentum state, it has negligible overlap with the core. In such cases, the polarization interaction provides the dominant contribution to the energy shift. This effect is utilized in resonant excitation Stark ionization spectroscopy (RESIS) [19–28]. RESIS experiments have been extremely successful in the high-precision determination of the ground-state polarizabilities of H_2^+ and D_2^+ [21], Ne^+ [19], Na-like Mg^+ [22], Na-like Si^{3+} [23], Mg-like Si^{2+} [20], Zn-like Kr^{6+} [28], Ba^+ [24], Hg-like Pb^{2+} [25], Fr-like Th^{3+} [26], and Rn-like Th^{3+} [27]. Quadrupole polarizabilities and transition matrix elements have also been determined for some of these systems.

To the best of our knowledge, RESIS experiments provide the most precise values known to date for the polarizability of any divalent atomic system. The most precise measurement has been carried out for the $3s^2\,{}^1S_0$ ground state of the Si^{2+} ion; $\alpha_0 = 11.666(4)$ a.u. [20]. Later analysis of the RESIS data that included additional terms in the polarization expansion yielded $\alpha_0 = 11.669(9)$ a.u. [29]. Therefore, the Si^{2+} RESIS experiment presents an excellent opportunity for a high-precision benchmark comparison of theory and experiment.

In this paper, we use a recently developed configuration iteration (CI) + all-order method [30–32] to calculate the properties of Si^{2+}. Our value for the ground-state electric dipole polarizability of 11.670(13) a.u. is in excellent agreement with the RESIS result. Our previous calculation of the Hg-like Pb^{2+} ground-state polarizability [33] was also in agreement with the RESIS value (accurate to 0.6%) within our estimated accuracy.

We note that Mg-like Si^{2+} was a particularly interesting test system due to its similarity with Mg-like Al^+, which was used to construct an optical clock with a fractional frequency uncertainty of 8.6×10^{-18} [34], the smallest such uncertainty yet attained. At room temperature, one of the largest contributions to the uncertainty budget of this clock is the blackbody radiation (BBR) shift. The BBR frequency shift in a clock transition is related to the difference in the static electric dipole polarizabilities between the two clock states [35]. We have recently calculated this effect in Al^+ using the same CI + all-order approach. Excellent agreement of our present calculation with the experiment in the ground state of Si^{2+} provides an additional test of the approach.

II. METHOD

To evaluate uncertainties of the final results, we carry out three calculations in different approximations: CI [36], CI + many-body perturbation theory (MBPT) [37], and CI + all-order [30–32]. These methods have been described in a number of papers [30,31,36,37], and we provide only a brief outline of these approaches and a few details relevant to this particular paper.

Our point of departure is a solution of the Dirac-Fock (DF) equations,

$$\hat{H}_0\,\psi_c = \varepsilon_c\,\psi_c,$$

where H_0 is the relativistic DF Hamiltonian [31,37] and ψ_c and ε_c are single-electron wave functions and energies. Self-consistent calculations were performed for the $[1s^2 2s^2 2p^6]$ closed core, and the $3s$, $3p$, $3d$, $4s$, $4p$, and $4d$ orbitals were formed in this potential. We constructed the B-spline basis set consisting of $N = 35$ orbitals for each of the $s, p_{1/2}, p_{3/2}, \ldots,$ partial waves up to $l \leqslant 5$. The basis set is formed in a spherical cavity with radius 60 a.u. The CI space is effectively complete and includes 23 orbitals for each partial wave with $l = 0 \cdots 4$.

The wave functions and the low-lying energy levels are determined by solving the multiparticle relativistic equation for two valence electrons [36],

$$H_{\rm eff}(E_n)\Phi_n = E_n\Phi_n.$$

The effective Hamiltonian is defined as

$$H_{\rm eff}(E) = H_{\rm FC} + \Sigma(E),$$

where $H_{\rm FC}$ is the Hamiltonian in the frozen-core approximation. The energy-dependent operator $\Sigma(E)$ takes into account virtual core excitations. It is zero in a pure CI calculation. The $\Sigma(E)$ part of the effective Hamiltonian is constructed using second-order perturbation theory in the CI + MBPT approach [37] and linearized single-double coupled-cluster method in the CI + all-order approach [31]. Construction of the effective Hamiltonian in the CI + MBPT and CI + all-order approximations is described in detail in Refs. [31,37]. The dominant part of the Breit interaction is included as described in Ref. [38].

The scalar polarizability α_0 is separated into a valence polarizability α_0^v, ionic-core polarizability α_c, and a small term α_{vc} that modifies ionic-core polarizability due to the presence of two valence electrons. The last two terms are evaluated in the random-phase approximation (RPA). Their uncertainty is determined by comparing the DF and RPA values. The small α_{vc} term is calculated by adding vc contributions from the individual electrons, i.e., $\alpha_{vc}(3s^2) = 2\alpha_{vc}(3s)$ and $\alpha_{vc}(3s3p) = \alpha_{vc}(3s) + \alpha_{vc}(3p)$.

The valence part of the polarizability is determined by solving the inhomogeneous equation in valence space, which is approximated as [39]

$$(E_v - H_{\rm eff})|\Psi(v,M')\rangle = D_{\rm eff}|\Psi_0(v,J,M)\rangle \tag{1}$$

TABLE I. Comparison of experimental [40] and theoretical energy levels in $\rm cm^{-1}$. Two-electron binding energies are given in the first row, energies in other rows are given relative to the ground state. Results of the CI, CI + MBPT, and CI + all-order calculations are given in columns labeled "CI," "CI + MBPT," and "CI + all." Corresponding relative differences of these three calculations with the experiment are given in percentages in the last three columns.

					Differences ($\rm cm^{-1}$)			Differences (%)		
State	Expt.	CI	CI + MBPT	CI + all	CI	CI + MBPT	CI + all	CI	CI + MBPT	CI + all
$3s^2\,{}^1S_0$	634 232	628 511	634 110	634 226	−5722	−123	−7	−0.9	−0.019	−0.001
$3p^2\,{}^1D_2$	122 215	120 224	122 225	122 294	−1991	10	80	−1.6	0.008	0.065
$3p^2\,{}^3P_0$	129 708	128 589	129 745	129 753	−1119	36	45	−0.9	0.028	0.035
$3p^2\,{}^3P_1$	129 842	128 717	129 878	129 887	−1125	36	45	−0.9	0.028	0.035
$3p^2\,{}^3P_2$	130 101	128 964	130 136	130 145	−1137	35	44	−0.9	0.027	0.034
$3s3d\,{}^3D_3$	142 944	141 676	142 953	142 944	−1268	10	1	−0.9	0.007	0.000
$3s3d\,{}^3D_2$	142 946	141 678	142 955	142 946	−1267	10	1	−0.9	0.007	0.000
$3s3d\,{}^3D_1$	142 948	141 681	142 957	142 948	−1268	9	0	−0.9	0.006	0.000
$3s4s\,{}^3S_1$	153 377	151 756	153 357	153 403	−1621	−20	26	−1.1	−0.013	0.017
$3p^2\,{}^1S_0$	153 444	152 674	153 631	153 613	−771	187	169	−0.5	0.122	0.110
$3s4s\,{}^1S_0$	159 070	157 543	159 079	159 116	−1527	9	47	−1.0	0.006	0.029
$3s3d\,{}^1D_2$	165 765	165 071	165 937	165 898	−694	172	133	−0.4	0.104	0.080
$3s3p\,{}^3P_0$	52 725	51 559	52 722	52 770	−1166	−3	45	−2.2	−0.006	0.086
$3s3p\,{}^3P_1$	52 853	51 682	52 849	52 897	−1171	−4	44	−2.2	−0.008	0.083
$3s3p\,{}^3P_2$	53 115	51 934	53 110	53 159	−1181	−5	44	−2.2	−0.010	0.082
$3s3p\,{}^1P_1$	82 884	82 998	82 969	82 933	113	84	48	0.1	0.102	0.058
$3s4p\,{}^3P_0$	175 230	173 409	175 202	175 249	−1821	−28	19	−1.0	−0.016	0.011
$3s4p\,{}^3P_1$	175 263	173 441	175 235	175 282	−1822	−28	19	−1.0	−0.016	0.011
$3s4p\,{}^3P_2$	175 336	173 511	175 308	175 355	−1825	−28	18	−1.0	−0.016	0.011
$3s4p\,{}^1P_1$	176 487	174 807	176 469	176 511	−1680	−18	23	−1.0	−0.010	0.013

TABLE II. Contributions to the $3s^2\,{}^1S_0$, $3s3p\,{}^3P_0$, and $3s3p\,{}^1P_1$ polarizabilities of Si^{2+} in a.u. The dominant contributions to the valence polarizabilities are listed separately with the corresponding absolute values of electric dipole reduced matrix elements given in columns labeled "D." The theoretical and experimental [40] transition energies are given in columns "$\Delta E_{\rm th}$" and "$\Delta E_{\rm expt}$." The remaining contributions to valence polarizability are given in rows labeled "Other." The contributions from the core and vc terms are given in rows "α_c" and "α_{vc}," respectively. The dominant contributions to α_0 listed in columns "α_0 (A)" and "α_0 (B)" are calculated with CI + all-order and experimental energies [40], respectively.

State	Contribution	$\Delta E_{\rm expt}$	$\Delta E_{\rm th}$	D	α_0 (A)	α_0 (B)
$3s^2\,{}^1S_0$	$3s^2\,{}^1S_0 - 3s3p\,{}^1P_1$	82 884	82 933	2.539	11.375	11.382
	$3s^2\,{}^1S_0 - 3s4p\,{}^1P_1$	176 487	176 511	0.198	0.032	0.032
	Other				0.105	0.105
	α_c				0.162	0.162
	α_{vc}				− 0.011	− 0.011
	Total				11.664	11.670
$3s3p\,{}^3P_0$	$3s3p\,{}^3P_0 - 3p^2\,{}^3P_1$	77 117	77 117	1.516	4.359	4.359
	$3s3p\,{}^3P_0 - 3s3d\,{}^3D_1$	90 224	90 179	1.779	5.137	5.135
	$3s3p\,{}^3P_0 - 3s4s\,{}^3S_1$	100 652	100 633	0.628	0.573	0.573
	Other				0.201	0.201
	α_c				0.162	0.162
	α_{vc}				− 0.006	− 0.006
	Total				10.427	10.425
$3s3p\,{}^1P_1$	$3s3p\,{}^1P_1 - 3s^2\,{}^1S_0$	− 82 884	− 82 933	2.539	− 3.792	− 3.794
	$3s3p\,{}^1P_1 - 3p^2\,{}^1D_2$	39 330	39 361	1.074	1.428	1.429
	$3s3p\,{}^1P_1 - 3p^2\,{}^1S_0$	70 560	70 680	1.776	2.178	2.181
	$3s3p\,{}^1P_1 - 3s4s\,{}^1S_0$	76 185	76 184	0.996	0.634	0.634
	$3s3p\,{}^1P_1 - 3s3d\,{}^1D_2$	82 881	82 965	4.450	11.642	11.654
	Other				0.440	0.440
	α_c				0.162	0.162
	α_{vc}				− 0.006	− 0.006
	Total				12.686	12.701

for state v with total angular momentum J and projection M. The wave function $\Psi(v,M')$ is composed of parts that have angular momenta of $J' = J, J \pm 1$ that allows us to determine the scalar and tensor polarizabilities of state $|v,J,M\rangle$ [39]. The effective dipole operator $D_{\rm eff}$ includes RPA corrections.

Unless stated otherwise, we use atomic units (a.u.) for all matrix elements and polarizabilities throughout this paper: The numerical values of the elementary charge e, the reduced Planck constant $\hbar = h/2\pi$, and the electron mass m_e, are set equal to 1. The atomic unit for polarizability can be converted to *Système International* units via α/h [Hz/(V/m)^2] = $2.488\,32 \times 10^{-8}\alpha$ (a.u.) where the conversion coefficient is $4\pi\epsilon_0 a_0^3/h$ and the Planck constant h is factored out in order to provide direct conversion into frequency units; a_0 is the Bohr radius, and ϵ_0 is the electric constant.

III. RESULTS

Comparison of the energy levels (in cm^{-1}) obtained in the CI, CI + MBPT, and CI + all-order approximations with experimental values [40] is given in Table I. Corresponding relative differences in these three calculations from the experiment are given in the last three columns. Two-electron binding energies are given in the first row of Table I, energies in other rows are measured from the ground state. For a few of the levels, the accuracy of the CI + MBPT calculation is already on the order of our expected precision. The accuracy of the ground-state two-electron binding energy is significantly improved in the CI + all-order calculation in comparison with the CI + MBPT one; the CI + MBPT value differs from the experiment by -123 cm^{-1}, whereas, our all-order value differs from the experiment by only -7 cm^{-1} (see line one of Table I). The inclusion of the all-order core-valence correlations significantly improves the differences between the singlet and the triplet states. For example, the CI + all-order value of the $3s3p\,{}^1P_1 - 3s3p\,{}^3P_1$ interval, 30 035 cm^{-1}, differs by only 4 cm^{-1} from the experimental value 30 031 cm^{-1}. The corresponding CI + MBPT value, 30 120 cm^{-1}, differs from the experiment by 89 cm^{-1}. As a result, the accuracy of the transition energies used in the polarizability calculations improves in the CI + all-order approach.

We separated the effect of the Breit interaction by comparing the results of the calculations with and without the Breit. The Breit contribution to the energies is very small, 0.01% or less. However, the inclusion of the Breit interaction significantly improves the splittings of all triplet states. For example, the $3s3p\,{}^3P_1 - 3s3p\,{}^3P_0$ and $3s3p\,{}^3P_2 - 3s3p\,{}^3P_0$ splittings are 136 and 413 cm^{-1} without Breit, respectively. The values of these splittings in our final calculations that include Breit, are 128 and 389 cm^{-1}, in excellent agreement with the experimental values 129 and 390 cm^{-1}.

We note that the transition energies relevant to the calculations of the $3s3p\,^3P_0$ polarizabilities are more accurate than the energies relative to the ground state listed in Table I.

While we do not use the sum-over-state approach in the calculation of the polarizabilities, it is useful to establish the dominant contributions to the final values. We combine our CI + all-order results for the electric dipole matrix elements and energies according to the sum-over-states formula for the valence polarizability [1],

$$\alpha_0^v = \frac{2}{3(2J+1)} \sum_n \frac{|\langle v||D||n\rangle|^2}{E_n - E_v} \quad (2)$$

to calculate the contribution of specific transitions. Here, J is the total angular momentum of state v, D is the electric dipole operator, and E_i is the energy of state i. The breakdown of the contributions to the $3s^2\,^1S_0$, $3s3p\,^3P_0$, and $3s3p\,^1P_1$ scalar polarizabilities α_0 of Si^{2+} in a.u. is given in Table II. Absolute values of the corresponding reduced electric dipole matrix elements are listed in the column labeled D in a_0e. The theoretical and experimental [40] transition energies are given in columns $\Delta E_{\rm th}$ and $\Delta E_{\rm expt}$. The remaining valence contributions are given in rows labeled Other. The contributions from the core and vc terms are listed in rows α_c and α_{vc}, respectively. The dominant contributions to α_0, listed in columns α_0 (A) and α_0 (B), are calculated with CI + all-order energies and experimental [40] energies, respectively. The differences between α_0 (A) and α_0 (B) values are small due to excellent agreement of the corresponding transition energies with the experiment. We take α_0 (B) results as final. Our study of the Breit interaction shows that it contributes only 0.03%–0.07% to the *ab initio* values of polarizabilities.

IV. EVALUATION OF THE UNCERTAINTY AND CONCLUSION

There are three contributions to the uncertainties in the final polarizability values that arise from the uncertainties in the valence α_0^v, core α_c, and α_{vc} polarizability terms. To evaluate uncertainty in the valence polarizabilities, we compare the results of the CI, CI + MBPT, CI + all-order calculations with our final CI + all-order calculation in which energies in the dominant contributions are replaced by their experimental values. The results of the last two calculations are given in Table II in columns α_0 (A) and α_0 (B). We summarize the results of all four calculations in Table III. For consistency, we refer to these calculations as CI (A), CI + MBPT (A), CI + all (A), and CI + all (B) since only theoretical energies (in the corresponding approximation) were used in the first three calculations. We evaluate the uncertainty of the final results in two different ways: (1) as the difference between the CI + all-order and the CI + MBPT calculations, listed in the row labeled "Difference all − MBPT," and (2) as the difference between the CI + all-order results with theoretical and experimental energies, listed in the row labeled "Difference (B) − (A)." We take the *largest* of the two uncertainties as the final uncertainty in the valence polarizability α_0^v. The uncertainty analysis is carried out separately for each state.

To evaluate the uncertainty in the α_c and α_{vc} contributions to the polarizability, we calculate these terms in both DF and RPA approximations. The DF values for the α_c and $\alpha_{vc}(3s^2)$ are 0.153 and −0.0086 a.u., respectively. The difference between the RPA and the DF results is taken to be the uncertainty. Uncertainties of the core and valence polarizabilities are added in quadrature to obtain uncertainties of the final values.

The final results, listed in the row labeled Total α_0, are compared with other theoretical [29,41] and experimental [20,29] values. Our value for the ground-state polarizability is in excellent agreement with both the original RESIS value [20] and the revised RESIS analysis [29]. Our values for the ground and $3s3p\,^1P_1$ state polarizabilities are in excellent agreement with theoretical values obtained with the large-scale CI calculation with semiempirical inclusion of the core polarization [29]. The CI result of Ref. [41] is consistent with other values; the small difference is probably due to the omission of the highly excited states in the valence CI and the restricted treatment of the core excitations in Ref. [41].

We note that the values of the $^1S_0$ and $^3P_0$ polarizabilities given in Table III are very similar; their difference is only 10% of the ground-state polarizability.

To summarize, we have carried out a benchmark test of the theoretical and experimental determinations of the ground-state polarizability of the Si^{2+} ion. Our final result is in excellent agreement with the RESIS experimental value [20,29]. High-precision recommended values are provided for the excited state $3s3p\,^3P_0$ and $3s3p\,^1P_1$ polarizabilities. The near cancellation of the $ns^2\,^1S_0$ ground state and the lowest $nsnp\,^3P_0$ polarizabilities reported for B^+, Al^+, In^+, Tl^+, and Pb^{2+} is also observed for the Si^{2+} ion.

TABLE III. Summary of the results for the $3s^2\,^1S_0$, $3s3p\,^3P_0$, and $3s3p\,^1P_1$ polarizabilities of Si^{2+} in a.u. and the evaluation of the uncertainties. First three rows give *ab initio* results for valence polarizabilities calculated in the CI, CI + MBPT, and CI + all-order approximations. In the CI + all (B) calculation, theoretical energies are replaced by the experimental values for the dominant contributions. The final results listed in row "Total α_0" are compared with other theoretical [29,41] and experimental [20,29] values.

Method	$3s^2\,^1S_0$	$3s3p\,^3P_0$	$3s3p\,^1P_1$
CI (A)	11.567	10.353	13.040
CI + MBPT (A)	11.502	10.262	12.539
CI + all (A)	11.512	10.271	12.530
CI + all (B)	11.519	10.268	12.545
Difference all − MBPT	0.010	0.009	−0.009
Difference (B) − (A)	0.007	−0.003	0.015
Final α_0^v	11.519(10)	10.268(9)	12.545(15)
α_c	0.162(9)	0.162(9)	0.162(9)
α_{vc}	−0.011(2)	−0.006(1)	−0.006(1)
Total α_0	11.670(13)	10.425(13)	12.701(17)
Theory [29]	11.688		12.707
Theory [41]	11.75		
Experiment [20]	11.666(4)		
Experiment [20,29][a]	11.669(9)		

[a]This value is a result of a revised analysis [29] of the RESIS experiment [20].

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[1] J. Mitroy, M. S. Safronova, and C. W. Clark, J. Phys. B **43**, 202001 (2010).

[2] M. S. Safronova, D. Jiang, B. Arora, C. W. Clark, M. G. Kozlov, U. I. Safronova, and W. R. Johnson, IEEE Trans. Ultrason. Ferroelectr. Freq. Control **57**, 94 (2010).

[3] C. R. Ekstrom, J. Schmiedmayer, M. S. Chapman, T. D. Hammond, and D. E. Pritchard, Phys. Rev. A **51**, 3883 (1995).

[4] A. Derevianko, W. R. Johnson, M. S. Safronova, and J. F. Babb, Phys. Rev. Lett. **82**, 3589 (1999).

[5] J. M. Amini and H. Gould, Phys. Rev. Lett. **91**, 153001 (2003).

[6] M. S. Safronova and C. W. Clark, Phys. Rev. A **69**, 040501 (2004).

[7] M. Auzinsh, K. Bluss, R. Ferber, F. Gahbauer, A. Jarmola, M. S. Safronova, U. I. Safronova, and M. Tamanis, Phys. Rev. A **75**, 022502 (2007).

[8] M. Gunawardena, D. S. Elliott, M. S. Safronova, and U. Safronova, Phys. Rev. A **75**, 022507 (2007).

[9] E. Iskrenova-Tchoukova and M. S. Safronova, Phys. Rev. A **78**, 012508 (2008).

[10] J. Mitroy and M. S. Safronova, Phys. Rev. A **79**, 012513 (2009).

[11] W. F. Holmgren, M. C. Revelle, V. P. A. Lonij, and A. D. Cronin, Phys. Rev. A **81**, 053607 (2010).

[12] A. Kortyna, C. Tinsman, J. Grab, M. S. Safronova, and U. I. Safronova, Phys. Rev. A **83**, 042511 (2011).

[13] S. G. Porsev, A. D. Ludlow, M. M. Boyd, and J. Ye, Phys. Rev. A **78**, 032508 (2008).

[14] T. Rosenband *et al.*, Science **319**, 1808 (2008).

[15] Y. Y. Jiang, A. D. Ludlow, N. D. Lemke, R. W. Fox, J. A. Sherman, L.-S. Ma, and C. W. Oates, Nat. Photonics **5**, 158 (2011).

[16] H. Hachisu, K. Miyagishi, S. G. Porsev, A. Derevianko, V. D. Ovsiannikov, V. G. Palchikov, M. Takamoto, and H. Katori, Phys. Rev. Lett. **100**, 053001 (2008).

[17] A. V. Gorshkov, A. M. Rey, A. J. Daley, M. M. Boyd, J. Ye, P. Zoller, and M. D. Lukin, Phys. Rev. Lett. **102**, 110503 (2009).

[18] *Atoms, Molecules and Clusters in Electric Fields. Theoretical Approaches to the Calculation of Electric Polarizability*, edited by G. Maroulis (Imperial College Press, London, 2006).

[19] R. F. Ward Jr., W. G. Sturrus, and S. R. Lundeen, Phys. Rev. A **53**, 113 (1996).

[20] R. A. Komara, M. A. Gearba, C. W. Fehrenbach, and S. R. Lundeen, J. Phys. B **38**, 87 (2005).

[21] P. L. Jacobson, R. A. Komara, W. G. Sturrus, and S. R. Lundeen, Phys. Rev. A **62**, 012509 (2000).

[22] E. L. Snow and S. R. Lundeen, Phys. Rev. A **77**, 052501 (2008).

[23] R. A. Komara, M. A. Gearba, S. R. Lundeen, and C. W. Fehrenbach, Phys. Rev. A **67**, 062502 (2003).

[24] E. L. Snow, M. A. Gearba, R. A. Komara, S. R. Lundeen, and W. G. Sturrus, Phys. Rev. A **71**, 022510 (2005).

[25] M. E. Hanni, J. A. Keele, S. R. Lundeen, C. W. Fehrenbach, and W. G. Sturrus, Phys. Rev. A **81**, 042512 (2010).

[26] J. A. Keele, M. E. Hanni, S. L. Woods, S. R. Lundeen, and C. W. Fehrenbach, Phys. Rev. A **83**, 062501 (2011).

[27] J. A. Keele, S. R. Lundeen, and C. W. Fehrenbach, Phys. Rev. A **83**, 062509 (2011).

[28] S. R. Lundeen and C. W. Fehrenbach, Phys. Rev. A **75**, 032523 (2007).

[29] J. Mitroy, Phys. Rev. A **78**, 052515 (2008).

[30] M. S. Safronova, M. G. Kozlov, and C. W. Clark, Phys. Rev. Lett. **107**, 143006 (2011).

[31] M. S. Safronova, M. G. Kozlov, W. R. Johnson, and D. Jiang, Phys. Rev. A **80**, 012516 (2009).

[32] M. G. Kozlov, Int. J. Quantum Chem. **100**, 336 (2004).

[33] M. S. Safronova, M. G. Kozlov, and U. I. Safronova, Phys. Rev. A **85**, 012507 (2012).

[34] C. W. Chou, D. B. Hume, J. C. J. Koelemeij, D. J. Wineland, and T. Rosenband, Phys. Rev. Lett. **104**, 070802 (2010).

[35] S. G. Porsev and A. Derevianko, Phys. Rev. A **74**, 020502(R) (2006).

[36] S. A. Kotochigova and I. I. Tupitsyn, J. Phys. B **20**, 4759 (1987).

[37] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996).

[38] M. G. Kozlov, S. G. Porsev, and I. I. Tupitsyn, e-print arXiv:physics/0004076.

[39] M. G. Kozlov and S. G. Porsev, Eur. Phys. J. D **5**, 59 (1999).

[40] Y. Ralchenko, A. Kramida, J. Reader, and the NIST ASD Team (2011). NIST Atomic Spectra Database (version 4.1) (online). Available at [http://physics.nist.gov/asd]. National Institute of Standards and Technology, Gaithersburg, MD.

[41] L. Hamonou and A. Hibbert, J. Phys. B **41**, 245004 (2008).