

Excitation energies, E1, M1, and E2 transition rates, and lifetimes in Ca^+ , Sr^+ , Cd^+ , Ba^+ , and Hg^+ ¹

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Abstract: Excitation energies of $ns_{1/2}$, np_j , and nd_j states in Cd^+ ($n = 5$), Hg^+ ($n = 5$) and $ns_{1/2}$, np_j , and $(n - 1)d_j$ states in Ca^+ ($n = 4$), Sr^+ ($n = 5$), and Ba^+ ($n = 6$) are evaluated using the linearized coupled-cluster (all-order) method. Reduced matrix elements, oscillator strengths, and transition rates are determined for the $ns-np_j-nd_j$ (or $ns-np_j-(n - 1)d_j$) possible electric dipole transitions in Ca^+ , Sr^+ , Ba^+ , Cd^+ , and Hg^+ . Electric quadrupole matrix elements are evaluated to obtain $ns_{1/2}-(n - 1)d_j$ transition rates in Ca^+ ($n = 5$), Sr^+ ($n = 5$), and Ba^+ ($n = 6$). The matrix elements are calculated using both relativistic many-body perturbation theory, complete through third order, and the relativistic all-order method restricted to single and double (SD) excitations. The SD lifetime results for the np and nd states in Ca^+ , Sr^+ , Ba^+ , Cd^+ , and Hg^+ , are compared with the latest available experimental measurements. The contribution of the magnetic dipole $nd_{3/2}-nd_{5/2}$ transition to the lifetimes of the lowest $nd_{5/2}$ level in Ca^+ , Sr^+ , and Ba^+ ions is discussed. These calculations provide a theoretical benchmark for comparison with experiment and theory as well as data needed for various applications.

PACS Nos: 31.15.A-, 31.15.ac, 31.15.ag, 31.15.ap

Résumé : Nous évaluons les énergies d'excitation des états $ns_{1/2}$, np_j et nd_j dans le $\text{Cd}^+(n = 5)$, $\text{Hg}^+(n = 6)$ et $ns_{1/2}$, np_j et $(n - 1)d_j$ dans le $\text{Ca}^+(n = 4)$, $\text{Sr}^+(n = 5)$ et $\text{Ba}^+(n = 6)$, en utilisant la méthode linéarisée paquet-paquet (*cluster-cluster*) à tous les ordres. Nous déterminons les éléments de matrice réduits, les forces d'oscillateur et les taux de transitions pour toutes les transitions dipôle électrique possibles $ns-np_j-nd_j$ (ou $ns-np_j-(n - 1)d_j$) dans Ca^+ , Sr^+ , Ba^+ , Cd^+ , et Hg^+ . Les éléments de matrice du quadripôle électrique sont calculés pour obtenir les taux de transition $ns_{1/2}-(n - 1)d_j$ dans Ca^+ ($n = 5$), Sr^+ ($n = 5$) et Ba^+ ($n = 6$). Les éléments de matrice sont calculés à l'aide de deux méthodes, la théorie relativiste des perturbations à N corps, jusqu'au troisième ordre et la méthode relativiste à tous les ordres, limitée aux excitations simples et doubles (SD). Nous comparons les temps de vie SD pour les états np et nd dans Ca^+ , Sr^+ , Ba^+ , Cd^+ et Hg^+ avec les plus récents résultats expérimentaux disponibles. Nous étudions la contribution de la transition dipôle magnétique $nd_{3/2}-nd_{5/2}$ au temps de vie du niveau $nd_{5/2}$ le plus bas dans les ions Ca^+ , Sr^+ et Ba^+ . Ces calculs fournissent une base de référence théorique pour comparer expérience avec théorie, aussi bien que pour déterminer les données expérimentales requises pour diverses applications.

[Traduit par la Rédaction]

1. Introduction

High-precision measurements of the atomic lifetimes for low-lying states were recently carried out for various atomic systems [1–4]. The lifetime of the $1s^2 2s^2 2p^2 \text{P}_{3/2}$ metastable level of boron-like Ar^{13+} was determined at the Heidelberg Electron Beam Ion Trap by Lapiere et al. [1]. The measurement of the $6s$ level lifetime in neutral rubidium using a time-correlated single-photon counting technique was reported by Gomez et al. [2]. The measurement of the $3d^2 \text{D}_j$ metastable state lifetime of a single laser-cooled $^{40}\text{Ca}^+$ ion in a linear Paul trap was presented in ref. 3. The precision measurements of the $5p^2 \text{P}_j$ level lifetimes of a single trapped Cd^+ ion were reported in ref. 4. These measurements are important for various fields, such as optical frequency stand-

ards, quantum information, and astronomy [3]. The comparison of high-precision measurements with theoretical predictions tests the quality of the approximation method used to account for correlation and relativistic effects in high-precision atomic calculations.

In the present paper, we calculate the lifetimes of the np_j and nd_j states in Cd^+ ($n = 5$), Hg^+ ($n = 6$) and np_j and $(n - 1)d_j$ states in Ca^+ ($n = 4$), Sr^+ ($n = 5$), and Ba^+ ($n = 6$). Electric dipole (E1), electric quadrupole (E2), and magnetic dipole (M1) matrix elements are evaluated to calculate the lifetimes of above-mentioned states. The matrix elements are calculated using both relativistic many-body perturbation theory, complete through third order, and the relativistic all-order method restricted to single and double (SD) excitations.

Received 24 September 2010. Accepted 6 January 2011. Published at www.nrcresearchpress.com/cjp on 6 May 2011.

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¹This article is part of a Special Issue on the 10th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas.

Recently, relativistic many-body calculation of energies, lifetimes, hyperfine constants, and multipole polarizabilities in $^{137}\text{Ba}^+$ and $^{87}\text{Sr}^+$ were presented by Safronova [5, 6]. The $6s-np_j$ ($n = 6-9$) E1 matrix elements and the $6s-nd_j$ ($n = 5-7$) E2 matrix elements in Ba^+ were calculated by Iskrenova-Tchoukova and Safronova [7] using the relativistic all-order linearized coupled-cluster method. This set of matrix elements was used in ref. 7 for accurate calculation of the ground-state dipole and quadrupole polarizabilities and lifetimes of the $6p_j$ and $5d_j$ levels. Previously, the $n_1s-n_2p_j$ and $n_3d_{j_1} - n_2p_j$ ($n_1 = 6-8$, $n_2 = 6-8$, and $n_3 = 5-7$) E1 matrix elements were evaluated by Dzuba et al. [8] to determine the parity-nonconserving $6s-5d$ amplitudes in Ba^+ . Correlation corrections to the electron orbitals were calculated using the ‘‘correlation potential’’ method. Dzuba et al. [9] carried out accurate ab initio nonperturbative calculations of the Breit correction to the parity nonconserving amplitudes of the $6s-5d_{3/2}$ transition in Ba^+ . E1 and E2 transition amplitudes in Ba^+ were calculated by Gopakumar et al. [10] using the relativistic coupled-cluster method. Numerical values for the $n_1s-n_2p_j$ and $5d_{j_1} - n_2p_j$ ($n_1 = 6-8$ and $n_2 = 6-8$) E1 matrix elements were calculated in ref. 10 using the relativistic third-order many-body perturbation theory (RMBPT). A description of this method and explicit formulas for the associated diagrams were given in the paper by Blundell et al. [11].

Recently [12], the calculation of the $4d^2 D_J-4s^2 S_{1/2}$ E2 matrix elements in Sr^+ was performed using an ab initio relativistic all-order method, which sums infinite sets of many-body perturbation theory terms. These matrix elements were used to evaluate the $4d$ radiative lifetimes and their ratio [12]. In ref. 13, the relativistic coupled-cluster theory was used to perform accurate calculations of the lifetimes of the lowest excited $4d^2 D_J$ states in singly ionized strontium. The lifetimes of the $4d^2 D_J$ levels and other Sr^+ properties were recently evaluated by Mitroy et al. [14] by diagonalizing a semiempirical Hamiltonian in a large dimension single-electron basis.

Recently, relativistic configuration–interaction oscillator strengths for lowest E1 transitions in gold isoelectronic sequence were presented by Glowacki and Migdalek [15]. Numerical results for Hg II ion were listed only for the $6s-6p_j$ transitions. Relativistic corrections to the transition frequencies of Ag I, Dy I, Ho I, Yb II, Yb III, Au I, and Hg II ions were investigated recently by Dzuba and Flambaum [16] owing to the search for variation of the fine-structure constant. Relativistic many-body perturbation theory was used by Safronova and Johnson [17] to evaluate excitation energies, oscillator strengths, and lifetimes of ions along the gold isoelectronic sequence. Numerical results for the Hg II ion were presented for the $ns_{1/2}$ ($n = 6-9$), np_j ($n = 6-8$), nd_j ($n = 6-7$), and $5f_j$ states for excitation energies and oscillator strengths between those states.

In this paper, we conduct both RMBPT and SD all-order calculations of the Ca^+ , Sr^+ , Cd^+ , Ba^+ , and Hg^+ properties. Such calculations permit one to investigate the convergence of the perturbation theory and estimate the theoretical error of predicted data. In the present paper, we evaluate reduced matrix elements, transition rates, and lifetimes for the low-lying levels in Ca^+ , Sr^+ , Cd^+ , Ba^+ , and Hg^+ ions. Our results are compared with theoretical results from refs. 18–27.

2. Energies of Hg^+ , Ba^+ , Cd^+ , Sr^+ , and Ca^+

We start from the ‘‘no-pair’’ Hamiltonian [28]

$$H = H_0 + V_I \quad (1)$$

where H_0 and V_I can be written in a second-quantized form as

$$H_0 = \sum_i \varepsilon_i a_i^\dagger a_i \quad (2)$$

$$V_I = \frac{1}{2} \sum_{ijkl} g_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \quad (3)$$

and the negative energy (positron) states are excluded from the sums. The quantities ε_i are eigenvalues of the one-electron Dirac–Fock (DF) equations with a frozen core, the two-particle matrix element g_{ijkl} is the Coulomb matrix element, and a_i^\dagger , a_i are creation and annihilation operators, respectively.

We carry out our calculations starting from a V^{N-1} DF potential [Ar], [Kr], [Kr]4d¹⁰, [Kr]4d¹⁰5s²5p⁶, and [Kr]4d¹⁰4f¹⁴5s²5p⁶5d¹⁰ in the cases of Ca^+ , Sr^+ , Cd^+ , Ba^+ , and Hg^+ , respectively. There are a number of advantages associated with this potential, including a greatly reduced number of Goldstone diagrams [29], a clean separation of the core and valence states, and one set of single-particle states, leading to important simplifications in the calculation of excitation energies and transition matrix elements. Thus, the total energy of different valence states of a one-electron atom, can be written as

$$E = E_\nu + E_{\text{core}} \quad (4)$$

where E_{core} is the same for all valence states, ν . Because the first-order correlation correction to valence removal energies vanishes for a V^{N-1} DF potential, the first nonvanishing corrections are found in second order.

Despite the elimination of a large set of Goldstone diagrams owing to the use of the V^{N-1} DF potential, the third-order energy expression still contains 52 terms, given by Blundell et al. [30]. The third-order expression for the energy includes terms with one-, two-, three-, and four-particle sums over virtual states and sums over core states.

The all-order single–double method was discussed previously in refs. 31–37. Briefly, we represent the wave function Ψ_ν of an atom with one valence electron atom as $\Psi_\nu \cong \Psi_\nu^{\text{SD}}$ with

$$\Psi_\nu^{\text{SD}} = \left[1 + \sum_{ma} \rho_{ma} a_m^\dagger a_a + \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{m \neq \nu} \rho_{mv} a_m^\dagger a_\nu + \sum_{mna} \rho_{mnmva} a_m^\dagger a_n^\dagger a_a a_\nu \right] \Phi_\nu \quad (5)$$

where Φ_ν is the lowest-order atomic wave function, which is taken to be the frozen-core DF wave function of a state ν . We note that we again start from the V^{N-1} DF potential. Substituting the wave function Ψ_ν^{SD} into the many-body Schrödinger equation, with Hamiltonian given by the eqs. (1)–(3), one obtains the coupled equations for the single- and double-excita-

tion coefficients ρ_{mv} , ρ_{ma} , ρ_{mnva} , and ρ_{mnab} . The coupled equations for the excitation coefficients are solved iteratively. The resulting excitation coefficients are used to evaluate multipole matrix elements. This method allows inclusion of the contribution of certain classes of RMBPT terms to all orders.

The valence E_v^{SD} energy given by

$$E_v^{\text{SD}} = \sum_{ma} \tilde{g}_{vavm} \rho_{ma} + \sum_{mab} g_{abvm} \tilde{\rho}_{mvab} + \sum_{mma} g_{vamn} \tilde{\rho}_{mnva} \quad (6)$$

does not include a certain part of the third-order contribution associated with triple excitation. This part of the third-order contribution, $E_{\text{extra}}^{(3)}$, is given in ref. 34 and needs to be calculated separately. We use our third-order energy code to separate out $E_{\text{extra}}^{(3)}$ and add it to the E_v^{SD} . We drop the index v in the designations in the text and tables below.

We use B-splines [38] to generate a complete set of basis DF wave functions for use in the evaluation of RMBPT and all-order expressions. For Ca^+ , Sr^+ , Cd^+ , Ba^+ , and Hg^+ , we use 50 splines of order $k = 8$ for each angular momentum value. The basis orbitals are constrained to a spherical cavity. The cavity radius, $R = 65$ au, is chosen large enough to accommodate all $ns_{1/2}$ and nd_j orbitals considered here and small enough that 50 splines can approximate inner-shell DF wave functions with good precision ($10^{-4}\%$ – $10^{-5}\%$ for Ba^+ ion and $10^{-6}\%$ – $10^{-7}\%$ for Sr^+ ion).

Results of our calculations of energies for the lowest states of Hg^+ , Ba^+ , Cd^+ , Sr^+ , and Ca^+ ions are summarized in Table 1. The first six columns of Table 1 give the lowest-order DF energies $E^{(0)}$, second- and third-order Coulomb correlation energies, $E^{(2)}$ and $E^{(3)}$, first-order Breit contribution $B^{(1)}$, second-order Coulomb–Breit $B^{(2)}$ corrections, and Lamb shift contribution, E_{LS} . We take the sum of these six contributions to be our final third-order RMBPT results, $E_{\text{tot}}^{(3)}$, listed in the seventh column of Table 1. We list the all-order SD energies in the column labeled E^{SD} and the part of the third-order energies omitted in the SD calculation in column $E_{\text{extra}}^{(3)}$. We note that E^{SD} contains an $E^{(2)}$ contribution. We take the sum of the six terms $E^{(0)}$, E^{SD} , $E_{\text{extra}}^{(3)}$, $B^{(1)}$, $B^{(2)}$, and E_{LS} to be our final all-order results $E_{\text{tot}}^{\text{SD}}$ listed in the ninth column of Table 1. The recommended values from the National Institute of Standards and Technology (NIST) database [39] are given in the column labeled E_{NIST} . The differences between our calculations and the NIST data, $\delta E^{(3)} = E_{\text{tot}}^{(3)} - E_{\text{NIST}}$ and $\delta E^{\text{SD}} = E_{\text{tot}}^{\text{SD}} - E_{\text{NIST}}$, are given in the last two columns of Table 1.

As expected, the largest correlation contribution to the valence energy comes from the second-order term, $E^{(2)}$. Calculating this term is simple in comparison with calculating the $E^{(3)}$ and E^{SD} terms. Thus, we can calculate the $E^{(2)}$ term with better numerical accuracy than the $E^{(3)}$ and E^{SD} terms.

The second-order energy, $E^{(2)}$, includes partial waves up to $l_{\text{max}} = 8$ and is extrapolated to account for contributions from higher partial waves (see, for example, refs. 40, 41). As an example of the convergence of $E^{(2)}$ with the number of partial waves, l , we consider the $6s_{1/2}$ state in the Hg^+ ion. Calculations of $E^{(2)}$ with $l_{\text{max}} = 6$ and 8 yield $E^{(2)}(6s_{1/2}) = -18158.0$ and -18351.4 cm^{-1} , respectively. Extrapolation of these calculations yields -18387.3 and -18381.3 cm^{-1} , respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(6s_{1/2})$ of 6.0 cm^{-1} . It should be noted that the 193.3 cm^{-1} contribution from partial waves with $l > 6$ for

the $6s$ state is the largest among all the Hg^+ states considered in Table 1; smaller (about 16 – 17 cm^{-1}) contributions are obtained for the $6d_{3/2}$ and $6d_{5/2}$ states and much smaller contributions (2 – 3 cm^{-1}) are obtained for $n = 7$ states. Similar convergence patterns are found for all other ions considered.

Owing to computational complexity, we restrict $l \leq l_{\text{max}} = 6$ in the E^{SD} calculation. As noted above, the second-order contribution dominates E^{SD} ; therefore, we can use the extrapolated value of $E^{(2)}$, described above, to account for the contributions of the higher partial waves. Six partial waves are also used in the calculation of $E^{(3)}$. Since the asymptotic l -dependence of the second- and third-order energies are similar (both fall off as l^{-4}), we use the second-order remainder as a guide to estimate the remainder in the third-order contribution. The term $E_{\text{extra}}^{(3)}$ in Table 1, which accounts for that part of the third-order RMBPT energy missing from the SD energy, is smaller than $E^{(3)}$ by a factor of 2 – 3 for the states considered here.

The first-order Breit energies (column $B^{(1)}$ in Table 1) include retardation, whereas the second-order Coulomb–Breit energies (column $B^{(2)}$ in Table 1) are evaluated using the unretarded Breit operator. The Lamb shift, E_{LS} , is approximated as the sum of the one-electron self energy and the first-order vacuum-polarization energy. The vacuum-polarization contribution is calculated from the Uehling potential using the results of Fullerton and Rinker [42]. The self-energy contribution is estimated for the s , $p_{1/2}$, and $p_{3/2}$ orbitals by interpolating among the values obtained by Mohr [43–45] using Coulomb wave functions. For this purpose, an effective nuclear charge, Z_{eff} , is obtained by finding the value of Z_{eff} required to give a Coulomb orbital with the same $\langle r \rangle$ as the DF orbital. It should be noted that the values of E_{LS} are very small ($E_{\text{LS}} \leq 79$ cm^{-1} for Hg II and $E_{\text{LS}} \leq 8$ cm^{-1} for Ba II).

We find that the correlation corrections to energies were large for the ions considered in this work, especially for the nd states in Ba II , Sr II , and Ca II and for the ns states in Hg II and Cd II . For example, $E^{(2)}$ is about 13% of $E^{(0)}$, and $E^{(3)}$ is about 30% of $E^{(2)}$ for the $5d_j$ states of Ba II . Despite the evident slow convergence of the perturbation theory expansion, the $6s$ energy in Hg II from the third-order RMBPT calculation is within 1.3% of the measured energy.

As expected, the SD results are in better agreement with the recommended values than the third-order RMBPT results are, owing to more complete inclusion of the correlation correction. The differences between the all-order values and experiment, δE^{SD} , are smaller than the corresponding third-order differences, $\delta E^{(3)}$, by a factor of 3 – 5 as illustrated by the two last columns of Table 1. Better agreement of the all-order values with experiment demonstrates the importance of the higher-order correlation contributions.

3. E1 matrix elements, transition rates, and lifetimes in Ca^+ , Sr^+ , Cd^+ , Ba^+ , and Hg^+

3.1 E1 matrix elements

The one-body matrix element of the operator Z is given by [31]

$$Z_{wv} = \frac{\langle \Psi_w | Z | \Psi_v \rangle}{\sqrt{\langle \Psi_v | \Psi_v \rangle \langle \Psi_w | \Psi_w \rangle}} \quad (7)$$

Table 1. Zeroth-order (DF), second- and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb E^{SD} , $E_{\text{extra}}^{(3)}$, first-order Breit and second-order Coulomb–Breit corrections $B^{(n)}$ to the energies of Hg II, Ba II, Cd II, Sr II, and Ca II.

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(1)}$	$B^{(2)}$	E_{LS}	$E_{\text{tot}}^{(3)}$	E^{SD}	$E_{\text{extra}}^{(3)}$	$E_{\text{tot}}^{\text{SD}}$	E_{NIST}	$\delta E^{(3)}$	δE^{SD}
Hg II													
6s _{1/2}	-136471	-18374	5622	389	-756	79	-149510	-15850	1665	-150943	-151280	1770	337
6p _{1/2}	-89694	-11013	2811	269	-375	-2	-98003	-10585	878	-99508	-99795	1792	287
6p _{3/2}	-82029	-8885	2201	153	-272	1	-88832	-8886	740	-90293	-90672	1840	379
6d _{3/2}	-44308	-1985	410	28	-58	0	-45912	-2089	183	-46243	-46297	385	54
6d _{5/2}	-43866	-1870	368	23	-60	0	-45405	-2086	168	-45821	-45737	332	-84
Ba II													
6s _{1/2}	-75340	-6569	2326	70	-102	8	-79606	-5970	1010	-80324	-80687	1081	363
5d _{3/2}	-68139	-9124	2731	105	-257	0	-74684	-8394	1218	-75467	-75813	1129	346
5d _{5/2}	-67665	-8667	2537	78	-246	0	-73962	-8010	1132	-74711	-75012	1050	301
6p _{1/2}	-57266	-3630	1120	54	-48	0	-59770	-3517	516	-60262	-60425	655	163
6p _{3/2}	-55873	-3275	1008	39	-47	0	-58149	-3171	464	-58589	-58735	586	146
Cd II													
5s _{1/2}	-124568	-13474	3325	150	-250	23	-134794	-12408	1143	-135910	-136375	1581	465
5p _{1/2}	-84903	-7730	1616	107	-124	0	-91034	-7678	593	-92005	-92239	1205	234
5p _{3/2}	-82871	-7175	1479	76	-113	0	-88604	-7175	554	-89529	-89756	1152	227
5d _{3/2}	-45147	-1532	236	14	-26	0	-46454	-1665	122	-46702	-46686	232	-16
5d _{5/2}	-45010	-1503	230	11	-27	0	-46299	-1643	119	-46550	-46531	232	-19
Sr II													
5s _{1/2}	-84042	-5610	1237	49	-64	6	-88425	-5386	618	-88819	-88964	539	145
4d _{3/2}	-67385	-7908	1644	61	-162	0	-73750	-7719	758	-74446	-74408	659	-38
4d _{5/2}	-67242	-7728	1593	45	-157	0	-73490	-7546	733	-74169	-74128	638	-41
5p _{1/2}	-62512	-2982	572	38	-31	0	-64915	-3000	310	-65196	-65249	334	53
5p _{3/2}	-61828	-2844	544	28	-31	0	-64131	-2861	294	-64397	-64447	317	50
Ca II													
4s _{1/2}	-91440	-4786	858	24	-23	4	-95364	-4698	520	-95600	-95752	387	139
3d _{3/2}	-72617	-10333	1990	34	-100	0	-81027	-10579	1011	-82206	-82102	1075	-149
3d _{5/2}	-72593	-10278	1978	21	-98	0	-80970	-10521	1003	-82142	-82041	1071	-146
4p _{1/2}	-68037	-2675	412	20	-12	0	-70293	-2753	272	-70506	-70560	267	50
4p _{3/2}	-67837	-2643	406	14	-13	0	-70073	-2719	268	-70283	-70337	265	50

Note: The total energies ($E_{\text{tot}}^{(3)} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)} + E_{\text{LS}}$, $E_{\text{tot}}^{\text{SD}} = E^{(0)} + E^{\text{SD}} + E_{\text{extra}}^{(3)} + B^{(1)} + B^{(2)} + E_{\text{LS}}$) are compared with experimental energies, E_{NIST} [39], $\delta E = E_{\text{tot}} - E_{\text{NIST}}$. Units: cm^{-1} .

where Ψ_v is the exact wave function for the many-body “no-pair” Hamiltonian H

$$H|\Psi_v\rangle = E|\Psi_v\rangle \quad (8)$$

In RMBPT, we expand the many-electron wave function Ψ_v in powers of V_I as

$$|\Psi_v\rangle = |\Psi_v^{(0)}\rangle + |\Psi_v^{(1)}\rangle + |\Psi_v^{(2)}\rangle + |\Psi_v^{(3)}\rangle + \dots \quad (9)$$

The denominator in (7) arises from the normalization condition that contributes starting from the third order of RMBPT [46]. In the lowest order, we find

$$Z_{wv}^{(1)} = \langle \Psi_w^{(0)} | Z | \Psi_v^{(0)} \rangle = z_{wv} \quad (10)$$

where z_{wv} is the corresponding one-electron matrix element [47]. Since $\Psi_w^{(0)}$ is a DF function we use the $Z^{(\text{DF})}$ designation instead of $Z^{(1)}$ below.

The second-order Coulomb correction to the transition matrix element in the DF case with V^{N-1} potential is given by [48]

$$Z_{wv}^{(2)} = \sum_{na} \frac{z_{an}(g_{wnva} - g_{wnav})}{\epsilon_a + \epsilon_v - \epsilon_n - \epsilon_w} + \sum_{na} \frac{(g_{wavn} - g_{wanv})z_{na}}{\epsilon_a + \epsilon_w - \epsilon_n - \epsilon_v} \quad (11)$$

The second-order Breit corrections are obtained from (11) by changing g_{ijkl} to Breit matrix element b_{ijkl} [49].

In the all-order SD calculation, we substitute the all-order SD wave function, Ψ_v^{SD} , into the matrix element expression given by (7) and obtain the expression [31]

$$Z_{wv}^{(\text{SD})} = \frac{z_{wv} + Z^{(a)} + \dots + Z^{(t)}}{\sqrt{(1 + N_w)(1 + N_v)}} \quad (12)$$

where Z_{wv} is the lowest-order (DF) matrix element given by (10) and the terms $Z^{(k)}$, $k = a, \dots, t$ are linear or quadratic functions of the excitation coefficients introduced in (5). The normalization terms, N_w , are quadratic functions of the excitation coefficients. As a result, certain sets of many-body perturbation theory terms are summed to all orders in this method. Unlike the energy, the SD all-order matrix elements contain the entire third-order RMBPT contribution.

The calculation of the transition matrix elements provides another test of the quality of atomic structure calculations and another measure of the size of correlation corrections. Reduced E1 matrix elements between low-lying states of Hg II, Ba II, Cd II, Sr II, and Ca II calculated in the third order RMBPT and in the all-order SD approximation are presented in Table 2.

Table 2. Reduced E1 matrix elements in Hg II, Ba II, Cd II, Sr II, and Ca II calculated in first, second, third, and all orders of perturbation theory.

Transition	$Z^{(DF)}$	$Z^{(DF+2)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$
Hg II				
6p _{1/2} 6s _{1/2}	2.2875	1.7000	1.6248	1.6569
6p _{3/2} 6s _{1/2}	3.1820	2.4358	2.3087	2.3469
6p _{1/2} 6d _{3/2}	3.6018	3.2440	2.8418	2.9495
6p _{3/2} 6d _{3/2}	1.8765	1.7052	1.5320	1.5647
6p _{3/2} 6d _{5/2}	5.5565	5.0638	4.5254	4.5923
Ba II				
6p _{1/2} 6s _{1/2}	3.8909	3.4733	3.2763	3.3380
6p _{3/2} 6s _{1/2}	5.4775	4.9114	4.6188	4.7097
6p _{1/2} 5d _{3/2}	3.7454	3.3923	2.9063	3.0545
6p _{3/2} 5d _{3/2}	1.6354	1.4939	1.2650	1.3340
6p _{3/2} 5d _{5/2}	5.0011	4.5729	3.9183	4.1108
Cd II				
5p _{1/2} 5s _{1/2}	2.4271	2.0342	1.9168	1.9392
5p _{3/2} 5s _{1/2}	3.4280	2.8889	2.7191	2.7513
5p _{1/2} 5d _{3/2}	4.0144	3.7414	3.3870	3.4401
5p _{3/2} 5d _{3/2}	1.8684	1.7444	1.5917	1.6122
5p _{3/2} 5d _{5/2}	5.5857	5.2181	4.7554	4.8195
Sr II				
5p _{1/2} 5s _{1/2}	3.4848	3.2051	3.0504	3.0784
5p _{3/2} 5s _{1/2}	4.9211	4.5325	4.3104	4.3507
5p _{1/2} 4d _{3/2}	3.7292	3.4779	2.9787	3.0830
5p _{3/2} 4d _{3/2}	1.6572	1.5493	1.3217	1.3694
5p _{3/2} 4d _{5/2}	5.0025	4.6776	4.0117	4.1497
Ca II				
4p _{1/2} 4s _{1/2}	3.2012	3.0045	2.8826	2.8978
4p _{3/2} 4s _{1/2}	4.5269	4.2499	4.0773	4.0989
4p _{1/2} 3d _{3/2}	3.0825	2.9296	2.2998	2.4173
4p _{3/2} 3d _{3/2}	1.3764	1.3088	1.0260	1.0788
4p _{3/2} 3d _{5/2}	4.1348	3.9311	3.0882	3.2452

Table 3. The E1 transition rates, A , (10^7 s⁻¹) for transitions in Ba II calculated in the SD A_{SD}^{SD} approximation (i.e., SD data are used for both energies and matrix elements).

Transition	A_{SD}^{SD}	A_{NIST}^{SD}	$A^{(theor)}$	$A^{(expt)}$
6s _{1/2} 6p _{1/2}	9.115	9.390	9.368	9.5±0.9
6s _{1/2} 6p _{3/2}	11.54	11.89	11.94	10.6±0.9
5d _{3/2} 6p _{1/2}	3.323	3.443	3.493	3.77±0.24
5d _{3/2} 6p _{3/2}	0.433	0.449	0.425	0.469±0.029
5d _{5/2} 6p _{3/2}	3.587	3.691	3.261	3.38±0.19

Note: Data in the column A_{NIST}^{SD} are obtained by using NIST data for wavelengths and SD matrix elements. Our results are compared with theoretical, $A^{(theor)}$, and experimental, $A^{(expt)}$, data given in ref. 52 and refs. cited therein.

Our calculations of reduced matrix elements in the lowest-, second-, and third-orders, $Z^{(n)}$, in Hg II, Ba II, Cd II, Sr II, and Ca II ions are carried out following the method described above. The lowest order DF value is obtained from (10). The values of $Z^{(DF+2)}$ are the sum of the second-order correlation correction, $Z^{(2)}$, given by (11) and the DF matrix elements, $Z^{(DF)}$. It should be noted that the second-order Breit corrections, $B^{(2)}$, are rather small in comparison with the the second-order Coulomb corrections, $Z^{(2)}$ (the ratio of $B^{(2)}$ and $Z^{(2)}$ is about 0.2%–2%).

Table 4. Lifetimes, τ , of the nl levels in Ca II, Sr II, Ba II, Cd II, and Hg II.

Level	$\tau^{(SD)}$	τ^{theor}	τ^{expt}
Ba II, Z = 56			
6p _{1/2}	7.798	7.89 ^a	7.90±0.10 ^a
6p _{3/2}	6.245	6.30 ^a	6.32±0.10 ^a
Sr II, Z = 38			
5p _{1/2}	7.383	7.48 ^b	7.39±0.07 ^b
5p _{3/2}	6.660	6.74 ^b	6.63±0.07 ^b
Ca II, Z = 20			
4p _{1/2}	6.892	6.931 ^c	6.978±0.056 ^c
4p _{3/2}	6.702	6.881 ^c	6.926±0.036 ^c
Hg II, Z = 80			
6p _{1/2}	2.64	–	2.91±0.11 ^d
6p _{3/2}	1.61	–	1.80±0.06 ^d
6d _{3/2}	1.29	–	–
6d _{5/2}	1.60	–	–
Cd II, Z = 48			
5p _{1/2}	3.102	3.09 ^e	3.148±0.011 ^f
5p _{3/2}	2.612	2.60 ^e	2.647±0.010 ^f
5d _{3/2}	1.51	1.86 ^e	1.79±0.11 ^g
	[1.79]		
5d _{5/2}	1.61	1.67	1.85±0.15 ^g

Note: The lifetime of 5d_{3/2} level in Cd II 1.51[1.79] comes from two decay channels, 5p_{1/2}–5d_{3/2} and 5p_{3/2}–5d_{3/2}. The second number includes only the 5p_{1/2}–5d_{3/2} transition. The SD data are compared with other theoretical results and experimental measurements

^aFor Ba II from ref. 54 and references therein

^bFor Sr II from ref. 55 and references therein

^cFor Ca II from ref. 27

^dFor Hg II from ref. 22 and references therein

^eFor Cd II from ref. 26

^fRef. 4

^gRef. 23

The third-order matrix elements, $Z^{(DF+2+3)}$, include the DF values, the second-order, $Z^{(2)}$, results, and the third-order, $Z^{(3)}$, correlation correction, which includes random-phase-approximation terms (RPA) iterated to all orders, Brueckner orbital (BO) corrections, the structural radiation, $Z^{(SR)}$, and normalization, $Z^{(NORM)}$, terms (see [50] for detailed expressions for these terms).

The terms $Z^{(RPA)}$ and $Z^{(BO)}$ give the largest contributions to $Z^{(3)}$. The sum of terms $Z^{(RPA)}$ and $Z^{(BO)}$ is about 15%–25% of the $Z^{(DF)}$ term and has opposite sign. The smallest contributions (about 1%) come from the structural radiation, $Z^{(SR)}$, and normalization, $Z^{(NORM)}$, terms. The basis set used here is the same as in the calculation of the energy contributions. We find correlation corrections $Z^{(2+3)}$ to be very large, 10%–25% for many cases. All results given in Table 2 are obtained using the length form of the matrix elements. Length-form and velocity-form matrix elements differ typically by 5%–20% for the DF matrix elements and 2%–5% for the second-order matrix elements in this calculations.

E1 matrix elements evaluated in the all-order SD approximation (12) are given in the column labeled $Z^{(SD)}$ in Table 2. The SD matrix elements $Z^{(SD)}$ include $Z^{(3)}$ completely, along with important fourth- and higher-order corrections. The fourth-order corrections omitted from the SD matrix elements were discussed recently by Derevianko and Emmons [51].

Table 5. Reduced matrix elements of the E2 and M1 operators in first-, second-, third-, and all-order perturbation theory in Ba II, Sr II, and Ca II.

Transition		$Z^{(DF)}$	$Z^{(DF+2)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$	$Z^{(DF)}$	$Z^{(DF+2)}$	$Z^{(DF+2+3)}$	$Z^{(SD)}$
		E2 transitions				M1 transitions			
		Ba II				Ba II			
6s _{1/2}	5d _{3/2}	14.7633	15.6749	11.8208	12.4976	0.0000	0.0001	0.0140	0.0002
6s _{1/2}	5d _{5/2}	18.3840	19.5789	14.8623	15.6514	–	–	–	–
5d _{3/2}	5d _{5/2}	8.0914	9.2780	6.2769	6.6486	1.5489	1.5489	1.5315	1.5493
		Sr II				Sr II			
5s _{3/2}	4d _{3/2}	12.9681	13.2533	10.5854	11.0096	0.0000	0.0000	0.0093	0.0000
5s _{3/2}	5d _{5/2}	15.9721	16.3366	13.0956	13.6016	–	–	–	–
4d _{3/2}	4d _{5/2}	7.2603	8.5432	5.5821	5.9045	1.5491	1.5492	1.5385	1.5492
		Ca II				Ca II			
4s _{1/2}	3d _{3/2}	9.7673	9.7272	7.4009	7.78776	0.0000	0.0000	0.0050	0.0000
4s _{1/2}	3d _{5/2}	11.9782	11.9265	9.0914	9.56146	–	–	–	–
3d _{3/2}	3d _{5/2}	5.0183	4.9554	3.3275	3.68805	1.5491	1.5491	1.5421	1.5491

Table 6. Lifetimes τ of the nd levels in Ba⁺, Sr⁺, and Ca⁺ in sec.

Level	τ^{SD}	τ^{theor}	τ^{expt}
Ba II, $Z = 56$			
5d _{3/2}	83.26	81.5(1.2) ^a	89.4±15.6 ^b
5d _{5/2}	30.88	30.3(4) ^a	31.6±4.6 ^b
Sr II, $Z = 38$			
4d _{3/2}	0.4509	0.441(3) ^c	0.435±0.004 ^d
4d _{5/2}	0.4029	0.394(3) ^c	0.408±0.022 ^d
Ca II, $Z = 20$			
3d _{3/2}	1.243	1.196(11) ^e	1.176(11) ^e
3d _{5/2}	1.209	1.165(11) ^e	1.168(7) ^e

Note: The SD data are compared with theoretical recommended values and experimental measurements

^aFor Ba II from ref. 7

^bFor Ba II from ref. 20

^cFor Sr II from ref. 12

^dFor Sr II from ref. 25

^eFor Ca II from ref. 3

The $Z^{(SD)}$ values are smaller than the $Z^{(DF+2)}$ values and larger than the $Z^{(DF+2+3)}$ values for all transitions given in Table 2.

3.2 Transition rates and lifetimes in Ca⁺, Sr⁺, Cd⁺, Ba⁺, and Hg⁺

Transition rates, A , and lifetimes in Ca⁺, Sr⁺, Cd⁺, Ba⁺, and Hg⁺ calculated in SD approximation are summarized in Tables 3 and 4, respectively.

In Table 3, we compare transition rates, A (10^7 cm⁻¹), with available theoretical and experimental measurements given in ref. 52 for Ba II. The SD data are used for dipole matrix elements and energies in columns with headings A_{SD}^{SD} . In the column with headings A_{NIST}^{SD} , the NIST data are used for energies and SD data are used for the matrix elements. We include these values since the NIST data were also used in the theoretical results by Gopakumar et al. [52]. Experimental results given in the last column of Table 3 are taken from ref. 52. The accuracy of experimental results is not very high and does not allow us to make a firm decision as to which theoretical data in Table 3 are in better agreement with experimental values.

We calculate lifetimes of the np and nd states in Cd⁺ ($n = 5$) and Hg⁺ ($n = 6$), and np_j states in Ca⁺ ($n = 4$), Sr⁺ ($n = 5$), and Ba⁺ ($n = 6$) using SD results for dipole matrix elements and experimental energies. The lifetimes of the $(n - 1)d_j$ states in Sr⁺ ($n = 5$), Ba⁺ ($n = 6$), and Ra⁺ ($n = 7$) are discussed in the next section. We compare the lifetimes, $\tau^{(SD)}$, with available experimental measurements in Table 4. Our SD results are in good agreement with experimental measurements when we take into account the experimental uncertainties. The largest disagreement (about 1%) between the SD results and measurements by Pinnigton et al. [23] is observed for the 5d_j states in Cd II. We list two SD numbers for the lifetime of 5d_{3/2} level in Cd II 1.51[1.79]: the first number comes from two decay channels, 5p_{1/2}–5d_{3/2} and 5p_{3/2}–5d_{3/2}. The second number includes only the 5p_{1/2}–5d_{3/2} transition. We note that the second result agrees very well with experimental measurements given in ref. 23.

4. E2 and M1 transitions in Ca II, Sr II, and Ba II

Reduced matrix elements of the E2 and M1 operators in lowest-, second-, third-, and all-order perturbation theory are given in Table 5 for Ca II, Sr II, and Ba II. Detailed descriptions of the calculations of the reduced matrix elements of the E2 and M1 operators in lowest- and second- order perturbation theory were given by Safronova et al. [53] Third-order and all-order calculations are done in the same way as the calculations of E1 matrix elements.

As an additional test of accuracy of our ab initio SD values, we compare our results for the lifetimes of the nd levels for Ba II, Sr II, and Ca II with recommended theoretical values and experimental measurements from refs. 3, 7, 12, 20, and 25, in Table 6. Recommended theoretical values [3, 7, and 12] are from a similar all-order calculation, but include semi-empirical scaling that estimates the dominant class of missing correlation effects. The ratio of the M1 5d_{3/2}–5d_{5/2} and the E2 6s_{1/2}–5d_{5/2} transition is equal to 0.206, which decreases the lifetime of the 5d_{5/2} level by 17%. It is smaller than the ratio of the M1 4d_{3/2}–4d_{5/2} and the E2 5s_{1/2}–4d_{5/2} transition in Sr II (about 0.01%).

5. Conclusion

In summary, a systematic relativistic RMBPT study of the energies of ns , np , and nd states in Ca^+ , Sr^+ , Ba^+ , Cd^+ , and Hg^+ is presented. The energy values are in good agreement with existing experimental data. A systematic all-order SD study of the reduced matrix elements and transition rates for the $ns_{1/2}-np_j-nd_j$ and $ns_{1/2}-np_j-(n-1)d_j$ allowed E1 transitions in Cd^+ ($n=5$), Hg^+ ($n=6$) and in Ca^+ ($n=4$), Sr^+ ($n=5$), and Ba^+ ($n=6$) is conducted. The SD lifetime results for np and nd states in Ca^+ , Sr^+ , Ba^+ , Cd^+ , and Hg^+ are compared with the latest available experimental measurements. The contributions of the M1 $nd_{3/2}-nd_{5/2}$ transition to the lifetimes of the $nd_{5/2}$ level in Ca^+ ($n=4$), Sr^+ ($n=5$), and Ba^+ ($n=6$) ions are included. Our work provides data for analyzing existing experimental data and for planning future measurements.

Acknowledgment

The work of MSS was supported in part by US National Science Foundation Grant No. PHY-07-58088.

References

- J.R. Crespo-López-Urrutia, J. Braun, G. Brenner, H. Bruhns, I.N. Draganić, A.J. González-Martínez, A. Lapierre, V. Mironov, C. Osborne, et al. *Can. J. Phys.* **83**, 387 (2005). doi:10.1139/p05-015.
- E. Gomez, F. Baumer, A.D. Lange, G.D. Sprouse, and L.A. Orozco. *Phys. Rev. A*, **72**, 012502 (2005). doi:10.1103/PhysRevA.72.012502.
- A. Kreuter, C. Becher, G.P.T. Lancaster, A.B. Mundt, C. Russo, H. Häffner, C. Roos, W. Hänsel, F. Schmidt-Kaler, R. Blatt, and M. Safronova. *Phys. Rev. A*, **71**, 032504 (2005). doi:10.1103/PhysRevA.71.032504.
- D.L. Moehring, B.B. Blinov, D.W. Gidley, R.N. Kohn, M.J. Madsen, T.D. Sanderson, R.S. Vallery, and C. Monroe. *Phys. Rev. A*, **73**, 023413 (2006). doi:10.1103/PhysRevA.73.023413.
- U.I. Safronova. *Phys. Rev. A*, **81**, 052506 (2010). doi:10.1103/PhysRevA.81.052506.
- U.I. Safronova. *Phys. Rev. A*, **82**, 022504 (2010). doi:10.1103/PhysRevA.82.022504.
- E. Iskrenova-Tchoukova and M.S. Safronova. *Phys. Rev. A*, **78**, 012508 (2008). doi:10.1103/PhysRevA.78.012508.
- V.A. Dzuba, V.V. Flambaum, and J.S.M. Ginges. *Phys. Rev. A*, **63**, 062101 (2001). doi:10.1103/PhysRevA.63.062101.
- V.A. Dzuba, V.V. Flambaum, and M.S. Safronova. *Phys. Rev. A*, **73**, 022112 (2006). doi:10.1103/PhysRevA.73.022112.
- G. Gopakumar, H. Merlitz, R.K. Chaudhuri, B.P. Das, U.S. Mahapatra, and D. Mukherjee. *Phys. Rev. A*, **66**, 032505 (2002). doi:10.1103/PhysRevA.66.032505.
- S.A. Blundell, W.R. Johnson, and J. Sapirstein. *Phys. Rev. A*, **43**, 3407 (1991). doi:10.1103/PhysRevA.43.3407. PMID: 9905424.
- D. Jiang, B. Arora, M.S. Safronova, and C.W. Clark. *J. Phys. B*, **42**, 154020 (2009). doi:10.1088/0953-4075/42/15/154020.
- B.K. Sahoo, M.R. Islam, B.P. Das, R.K. Chaudhuri, and D. Mukherjee. *Phys. Rev. A*, **74**, 062504 (2006). doi:10.1103/PhysRevA.74.062504.
- J. Mitroy, J.Y. Zhang, and M.W.J. Bromley. *Phys. Rev. A*, **77**, 032512 (2008). doi:10.1103/PhysRevA.77.032512.
- L. Głowacki and J. Migdalek. *Phys. Rev. A*, **80**, 042505 (2009). doi:10.1103/PhysRevA.80.042505.
- V.A. Dzuba and V.V. Flambaum. *Phys. Rev. A*, **77**, 012515 (2008). doi:10.1103/PhysRevA.77.012515.
- U.I. Safronova and W.R. Johnson. *Phys. Rev. A*, **69**, 052511 (2004). doi:10.1103/PhysRevA.69.052511.
- E.H. Pinnington, R.W. Berends, and M. Lumsden. *J. Phys. B*, **28**, 2095 (1995). doi:10.1088/0953-4075/28/11/009.
- A.A. Madej and J.D. Sankey. *Phys. Rev. A*, **41**, 2621 (1990). doi:10.1103/PhysRevA.41.2621. PMID:9903395.
- C. Knab-Bernardini, H. Knab, F. Vedel, and G. Werth. *Z. Phys. D*, **24**, 339 (1992). doi:10.1007/BF01426681.
- N. Yu, W. Nagourney, and H. Dehmelt. *Phys. Rev. Lett.* **78**, 4898 (1997). doi:10.1103/PhysRevLett.78.4898.
- M. Henderson, L.J. Curtis, R. Matulioniene, D.G. Ellis, and C.E. Theodosiou. *Phys. Rev. A*, **56**, 1872 (1997). doi:10.1103/PhysRevA.56.1872.
- E.H. Pinnington, J.J. van Hunen, R.N. Gosselin, B. Guo, and R.W. Berends. *Phys. Scr.* **49**, 331 (1994). doi:10.1088/0031-8949/49/3/012.
- S. Mannervik, J. Lidberg, L.-O. Norlin, P. Royen, A. Schmitt, W. Shi, and X. Tordoir. *Phys. Rev. Lett.* **83**, 698 (1999). doi:10.1103/PhysRevLett.83.698.
- E. Biémont, J. Lidberg, S. Mannervik, L.-O. Norlin, P. Royen, A. Schmitt, W. Shi, and X. Tordoir. *Eur. Phys. J. D*, **11**, 355 (2000). doi:10.1007/s100530070063.
- U.I. Safronova, I.M. Savukov, M.S. Safronova, and W.R. Johnson. *Phys. Rev. A*, **68**, 062505 (2003). doi:10.1103/PhysRevA.68.062505.
- B.K. Sahoo, B.P. Das, and D. Mukherjee. *Phys. Rev. A*, **79**, 052511 (2009). doi:10.1103/PhysRevA.79.052511.
- J. Sucher. *Phys. Rev. A*, **22**, 348 (1980). doi:10.1103/PhysRevA.22.348.
- J. Goldstone. *Proc. R. Soc. Lond. A Math. Phys. Sci.* **239**, 267 (1957). doi:10.1098/rspa.1957.0037.
- S.A. Blundell, W.R. Johnson, and J. Sapirstein. *Phys. Rev. A*, **42**, 3751 (1990). doi:10.1103/PhysRevA.42.3751. PMID: 9904471.
- S.A. Blundell, W.R. Johnson, Z.W. Liu, and J. Sapirstein. *Phys. Rev. A*, **40**, 2233 (1989). doi:10.1103/PhysRevA.40.2233. PMID:9902395.
- Z.W. Liu. Ph.D. thesis, Notre Dame University. 1989.
- S.A. Blundell, W.R. Johnson, and J. Sapirstein. *Phys. Rev. A*, **43**, 3407 (1991). doi:10.1103/PhysRevA.43.3407. PMID: 9905424.
- M.S. Safronova, A. Derevianko, and W.R. Johnson. *Phys. Rev. A*, **58**, 1016 (1998). doi:10.1103/PhysRevA.58.1016.
- M.S. Safronova, W.R. Johnson, and A. Derevianko. *Phys. Rev. A*, **60**, 4476 (1999). doi:10.1103/PhysRevA.60.4476.
- U.I. Safronova and W.R. Johnson. *Phys. Rev. A*, **69**, 052511 (2004). doi:10.1103/PhysRevA.69.052511.
- U.I. Safronova, M.S. Safronova, and W.R. Johnson. *Phys. Rev. A*, **71**, 052506 (2005). doi:10.1103/PhysRevA.71.052506.
- W.R. Johnson, S.A. Blundell, and J. Sapirstein. *Phys. Rev. A*, **37**, 307 (1988). doi:10.1103/PhysRevA.37.307. PMID: 9899658.
- C.E. Moore. *Atomic Energy Levels - v. III, NSRDS-NBS 35*. U.S. Government Printing Office, Washington, DC, USA. 1971.
- M.S. Safronova, W.R. Johnson, and U.I. Safronova. *Phys. Rev. A*, **53**, 4036 (1996). doi:10.1103/PhysRevA.53.4036. PMID: 9913369.
- M.S. Safronova, W.R. Johnson, and U.I. Safronova. *J. Phys. B*, **30**, 2375 (1997). doi:10.1088/0953-4075/30/10/012.
- L.W. Fullerton and G.A. Rinker, Jr. *Phys. Rev. A*, **13**, 1283 (1976). doi:10.1103/PhysRevA.13.1283.

43. P.J. Mohr. *Ann. Phys.* **88**, 26 (1974). doi:10.1016/0003-4916(74)90398-4.
44. P.J. Mohr. *Ann. Phys.* **88**, 52 (1974). doi:10.1016/0003-4916(74)90399-6.
45. P.J. Mohr. *Phys. Rev. Lett.* **34**, 1050 (1975). doi:10.1103/PhysRevLett.34.1050.
46. S.A. Blundell, D.S. Guo, W.R. Johnson, and J. Sapirstein. *At. Data Nucl. Data Tables*, **37**, 103 (1987). doi:10.1016/0092-640X(87)90006-4.
47. W.R. Johnson, D.R. Plante, and J. Sapirstein. *Adv. At. Mol. Opt. Phys.* **35**, 255 (1995).
48. W.R. Johnson, Z.W. Liu, and J. Sapirstein. *At. Data Nucl. Data Tables*, **64**, 279 (1996). doi:10.1006/adnd.1996.0024.
49. W.R. Johnson, S.A. Blundell, and J. Sapirstein. *Phys. Rev. A*, **37**, 2764 (1988). doi:10.1103/PhysRevA.37.2764. PMID: 9900004.
50. W.R. Johnson, Z.W. Liu, and J. Sapirstein. *At. Data Nucl. Data Tables*, **64**, 279 (1996). doi:10.1006/adnd.1996.0024.
51. A. Derevianko and E.D. Emmons. *Phys. Rev. A*, **66**, 012503 (2002). doi:10.1103/PhysRevA.66.012503.
52. G. Gopakumar, H. Merlitz, R.K. Chaudhuri, B.P. Das, U.S. Mahapatra, and D. Mukherjee. *Phys. Rev. A*, **66**, 032505 (2002). doi:10.1103/PhysRevA.66.032505.
53. U.I. Safronova, W.R. Johnson, D. Kato, and S. Ohtani. *Phys. Rev. A*, **63**, 032518 (2001). doi:10.1103/PhysRevA.63.032518.
54. V.A. Dzuba, V.V. Flambaum, and J.S.M. Ginges. *Phys. Rev. A*, **63**, 062101 (2001). doi:10.1103/PhysRevA.63.062101.
55. C. Guet and W.R. Johnson. *Phys. Rev. A*, **44**, 1531 (1991). doi:10.1103/PhysRevA.44.1531. PMID:9906115.