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# Relativistic many-body calculation of energies, lifetimes, polarizabilities, and hyperpolarizabilities in Li-like $\text{Be}^+$

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Excitation energies of the  $ns$ ,  $np$ ,  $nd$ , and  $nf$  ( $n \leq 9$ ) states in Li-like  $\text{Be}^+$  are evaluated within the framework of relativistic many-body theory. First-, second-, third-, and all-order Coulomb energies and first- and second-order Breit corrections to energies are calculated. Two alternative treatments of the Breit interaction are investigated. In the first approach, we omit Breit contributions to the Dirac-Fock potential and evaluate Coulomb and Breit-Coulomb corrections through second order perturbatively. In the second approach, we include both Coulomb and Breit contributions on the same footing via the Breit-Dirac-Fock potential and then treat the residual Breit and Coulomb interactions perturbatively. The results obtained from the two approaches are compared and discussed. All-order calculations of reduced matrix elements, oscillator strengths, transition rates, and lifetimes are given for levels up to  $n = 9$ . Electric-dipole ( $2s - np$ ), electric-quadrupole ( $2s - nd$ ), and electric-octupole ( $2s - nf$ ), matrix elements are evaluated in order to obtain the corresponding ground state multipole polarizabilities using the sum-over-states approach. Recommended values are provided for a large number of electric-dipole matrix elements. Scalar and tensor polarizabilities for the  $ns$ ,  $np_{1/2}$ ,  $np_{3/2}$ ,  $nd_{3/2}$ , and  $nd_{5/2}$  states with  $n \leq 9$  are also calculated. Scalar hyperpolarizability for the ground  $2s$  state is evaluated and compared with non-relativistic calculation.

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## I. INTRODUCTION

In the present paper, we report a systematic *ab initio* relativistic study of  $\text{Be}^+$  properties, including calculations of excitation energies, oscillator strengths, transition rates, lifetimes, polarizabilities and hyperpolarizability in Li-like beryllium. The calculations are carried out using a high-precision relativistic all-order method which includes all single, double (SD), and partial triple excitations (SDpT) of the Dirac-Fock wave functions [1]. In 2012, all-order calculations of neutral Li oscillator strengths, lifetimes, and polarizabilities [2] were found in excellent agreement with benchmark high-precision results obtained with Hylleraas basis functions [3–7]. Recently, oscillator strengths, polarizabilities and hyperpolarizabilities in Li-like beryllium evaluated using Hylleraas basis functions were presented by Tang *et al.* [8, 9]. We compare our values with these calculations as well as provide a large number of recommended data for other states. These calculations provide recommended values critically evaluated for their accuracy for a number of  $\text{Be}^+$  atomic properties useful for a variety of applications.

We start with a review of relevant theoretical and experimental studies. Most accurate calculations of the oscillator strengths, lifetimes, polarizabilities in neutral lithium were obtained using Hylleraas basis functions [3–7, 10–21]. A review of Li polarizabilities was recently given in [22].

Early theoretical calculations and measurements of en-

ergies, wavelengths, oscillator strengths, transition rates, polarizabilities, and lifetimes in  $\text{Be}^+$  were presented in Refs. [14, 23–62]. Recently published comprehensive critical NIST compilation by Fuhr and Wiese [63] included the energies, wavelengths and transition rates for allowed and forbidden transitions of  $\text{Be}^+$ . Recommended values of the line strengths, oscillator strengths, and transition rates in Ref. [63] were based on accurate theoretical calculations presented by Yan *et al.* [14], Godefroid *et al.* [23], Froese Fisher *et al.* [27], Qu *et al.* [25, 26], Chung [34], and Peach *et al.* [40].

The Hylleraas-type variational method was used in Ref. [14] to calculate the energies of the lithium  $2s$  and  $2p$  isoelectronic sequences up to  $Z = 20$ . The oscillator strengths for the  $2s \rightarrow 2p$  transitions were evaluated for  $Z$  up to 20 including finite nuclear mass effects; the corresponding lifetimes were also determined [14]. The multiconfiguration Hartree-Fock method was used in [23] to calculate wavefunctions in the infinite nuclear mass limit for the  $1s^2ns \ ^2S$  ( $n = 2-4$ ),  $1s^2np \ ^2P$  ( $n = 2-3$ ), and  $1s^23d \ ^2D$  terms of lithium-like ions ( $3 \leq Z \leq 8$ ). Line strength and transition rates were evaluated for the  $2s - 2p$ ,  $2s - 3p$ ,  $3s - 3p$ ,  $2p - 3s$ ,  $2p - 4s$ ,  $3p - 4s$ ,  $2p - 3d$ , and  $3p - 3d$  transitions [23]. Multiconfiguration Breit-Pauli energy levels, lifetimes, and transition data were presented by Froese Fisher *et al.* [27] for the lithium sequence in the range  $Z \leq 8$ . All  $J$ -levels of the six lowest  $2L$  terms, namely those with configuration labels  $2s$ ,  $2p$ ,  $3s$ ,  $3p$ ,  $3d$ , and  $4s$  were included. The nonrelativistic

dipole length, velocity, and acceleration absorption oscillator strengths for the  $2s - np$  ( $3 \leq Z \leq 9$ ) transitions of the lithium isoelectronic sequence up to  $Z = 10$  were calculated by using the energies and the multiconfiguration wave functions obtained from a full core plus correlation (FCPC) method [25]. Authors underlined that in most cases, the  $f$ -values from the length and velocity formulae were in agreement up to forth or fifth digit [25]. The same method was used in Refs. [24, 26] to evaluate oscillator strengths for the  $2p - nd$  ( $3 \leq n \leq 9$ ) and  $3d - nd$  ( $4 \leq n \leq 9$ ) transitions of the lithium isoelectronic sequence up to  $Z = 10$ . Theoretical wavelengths, oscillator strengths, line strengths, and transition probabilities for the E1, M1, and E2 transitions among states in Li isoelectronic sequence were evaluated by Cheng *et al.* [43]. The multiconfiguration Dirac-Fock technique was used to calculate necessary energy levels and wave functions. In addition to relativistic effects arising from the Dirac Hamiltonian and the Breit operator, authors included the Lamb shift of the  $1s$ ,  $2s$ , and  $2p_{1/2}$  electrons [43].

The oscillator strengths of all allowed transitions between the singly excited states of  $\text{Be}^+$  with principal quantum numbers up to  $n = 11$  were calculated within the Coulomb approximation with a Hartree-Slater core (CAHS) approach [37]. The results were subsequently combined to obtain the radiative lifetimes of the excited states. Tabulated results were given by Theodosiou [37] for the  $ns$ ,  $np$ ,  $nd$ ,  $nf$ , and  $ng$  states up to  $n = 12$ . Lifetime of the  $2p_{1/2}$  and  $2p_{3/2}$  levels in the lithium isoelectronic sequence were computed by Theodosiou *et al.* [38] using the semiempirical Coulomb approximation with a Hartree-Slater core. Isoelectronic trends of line strength data in the Li isoelectronic sequences were presented by Träbert and Curtis [64]. Authors proposed that the decays of the  $2p_{1/2}$  and  $2p_{3/2}$  levels of Li-like ions can be used as simple-atom test beds for lifetime measurements and for the development of accurate calculations of the transition rates. The experimental data were summarized and filtered in order to obtain consistent data sets and isoelectronic trends that can be compared with theoretical predictions. The graphical presentation of line strength data enables direct comparison and evaluation of the merit of data along extended isoelectronic sequences [64].

The energy levels of the  $ns$ ,  $np_{1/2}$ ,  $2p_{3/2}$  ( $n = 2-3$ ),  $3d_{3/2}$ , and  $3d_{5/2}$  levels of Li-like ions with  $Z = 2-16$  were calculated by Safronova [52] using the perturbation theory method (MZ code). The  $Z$ -expansion method allowed to describe the correlation part of the energy in the first, second, and higher orders of the perturbation theory. Relativistic effects were taken into account by the Breit-Pauli operators [52]. Relativistic all-order calculations of energies and matrix elements for Li and  $\text{Be}^+$  were presented by Blundell *et al.* [39]. Valence removal energies, hyperfine constants, and E1 transition amplitudes were calculated for the  $2s$ ,  $2p_{1/2}$ ,  $2p_{3/2}$ , and  $3s$ , states of Li and  $\text{Be}^+$ . This calculation was a significant improve-

ment over the earlier second- and third-order many-body perturbation theory (MBPT) calculations, and included infinite subset of MBPT terms evaluated using all-order methods [39]. The nonrelativistic energies of the lithiumlike  $ns$ ,  $nd$  ( $n = 3, 4$ , and  $5$ ), and  $nf$  ( $n = 4$  and  $5$ ) states for  $Z = 3$  to  $10$  were calculated by Wang *et al.* [35, 36] using a full-core-plus-correlation method with multiconfiguration-interaction wave functions. Relativistic and mass-polarization effects were treated as the first-order perturbation corrections. The quantum-electrodynamic (QED) correction to the energy was included using effective nuclear charge [35, 36].

The dipole polarizabilities of the lithium-like ground states,  $2s$  were calculated by Wang and Chung [33] using the full-core plus correlation (FCFC) wavefunctions. The non-relativistic polarizabilities were obtained by using a variation-perturbation method. Based on the relativistic and QED correction to the energy, the dipole polarizabilities were corrected using an oscillator strength formula [33]. The same approximation was used by Chen and Wang [65] to evaluate the quadrupole and octupole polarizabilities for the ground states of lithiumlike systems from  $Z = 3$  to  $20$ . The polarizabilities and hyperpolarizabilities of the  $\text{Be}^+$  ion in the  $2s$  and  $2p$  states were determined by Tang *et al.* [8]. Calculations were performed using two independent methods: variationally determined wave functions using Hylleraas basis set expansions and single-electron calculations utilizing a frozen-core Hamiltonian. The dynamic dipole polarizabilities for Li atoms and  $\text{Be}^+$  ions in the  $2s$  and  $2p$  states were calculated using the variational method with a Hylleraas basis in [9]. Corrections due to relativistic effects were also estimated. Analytic representations of the polarizabilities for frequency ranges encompassing the  $n = 3$  excitations were presented in Ref. [9].

In the present paper, we investigate all of the above properties of the ground and excited states of Li-like  $\text{Be}^+$  using the relativistic all-order method described in [1]. In particular, we evaluate excitation energies of  $ns$ ,  $np$ ,  $nd$ , and  $nf$  states with  $n \leq 10$ , reduced matrix elements, oscillator strengths, transition rates, and lifetimes for levels with  $n \leq 9$ , ground state E1, E2, and E3 static polarizabilities, scalar and tensor polarizabilities for the  $np_{1/2}$ ,  $np_{3/2}$  ( $n = 2-9$ ),  $nd_{3/2}$ , and  $nd_{5/2}$  ( $n = 3-9$ ) states. Scalar hyperpolarizability for the ground  $2s_{1/2}$  state is evaluated and compared with non-relativistic calculations. We use a complete set of DF wave functions on a nonlinear grid generated using B-splines [66] constrained to a spherical cavity. A cavity radius of  $220 a_0$  is chosen to accommodate all valence orbitals with  $n < 13$  so we can use experimental energies for these states. The basis set consists of 70 splines of order 11 for each value of the relativistic angular quantum number  $\kappa$ .

TABLE I: Energy calculated with a Dirac-Fock (DF) and Breit-Dirac-Fock (BDF) potentials. Zeroth-orders (DF) and (BDF), single-double Coulomb energies  $E^{(SD)}$ ,  $E^{(BSD)}$ ,  $E_{\text{extra}}^{(3)}$ , first-order  $B^{(1)}$  and second-order Breit-Coulomb ( $B^{(2)}$  and  $BB^{(2)}$ ) corrections, Lamb shift  $E_{\text{LS}}$  corrections in  ${}^9\text{Be}^+$  are listed. The total energies ( $E_{\text{tot}}^{(SD)} = E^{(DF)} + E^{(SD)} + E_{\text{extra}}^{(3)} + B^{(1)} + B^{(2)} + E_{\text{LS}}$  and  $E_{\text{tot}}^{(BSD)} = E^{(BDF)} + E^{(BSD)} + E_{\text{extra}}^{(3)} + BB^{(2)} + E_{\text{LS}}$ ) are compared with experimental energies  $E_{\text{NIST}}$  [73],  $\delta E = E_{\text{tot}} - E_{\text{NIST}}$ . Units:  $\text{cm}^{-1}$ . The value of the infinite mass Rydberg constant used to convert numerical data from a.u. to  $\text{cm}^{-1}$  is  $R_y = 10973.7316$ .

$nlj$	$E^{(DF)}$	$E^{(SD)}$	$E_{\text{extra}}^{(3)}$	$B^{(1)}$	$B^{(2)}$	$E_{\text{LS}}$	$E_{\text{tot}}^{(SD)}$	$E^{(BDF)}$	$E^{(BSD)}$	$BB^{(2)}$	$E_{\text{tot}}^{(BSD)}$	$E_{\text{NIST}}$	$\delta E^{(SD)}$	$\delta E^{(BSD)}$
$2s_{1/2}$	-146210.3	-690.27	2.45	5.64	-1.77	1.10	-146893.2	-146205.1	-690.32	-1.33	-146893.2	-146882.9	-10.3	-10.4
$2p_{1/2}$	-114005.4	-959.58	4.06	5.99	-1.30	0.00	-114956.2	-114000.3	-959.52	-0.44	-114956.2	-114954.1	-2.1	-2.1
$2p_{3/2}$	-113996.5	-958.77	4.05	2.88	-1.19	0.00	-114949.5	-113994.5	-958.84	-0.34	-114949.6	-114947.5	-2.0	-2.1
$3s_{1/2}$	-58495.1	-161.28	0.35	1.43	-0.47	0.22	-58654.9	-58493.8	-161.30	-0.35	-58654.9	-58650.9	-3.9	-3.9
$3p_{1/2}$	-50133.8	-257.80	0.98	1.87	-0.42	0.00	-50389.2	-50132.2	-257.79	-0.16	-50389.2	-50387.5	-1.7	-1.7
$3p_{3/2}$	-50131.1	-257.57	0.97	0.88	-0.38	0.00	-50387.2	-50130.5	-257.59	-0.13	-50387.3	-50385.6	-1.7	-1.7
$3d_{3/2}$	-48788.5	-42.99	0.41	0.02	0.00	0.00	-48831.1	-48788.5	-43.00	0.01	-48831.1	-48828.3	-2.8	-2.8
$3d_{5/2}$	-48788.0	-42.99	0.41	0.00	0.00	0.00	-48830.5	-48788.0	-43.00	0.01	-48830.9	-48827.8	-2.8	-3.2
$4s_{1/2}$	-31358.9	-62.14	0.11	0.57	-0.19	0.09	-31420.4	-31358.4	-62.14	-0.14	-31420.4	-31418.4	-2.0	-2.0
$4p_{1/2}$	-28019.4	-105.13	0.39	0.79	-0.18	0.00	-28123.5	-28018.7	-105.13	-0.07	-28123.5	-28122.3	-1.2	-1.2
$4p_{3/2}$	-28018.3	-105.04	0.39	0.37	-0.16	0.00	-28122.7	-28018.0	-105.05	-0.06	-28122.7	-28121.5	-1.2	-1.2
$4d_{3/2}$	-27443.8	-19.68	0.18	0.00	0.00	0.00	-27463.3	-27443.8	-19.68	0.00	-27463.3	-27461.7	-1.6	-1.6
$4d_{5/2}$	-27443.5	-19.68	0.18	0.00	0.00	0.00	-27463.0	-27443.5	-19.68	0.00	-27463.2	-27461.4	-1.6	-1.8
$4f_{5/2}$	-27434.6	-3.38	0.04	0.00	0.00	0.00	-27437.9	-27434.6	-3.38	0.00	-27438.0	-27436.3	-1.7	-1.7
$4f_{7/2}$	-27434.5	-3.37	0.04	0.00	0.00	0.00	-27437.8	-27434.5	-3.38	0.00	-27437.8	-27436.1	-1.7	-1.7
$5s_{1/2}$	-19518.9	-30.31	0.05	0.29	-0.09	0.04	-19548.9	-19518.7	-30.31	-0.07	-19549.0	-19547.7	-1.2	-1.2
$5p_{1/2}$	-17859.6	-52.94	0.19	0.40	-0.09	0.00	-17912.0	-17859.2	-52.94	-0.04	-17912.0	-17911.2	-0.8	-0.8
$5p_{3/2}$	-17859.0	-52.89	0.19	0.20	-0.08	0.00	-17911.6	-17858.9	-52.90	-0.03	-17911.6	-17910.8	-0.8	-0.8
$5d_{3/2}$	-17563.4	-10.44	0.09	0.00	0.00	0.00	-17573.8	-17563.4	-10.44	0.00	-17573.8	-17572.7	-1.0	-1.0
$5d_{5/2}$	-17563.3	-10.43	0.09	0.00	0.00	0.00	-17573.6	-17563.3	-10.44	0.00	-17573.7	-17572.6	-1.0	-1.1
$5f_{5/2}$	-17558.1	-1.93	0.02	0.00	0.00	0.00	-17560.1	-17558.1	-1.93	0.00	-17560.1	-17559.0	-1.0	-1.1
$5f_{7/2}$	-17558.1	-1.93	0.02	0.00	0.00	0.00	-17560.0	-17558.1	-1.93	0.00	-17560.0	-17558.9	-1.0	-1.1
$6s_{1/2}$	-13310.4	-17.02	0.03	0.15	-0.05	0.02	-13327.3	-13310.3	-17.02	-0.04	-13327.3	-13326.4	-0.8	-0.8
$6p_{1/2}$	-12368.1	-30.34	0.11	0.24	-0.05	0.00	-12398.2	-12367.9	-30.34	-0.02	-12398.2	-12397.5	-0.7	-0.7
$6p_{3/2}$	-12367.8	-30.31	0.11	0.11	-0.05	0.00	-12397.9	-12367.7	-30.32	-0.02	-12397.9	-12397.3	-0.7	-0.7
$6d_{3/2}$	-12196.4	-6.15	0.06	0.00	0.00	0.00	-12202.5	-12196.4	-6.15	0.00	-12202.5	-12201.7	-0.8	-0.8
$6d_{5/2}$	-12196.3	-6.15	0.06	0.00	0.00	0.00	-12202.4	-12196.3	-6.15	0.00	-12202.5	-12201.7	-0.7	-0.8
$6f_{5/2}$	-12193.2	-1.18	0.01	0.00	0.00	0.00	-12194.3	-12193.2	-1.18	0.00	-12194.3	-12193.7	-0.7	-0.7
$6f_{7/2}$	-12193.1	-1.18	0.01	0.00	0.00	0.00	-12194.3	-12193.1	-1.18	0.00	-12194.3	-12193.6	-0.6	-0.7
$7s_{1/2}$	-9654.3	-10.49	0.02	0.09	-0.03	0.02	-9664.7	-9654.2	-10.49	-0.02	-9664.7	-9664.1	-0.6	-0.6
$7p_{1/2}$	-9068.6	-18.99	0.07	0.15	-0.03	0.00	-9087.4	-9068.5	-18.99	-0.01	-9087.4	-9086.9	-0.5	-0.5
$7p_{3/2}$	-9068.4	-18.97	0.07	0.07	-0.03	0.00	-9087.2	-9068.3	-18.97	-0.01	-9087.2	-9086.7	-0.5	-0.5
$7d_{3/2}$	-8960.3	-3.92	0.04	0.00	0.00	0.00	-8964.2	-8960.3	-3.92	0.00	-8964.2	-8963.7	-0.5	-0.5
$7d_{5/2}$	-8960.3	-3.92	0.00	0.00	0.00	0.00	-8964.2	-8960.3	-3.92	0.00	-8964.2	-8963.7	-0.5	-0.5
$7f_{5/2}$	-8958.2	-0.77	0.01	0.00	0.00	0.00	-8959.0	-8958.2	-0.77	0.00	-8959.0	-8958.5	-0.4	-0.4
$7f_{7/2}$	-8958.2	-0.76	0.01	0.00	0.00	0.00	-8959.0	-8958.2	-0.77	0.00	-8959.0	-8958.5	-0.4	-0.4
$8s_{1/2}$	-7321.3	-6.92	0.01	0.07	-0.02	0.00	-7328.2	-7321.2	-6.92	-0.02	-7328.2	-7327.7	-0.5	-0.5
$8p_{1/2}$	-6932.6	-12.66	0.05	0.09	-0.02	0.00	-6945.2	-6932.5	-12.66	-0.01	-6945.2	-6944.8	-0.4	-0.4
$8p_{3/2}$	-6932.5	-12.65	0.05	0.04	-0.02	0.00	-6945.1	-6932.5	-12.65	-0.01	-6945.1	-6944.7	-0.4	-0.4
$8d_{3/2}$	-6860.1	-2.64	0.02	0.00	0.00	0.00	-6862.7	-6860.1	-2.64	0.00	-6862.7	-6862.3	-0.4	-0.4
$8d_{5/2}$	-6860.1	-2.64	0.00	0.00	0.00	0.00	-6862.7	-6860.1	-2.64	0.00	-6862.7	-6862.3	-0.4	-0.4
$8f_{5/2}$	-6858.6	-0.52	0.01	0.00	0.00	0.00	-6859.2	-6858.6	-0.52	0.00	-6859.2	-6858.7	-0.4	-0.4
$8f_{7/2}$	-6858.6	-0.52	0.01	0.00	0.00	0.00	-6859.1	-6858.6	-0.52	0.00	-6859.1	-6858.7	-0.4	-0.4
$9s_{1/2}$	-5742.2	-4.81	0.01	0.04	-0.02	0.00	-5746.9	-5742.1	-4.81	-0.01	-5746.9	-5746.6	-0.4	-0.4
$9p_{1/2}$	-5471.2	-8.87	0.03	0.07	-0.02	0.00	-5479.9	-5471.1	-8.87	-0.01	-5479.9	-5479.6	-0.3	-0.3
$9p_{3/2}$	-5471.1	-8.86	0.03	0.02	-0.02	0.00	-5479.9	-5471.0	-8.86	-0.01	-5479.9	-5479.5	-0.3	-0.3
$9d_{3/2}$	-5420.2	-1.86	0.00	0.00	0.00	0.00	-5422.1	-5420.2	-1.86	0.00	-5422.1	-5421.7	-0.3	-0.3
$9d_{5/2}$	-5420.2	-1.86	0.00	0.00	0.00	0.00	-5422.0	-5420.2	-1.86	0.00	-5422.0	-5421.7	-0.3	-0.3
$9f_{5/2}$	-5419.2	-0.37	0.00	0.00	0.00	0.00	-5419.5	-5419.2	-0.37	0.00	-5419.5	-5419.2	-0.3	-0.3
$9f_{7/2}$	-5419.2	-0.37	0.00	0.00	0.00	0.00	-5419.5	-5419.2	-0.37	0.00	-5419.5	-5419.2	-0.3	-0.3
$10s_{1/2}$	-4623.9	-3.48	0.00	0.02	-0.02	0.00	-4627.3	-4623.8	-3.48	-0.01	-4627.3	-4627.0	-0.3	-0.3
$10p_{1/2}$	-4427.4	-6.49	0.02	0.04	-0.02	0.00	-4433.9	-4427.4	-6.49	-0.01	-4433.9	-4433.6	-0.3	-0.3
$10p_{3/2}$	-4427.4	-6.46	0.02	0.02	-0.02	0.00	-4433.8	-4427.4	-6.46	-0.01	-4433.8	-4433.5	-0.3	-0.3
$10f_{5/2}$	-4389.5	-0.27	0.00	0.00	0.00	0.00	-4389.8	-4389.5	-0.27	0.00	-4389.8	-4389.5	-0.3	-0.3
$10f_{7/2}$	-4389.5	-0.27	0.00	0.00	0.00	0.00	-4389.8	-4389.5	-0.27	0.00	-4389.8	-4389.5	-0.3	-0.3

TABLE II: Recommended values of the reduced electric-dipole matrix elements in Li-like  $\text{Be}^+$  in atomic units. Final recommended values and their uncertainties are given in the  $Z^{\text{final}}$  column.

Transition	$Z^{\text{final}}$	Transition	$Z^{\text{final}}$	Transition	$Z^{\text{final}}$	Transition	$Z^{\text{final}}$	Transition	$Z^{\text{final}}$
$2s - 2p_{1/2}$	1.8506(2)	$3s - 2p_{1/2}$	0.8675(1)	$4s - 2p_{1/2}$	0.2838(0)	$5s - 2p_{1/2}$	0.1597(0)	$6s - 2p_{1/2}$	0.1079(0)
$2s - 2p_{3/2}$	2.6172(3)	$3s - 2p_{3/2}$	1.2271(3)	$4s - 2p_{3/2}$	0.4013(1)	$5s - 2p_{3/2}$	0.2258(1)	$6s - 2p_{3/2}$	0.1526(0)
$2s - 3p_{1/2}$	0.4347(0)	$3s - 3p_{1/2}$	4.6951(3)	$4s - 3p_{1/2}$	2.1611(3)	$5s - 3p_{1/2}$	0.6810(1)	$6s - 3p_{1/2}$	0.3774(0)
$2s - 3p_{3/2}$	0.6145(1)	$3s - 3p_{3/2}$	6.6400(4)	$4s - 3p_{3/2}$	3.0568(7)	$5s - 3p_{3/2}$	0.9632(1)	$6s - 3p_{3/2}$	0.5338(1)
$2s - 4p_{1/2}$	0.2403(0)	$3s - 4p_{1/2}$	0.7008(0)	$4s - 4p_{1/2}$	8.6922(6)	$5s - 4p_{1/2}$	3.9845(4)	$6s - 4p_{1/2}$	1.2201(1)
$2s - 4p_{3/2}$	0.3397(0)	$3s - 4p_{3/2}$	0.9907(3)	$4s - 4p_{3/2}$	12.2927(8)	$5s - 4p_{3/2}$	5.636(1)	$6s - 4p_{3/2}$	1.7257(2)
$2s - 5p_{1/2}$	0.1590(1)	$3s - 5p_{1/2}$	0.3941(0)	$4s - 5p_{1/2}$	1.0130(1)	$5s - 5p_{1/2}$	13.8507(9)	$6s - 5p_{1/2}$	6.3388(7)
$2s - 5p_{3/2}$	0.2249(0)	$3s - 5p_{3/2}$	0.5572(0)	$4s - 5p_{3/2}$	1.4319(5)	$5s - 5p_{3/2}$	19.588(1)	$6s - 5p_{3/2}$	8.966(2)
$2s - 6p_{1/2}$	0.1159(1)	$3s - 6p_{1/2}$	0.2641(1)	$4s - 6p_{1/2}$	0.5688(2)	$5s - 6p_{1/2}$	1.3737(3)	$6s - 6p_{1/2}$	20.172(1)
$2s - 6p_{3/2}$	0.1639(1)	$3s - 6p_{3/2}$	0.3734(1)	$4s - 6p_{3/2}$	0.8042(1)	$5s - 6p_{3/2}$	1.9416(2)	$6s - 6p_{3/2}$	28.527(2)
$2s - 7p_{1/2}$	0.0897(1)	$3s - 7p_{1/2}$	0.1948(1)	$4s - 7p_{1/2}$	0.3813(2)	$5s - 7p_{1/2}$	0.7669(3)	$6s - 7p_{1/2}$	1.7844(3)
$2s - 7p_{3/2}$	0.1268(1)	$3s - 7p_{3/2}$	0.2754(1)	$4s - 7p_{3/2}$	0.5391(1)	$5s - 7p_{3/2}$	1.0842(1)	$6s - 7p_{3/2}$	2.5221(4)
$2s - 8p_{1/2}$	0.0722(1)	$3s - 8p_{1/2}$	0.1522(1)	$4s - 8p_{1/2}$	0.2818(2)	$5s - 8p_{1/2}$	0.5120(4)	$6s - 8p_{1/2}$	0.9892(6)
$2s - 8p_{3/2}$	0.1020(1)	$3s - 8p_{3/2}$	0.2152(1)	$4s - 8p_{3/2}$	0.3985(2)	$5s - 8p_{3/2}$	0.7239(3)	$6s - 8p_{3/2}$	1.3985(3)
$2s - 9p_{1/2}$	0.0598(1)	$3s - 9p_{1/2}$	0.1236(2)	$4s - 9p_{1/2}$	0.2209(4)	$5s - 9p_{1/2}$	0.3777(7)	$6s - 9p_{1/2}$	0.657(1)
$2s - 9p_{3/2}$	0.0845(1)	$3s - 9p_{3/2}$	0.1748(1)	$4s - 9p_{3/2}$	0.3124(2)	$5s - 9p_{3/2}$	0.5344(4)	$6s - 9p_{3/2}$	0.9290(5)
$2p_{1/2} - 3d_{3/2}$	2.5084(0)	$2p_{1/2} - 4d_{3/2}$	0.9608(1)	$2p_{1/2} - 5d_{3/2}$	0.5596	$2p_{1/2} - 6d_{3/2}$	0.3837	$2p_{1/2} - 7d_{3/2}$	0.2867
$2p_{3/2} - 3d_{3/2}$	1.1219(1)	$2p_{3/2} - 4d_{3/2}$	0.4297(1)	$2p_{3/2} - 5d_{3/2}$	0.2503	$2p_{3/2} - 6d_{3/2}$	0.1716	$2p_{3/2} - 7d_{3/2}$	0.1282
$2p_{3/2} - 3d_{5/2}$	3.3657(2)	$2p_{3/2} - 4d_{5/2}$	1.2892(2)	$2p_{3/2} - 5d_{5/2}$	0.7508	$2p_{3/2} - 6d_{5/2}$	0.5148	$2p_{3/2} - 7d_{5/2}$	0.3846
$3p_{1/2} - 3d_{3/2}$	5.8534(7)	$3p_{1/2} - 4d_{3/2}$	3.8426(3)	$3p_{1/2} - 5d_{3/2}$	1.6090(1)	$3p_{1/2} - 6d_{3/2}$	0.9661(0)	$3p_{1/2} - 7d_{3/2}$	0.6736(0)
$3p_{3/2} - 3d_{3/2}$	2.6177(3)	$3p_{3/2} - 4d_{3/2}$	1.7187(3)	$3p_{3/2} - 5d_{3/2}$	0.7196(1)	$3p_{3/2} - 6d_{3/2}$	0.4321(0)	$3p_{3/2} - 7d_{3/2}$	0.3012(0)
$3p_{3/2} - 3d_{5/2}$	7.853(1)	$3p_{3/2} - 4d_{5/2}$	5.1560(8)	$3p_{3/2} - 5d_{5/2}$	2.1588(2)	$3p_{3/2} - 6d_{5/2}$	1.2962(0)	$3p_{3/2} - 7d_{5/2}$	0.9038(0)
$4p_{1/2} - 3d_{3/2}$	0.9972(0)	$4p_{1/2} - 4d_{3/2}$	12.0562(8)	$4p_{1/2} - 5d_{3/2}$	5.4853(5)	$4p_{1/2} - 6d_{3/2}$	2.3276(2)	$4p_{1/2} - 7d_{3/2}$	1.4058(1)
$4p_{3/2} - 3d_{3/2}$	0.4458(1)	$4p_{3/2} - 4d_{3/2}$	5.3917(4)	$4p_{3/2} - 5d_{3/2}$	2.4536(5)	$4p_{3/2} - 6d_{3/2}$	1.0410(2)	$4p_{3/2} - 7d_{3/2}$	0.6288(1)
$4p_{3/2} - 3d_{5/2}$	1.3375(2)	$4p_{3/2} - 4d_{5/2}$	16.175(1)	$4p_{3/2} - 5d_{5/2}$	7.360(1)	$4p_{3/2} - 6d_{5/2}$	3.1231(4)	$4p_{3/2} - 7d_{5/2}$	1.8863(2)
$5p_{1/2} - 3d_{3/2}$	0.3563(0)	$5p_{1/2} - 4d_{3/2}$	2.2833(1)	$5p_{1/2} - 5d_{3/2}$	19.905(1)	$5p_{1/2} - 6d_{3/2}$	7.430(1)	$5p_{1/2} - 7d_{3/2}$	3.1418(4)
$5p_{3/2} - 3d_{3/2}$	0.1593(0)	$5p_{3/2} - 4d_{3/2}$	1.0208(2)	$5p_{3/2} - 5d_{3/2}$	8.9016(6)	$5p_{3/2} - 6d_{3/2}$	3.3237(9)	$5p_{3/2} - 7d_{3/2}$	1.4052(2)
$5p_{3/2} - 3d_{5/2}$	0.4779(0)	$5p_{3/2} - 4d_{5/2}$	3.0628(5)	$5p_{3/2} - 5d_{5/2}$	26.705(2)	$5p_{3/2} - 6d_{5/2}$	9.971(2)	$5p_{3/2} - 7d_{5/2}$	4.2158(6)
$6p_{1/2} - 3d_{3/2}$	0.2013(1)	$6p_{1/2} - 4d_{3/2}$	0.8078(2)	$6p_{1/2} - 5d_{3/2}$	4.0169(4)	$6p_{1/2} - 6d_{3/2}$	29.455(2)	$6p_{1/2} - 7d_{3/2}$	9.6778(2)
$6p_{3/2} - 3d_{3/2}$	0.0900(0)	$6p_{3/2} - 4d_{3/2}$	0.3612(0)	$6p_{3/2} - 5d_{3/2}$	1.7959(1)	$6p_{3/2} - 6d_{3/2}$	13.1728(9)	$6p_{3/2} - 7d_{3/2}$	4.3290(6)
$6p_{3/2} - 3d_{5/2}$	0.2701(1)	$6p_{3/2} - 4d_{5/2}$	1.0837(1)	$6p_{3/2} - 5d_{5/2}$	5.3883(1)	$6p_{3/2} - 6d_{5/2}$	39.518(2)	$6p_{3/2} - 7d_{5/2}$	12.9870(8)
$4f_{7/2} - 3d_{5/2}$	9.4461(4)	$4f_{5/2} - 3d_{5/2}$	2.1122(1)	$4f_{5/2} - 3d_{3/2}$	7.9031(4)	$5f_{7/2} - 3d_{5/2}$	3.0718	$6f_{7/2} - 3d_{5/2}$	1.6663(6)
$4f_{7/2} - 4d_{5/2}$	14.707(1)	$4f_{5/2} - 4d_{5/2}$	3.2885(3)	$4f_{5/2} - 4d_{3/2}$	12.304(1)	$5f_{7/2} - 4d_{5/2}$	12.9685(1)	$6f_{7/2} - 4d_{5/2}$	4.7877(3)
$4f_{7/2} - 5d_{5/2}$	1.5595(0)	$4f_{5/2} - 5d_{5/2}$	0.3487(0)	$4f_{5/2} - 5d_{3/2}$	1.3048(0)	$5f_{7/2} - 5d_{5/2}$	27.790(2)	$6f_{7/2} - 5d_{5/2}$	17.1194(1)
$4f_{7/2} - 6d_{5/2}$	0.5297(1)	$4f_{5/2} - 6d_{5/2}$	0.1184(0)	$4f_{5/2} - 6d_{3/2}$	0.4432(1)	$5f_{7/2} - 6d_{5/2}$	3.4248(1)	$6f_{7/2} - 6d_{5/2}$	43.316(3)
$4f_{7/2} - 7d_{5/2}$	0.2873(1)	$4f_{5/2} - 7d_{5/2}$	0.0642(0)	$4f_{5/2} - 7d_{3/2}$	0.2403(1)	$5f_{7/2} - 7d_{5/2}$	1.1788(1)	$6f_{7/2} - 7d_{5/2}$	5.8748(4)
$4f_{7/2} - 8d_{5/2}$	0.1888(1)	$4f_{5/2} - 8d_{5/2}$	0.0422(0)	$4f_{5/2} - 8d_{3/2}$	0.1580(1)	$5f_{7/2} - 8d_{5/2}$	0.6406(2)	$6f_{7/2} - 8d_{5/2}$	2.0345(5)
$4f_{7/2} - 9d_{5/2}$	0.1375(1)	$4f_{5/2} - 9d_{5/2}$	0.0307(0)	$4f_{5/2} - 9d_{3/2}$	0.1151(1)	$5f_{7/2} - 9d_{5/2}$	0.4209(2)	$6f_{7/2} - 9d_{5/2}$	1.1060(5)

## II. ALL-ORDER MBPT CALCULATIONS OF ENERGIES

Energies of  $nl_j$  states are evaluated for  $n \leq 10$  and  $l \leq 3$  using the single-double all-order (SD) method discussed in Ref. [67], in which all single and double excitations of Dirac-Fock (DF) wave functions are iterated to all orders. Results of our energy calculations are summarized in Table I. Columns 2–8 of Table I give the lowest-order DF energies  $E^{(\text{DF})}$ , the all-order SD energies in the column labeled  $E^{(\text{SD})}$ , and the part of the third-order energies missing from  $E^{(\text{SD})}$  in the column labeled  $E_{\text{extra}}^{(3)}$ . The first-order and second-order Breit corrections  $B^{(1)}$  and  $B^{(2)}$  and an estimated Lamb shift contribution,  $E_{\text{LS}}$ , are listed in columns 5–7. The sum of these contributions  $E_{\text{tot}}^{(\text{SD})}$ , listed in the eighth column of

Table I, is the final all-order result. The Lamb shift correction for  $ns$  states is estimated by scaling the  $2s$  Lamb shift ( $X_\alpha = 2/3$  case) given by Sapirstein and Cheng [68] with  $1/n^3$ . The  $2s$  Lamb shift from [68] is consistent with values found in Refs. [69, 70]. For states with  $l > 0$ , the Lamb-shift is estimated to be smaller than  $0.01 \text{ cm}^{-1}$  using scaled Coulomb values and can be omitted at the present level of precision.

As expected, the largest correlation contribution to the valence energy comes from the second-order term  $E^{(2)}$ . Therefore, we calculate this term with higher numerical accuracy. The second-order energy includes partial waves up to  $l_{\text{max}} = 8$  and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [71, 72]). As an example of the convergence of  $E^{(2)}$  with the number of partial waves  $l$ , consider the  $2s$  state.

TABLE III: Transition rates  $A_r$  ( $s^{-1}$ ), oscillator strengths ( $f$ ), and line strengths  $S$  (a.u.) for transitions in  $Be^+$  calculated using our recommended values of reduced electric-dipole matrix elements  $Z^{(final)}$  and their uncertainties. Our relativistic values are averaged over  $j$ . The relative uncertainties in the values of transition rates, oscillator strengths, and line strengths are the same. They are listed in the column labeled “Unc.” in percentages. Numbers in brackets represent powers of 10. Wavelengths  $\lambda$  ( $\text{\AA}$ ) are from NIST data [63].

Transitions	$\lambda$ $\text{\AA}$	$A_r$ $s^{-1}$	$f$	$S$ a.u.	Unc. %	Transitions	$\lambda$ $\text{\AA}$	$A_r$ $s^{-1}$	$f$	$S$ a.u.	Unc. %
$2^2S - 2^2P$	3131.5	1.130[8]	4.983[-1]	1.027[ 1]	0.015	$2^2P - 7^2D$	943.52	5.947[7]	1.323[-2]	2.465[-1]	0.036
$2^2S - 3^2P$	1036.3	1.719[8]	8.305[-2]	5.666[-1]	0.027	$2^2P - 8^2D$	925.18	3.915[7]	8.372[-3]	1.530[-1]	0.045
$2^2S - 4^2P$	842.03	9.793[7]	3.123[-2]	1.731[-1]	0.015	$2^2P - 9^2D$	913.01	2.716[7]	5.656[-3]	1.020[-1]	0.058
$2^2S - 5^2P$	775.36	5.497[7]	1.486[-2]	7.586[-2]	0.033	$3^2P - 3^2D$	64177	7.879[4]	8.109[-2]	1.028[ 2]	0.014
$2^2S - 6^2P$	743.57	3.310[7]	8.229[-3]	4.029[-2]	0.078	$3^2P - 4^2D$	4362.1	1.082[8]	5.141[-1]	4.430[ 1]	0.025
$2^2S - 7^2P$	725.71	2.131[7]	5.049[-3]	2.413[-2]	0.093	$3^2P - 5^2D$	3047.5	5.560[7]	1.290[-1]	7.767[ 0]	0.013
$2^2S - 8^2P$	714.60	1.445[7]	3.319[-3]	1.561[-2]	0.126	$3^2P - 6^2D$	2618.9	3.159[7]	5.414[-2]	2.800[ 0]	0.007
$2^2S - 9^2P$	707.20	1.023[7]	2.301[-3]	1.072[-2]	0.184	$3^2P - 7^2D$	2414.1	1.960[7]	2.855[-2]	1.361[ 0]	0.007
$3^2S - 3^2P$	12096	1.261[7]	8.301[-1]	6.613[ 1]	0.015	$3^2P - 8^2D$	2297.6	1.300[7]	1.714[-2]	7.779[-1]	0.007
$3^2S - 4^2P$	3275.6	1.415[7]	6.828[-2]	1.473[ 0]	0.040	$4^2P - 4^2D$	151450	2.544[4]	1.458[-1]	4.361[ 2]	0.014
$3^2S - 5^2P$	2454.6	1.064[7]	2.882[-2]	4.658[-1]	0.009	$4^2P - 5^2D$	9479.4	2.148[7]	4.822[-1]	9.029[ 1]	0.025
$4^2S - 4^2P$	30326	2.742[6]	1.135[ 0]	2.266[ 2]	0.015	$4^2P - 6^2D$	6281.4	1.329[7]	1.310[-1]	1.626[ 1]	0.014
$4^2S - 5^2P$	7403.3	2.561[6]	6.312[-2]	3.076[ 0]	0.041	$4^2P - 7^2D$	5219.7	8.448[6]	5.752[-2]	5.929[ 0]	0.014
$5^2S - 5^2P$	61090	8.523[5]	1.431[ 0]	5.755[ 2]	0.015	$4^2P - 8^2D$	4703.8	5.659[6]	3.128[-2]	2.907[ 0]	0.014
$2^2P - 3^2S$	1776.2	4.082[8]	6.437[-2]	2.259[ 0]	0.027	$5^2P - 5^2D$	295600	9.323[3]	2.036[-1]	1.189[ 3]	0.014
$2^2P - 4^2S$	1197.2	1.427[8]	1.022[-2]	2.415[-1]	0.027	$5^2P - 6^2D$	17511	6.247[6]	4.788[-1]	1.657[ 2]	0.028
$2^2P - 5^2S$	1048.2	6.729[7]	3.694[-3]	7.649[-2]	0.042	$5^2P - 7^2D$	11174	4.299[6]	1.342[-1]	2.962[ 1]	0.014
$2^2P - 6^2S$	984.03	3.714[7]	1.797[-3]	3.493[-2]	0.042	$5^2P - 8^2D$	9050.8	2.940[6]	6.018[-2]	1.076[ 1]	0.025
$2^2P - 7^2S$	949.80	2.270[7]	1.023[-3]	1.919[-2]	0.045	$3^2D - 4^2P$	4829.5	8.941[6]	1.875[-2]	2.982[ 0]	0.024
$3^2P - 4^2S$	5272.1	9.690[7]	1.346[-1]	1.401[ 1]	0.027	$3^2D - 5^2P$	3234.5	3.800[6]	3.575[-3]	3.807[-1]	0.009
$3^2P - 5^2S$	3242.7	4.135[7]	2.172[-2]	1.392[ 0]	0.015	$4^2D - 5^2P$	10468	4.600[6]	4.535[-2]	1.564[ 1]	0.024
$3^2P - 6^2S$	2698.3	2.204[7]	8.018[-3]	4.273[-1]	0.027	$3^2D - 4^2F$	4674.7	2.212[8]	1.015[ 0]	1.562[ 2]	0.007
$3^2P - 7^2S$	2455.7	1.322[7]	3.985[-3]	1.933[-1]	0.027	$3^2D - 5^2F$	3198.1	7.307[7]	1.568[-1]	1.651[ 1]	0.020
$4^2P - 5^2S$	11660	3.042[7]	2.068[-1]	4.764[ 1]	0.027	$3^2D - 6^2F$	2729.7	3.457[7]	5.408[-2]	4.860[ 0]	0.056
$4^2P - 6^2S$	6758.9	1.466[7]	3.345[-2]	4.467[ 0]	0.015	$3^2D - 7^2F$	2508.2	1.946[7]	2.569[-2]	2.121[ 0]	0.056
$4^2P - 7^2S$	5417.8	8.482[6]	1.244[-2]	1.331[ 0]	0.015	$3^2D - 8^2F$	2382.7	1.216[7]	1.449[-2]	1.137[ 0]	0.070
$5^2P - 6^2S$	21807	1.177[7]	2.798[-1]	1.206[ 2]	0.027	$3^2D - 9^2F$	2303.7	8.156[6]	9.084[-3]	6.889[-1]	0.084
$5^2P - 7^2S$	12122	6.151[6]	4.520[-2]	1.082[ 1]	0.015	$4^2F - 5^2D$	10138	8.275[5]	9.109[-3]	4.257[ 0]	0.007
$2^2P - 3^2D$	1512.4	1.106[9]	6.320[-1]	1.888[ 1]	0.013	$5^2F - 6^2D$	18666	6.394[5]	2.386[-2]	2.053[ 1]	0.017
$2^2P - 4^2D$	1143.0	3.759[8]	1.227[-1]	2.770[ 0]	0.018	$6^2F - 7^2D$	30960	4.123[5]	4.232[-2]	6.040[ 1]	0.020
$2^2P - 5^2D$	1026.9	1.758[8]	4.631[-2]	9.395[-1]	0.038	$7^2F - 8^2D$	47704	2.599[5]	6.334[-2]	1.393[ 2]	0.047
$2^2P - 6^2D$	973.25	9.707[7]	2.298[-2]	4.416[-1]	0.031	$8^2F - 9^2D$	69588	1.663[5]	8.626[-2]	2.767[ 2]	0.010

Calculations of  $E^{(2)}$  with  $l_{\max} = 6$  and 8 yield  $E^{(2)}(2s) = -637.021$  and  $-638.021 \text{ cm}^{-1}$ , respectively. Extrapolation of these calculations yields  $-638.814$  and  $-638.873 \text{ cm}^{-1}$ , respectively. Thus, in this particular case, we have a numerical uncertainty in  $E^{(2)}(2s)$  of  $0.059 \text{ cm}^{-1}$ . It should be noted that the  $1.85 \text{ cm}^{-1}$  contribution from partial waves with  $l > 8$  for the  $2s$  state is the largest among all states considered in Table I; a smaller ( $1.00 \text{ cm}^{-1}$ ) contribution is obtained for two other  $n = 2$  states and much smaller contributions ( $0.01$ – $0.32 \text{ cm}^{-1}$ ) were found for the  $n = 3$  states.

Owing to numerical complexity, we restrict  $l \leq l_{\max} = 6$  in all third-order and all-order calculations. As noted above, the second-order contribution dominates, therefore, we can use the extrapolated values of  $E^{(2)}$  described above to account for the contributions of the higher partial waves. 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 I, which accounts for that part of the third-order MBPT energy missing from the SD expression for the energy, is smaller than the total third-order contribution  $E^{(3)}$  by an order of magnitude for the states considered here.

Recommended energies from the National Institute of Standards and Technology (NIST) database [73] are given in the column labeled  $E_{\text{NIST}}$ . Differences between our the all-order calculations and experimental data  $\delta E^{(\text{SD})} = E_{\text{tot}}^{(\text{SD})} - E_{\text{NIST}}$ , are given in the  $\delta E^{(\text{SD})}$  column of Table I.

The first-order and second-order Breit corrections  $B^{(1)}$  and  $B^{(2)}$  given in columns 5 a 6 of Table I are obtained with the Dirac-Fock potential were the Breit interaction was omitted. We evaluate Coulomb and Breit- Coulomb

TABLE IV: Oscillator strengths ( $f$ ) for transitions in  $\text{Be}^+$  calculated using our recommended values of reduced electric-dipole matrix elements  $Z^{(\text{final})}$  and their uncertainties. Our relativistic values  $f(nlj, n'l'j')$  are averaged over  $j$  and  $j'$ . Oscillator strengths calculated by Hylleraas bases functions [8, 14], FCCI[25] and MCHF[23] methods are compared with our results.

Transitions	Present	[8]	Theory
$2^2S - 2^2P$	0.49830(7)	0.49806736(6)	0.498067381(25)[14]
$2^2S - 3^2P$	0.08305(2)	0.08316525(18)	0.08136 [25]
$3^2S - 3^2P$	0.8301(1)	0.8297696(15)	
$2^2P - 3^2S$	0.06437(2)	0.06434157(29)	
$2^2P - 4^2S$	0.010216(3)	0.01021583(30)	
$3^2P - 4^2S$	0.13457(4)	0.1345245(13)	
$2^2P - 3^2D$	0.63195(8)	0.6319828(11)	0.63199[23]
$3^2P - 3^2D$	0.08109(1)	0.08103350(17)	
$3^2D - 4^2F$	1.0146(1)	1.01460194(11)	

corrections through second order perturbatively in such approach. In the second more accurate approach, we include both Coulomb and Breit contributions to the Breit-Dirac-Fock (BDF) potential and then treat the residual Breit and Coulomb interactions perturbatively. In this approximation the first-order Breit corrections  $B^{(1)}$  is equal to zero. The value of the second-order Breit corrections  $BB^{(2)}$  given in column 11 of Table I is smaller than the value of  $B^{(2)}$  (column 6) because the random-phase-approximation (RPA) diagram was removed from the  $B^{(2)}$  correction (see Sect. III of Ref. [74] for detail). Such RPA contribution is explicitly included by the use of the BDF potential. We find that the difference between the all-order contributions calculated with DF and BDF potentials is very small, less than 0.01%. We did not recalculate the extra third order correction since its contribution is small. The largest difference between two approximations is in the Breit correction as well as in the DF and BDF ( $E^{(\text{DF})}$   $E^{(\text{BDF})}$ ) energies.

The three terms  $E^{(\text{BDF})}$ ,  $E^{\text{BSD}}$ , and  $BB^{(2)}$  evaluated using the Breit-Dirac-Fock potential are displayed in columns 8, 9, and 10 of Table I. The final all-order result  $E_{\text{tot}}^{\text{BSD}}$  given in column 11 of Table I is obtained as a sum of the  $E^{(\text{BDF})}$ ,  $E^{\text{BSD}}$ ,  $BB^{(2)}$ ,  $E_{\text{extra}}^{(3)}$ , and  $E_{\text{LS}}$  terms. Differences between our the all-order calculations and experimental data  $\delta E^{(\text{BSD})} = E_{\text{tot}}^{(\text{BSD})} - E_{\text{NIST}}$ , are given in the  $\delta E^{(\text{SD})}$  column of Table I. We find that the higher-order Breit corrections that are included using the BDF potential are negligible for  $\text{Be}^+$ , since the results given in two last columns are almost identical.

### III. ELECTRIC-DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN LI-LIKE $\text{Be}^+$

#### A. Electric-dipole matrix elements

In Table II, we list our recommended values for 190 E1  $ns - n'p$ ,  $np - n'd$ , and  $nf - n'd$  transitions. The absolute values in atomic units ( $a_0e$ ) are given in all cases. We refer to these values as the recommended matrix elements. We note that we have calculated 489 E1 matrix elements that included all dipole transitions between the  $ns$ ,  $np_j$ ,  $nd_j$ , and  $nf_j$ , states with  $n \leq 10$  for our calculation of the polarizabilities and hyperpolarizability. We only list the matrix elements that give significant contributions to the atomic properties calculated in the other sections. To evaluate the uncertainties of these values, we carried out several calculations by different methods of increasing accuracy: lowest-order DF, second-order relativistic many-body perturbation theory (RMBPT), third-order RMBPT, and all-order methods. The many-body perturbation theory (MBPT) calculations are carried out following the method described in Ref. [75]. The third-order RMBPT includes random-phase-approximation terms (RPA) iterated to all orders, Brueckner orbital (BO) corrections, the structural radiation, and normalization terms (see [75] for definition of these terms). Comparisons of the values obtained in different approximations allow us to evaluate the size of the second, third, and higher-order correlation corrections.

The evaluation of the uncertainty of the matrix elements in this approach was described in detail in [76–78]. Four all-order calculations were carried out. Two of these were *ab initio* all-order calculations with (SDpT) and without (SD) the inclusion of the partial triple excitations. We have developed some general criteria to establish the final values for all transitions and evaluate uncertainties owing to the need to analyze a very large number of transitions. The scaling procedure and evaluation of the uncertainties are described in detail in [76–78]. We note that it is a rather complicated procedure that involves complete recalculation of the matrix elements with new values of the valence excitation coefficients. The scaling factors depend on the correlation energy given by the particular calculation and are different for the SD and SDpT calculations, therefore these values have to be scaled separately. The results were listed in Refs. [76–78] with subscript “sc”. To limit the size of the table, we displayed here only final results  $Z^{(\text{final})}$  with uncertainties.

The values of uncertainties in Li-like  $\text{Be}^+$  are smaller than the values of uncertainties in  $\text{Ca}^{2+}$  [76], K-like  $\text{Sc}^{2+}$  [78], Rb-like  $\text{Sr}^+$  [79], and neutral Rb [77], as expected. The relative uncertainties of the final values are to be 0.01% - 0.001%. We note that some other contributions (such as Breit and QED corrections) may start to contribute at this level. The present uncertainties represent our best estimate of the uncertainty of the Coulomb

TABLE V: Comparison of the  $\text{Be}^+$  lifetimes (in nsec) with other theory and experiment. Uncertainties are given in parenthesis. References are given in square brackets.

Level	Present	Theory	Ref.	Expt.	Level	Present	Theory [37]
$2p_{1/2}$	8.850(2)	8.853	[27]	8.1(4)[58]	$7s_{1/2}$	17.918(4)	18.02
$2p_{3/2}$	8.850(2)	8.847	[27]		$7p_{1/2}$	29.78(3)	29.19
$3s_{1/2}$	2.451(1)	2.450	[27]	3.3(3)[58]	$7p_{3/2}$	29.78(2)	
$3p_{1/2}$	5.417(1)	5.418	[27]		$7d_{3/2}$	10.522(1)	10.61
$3p_{3/2}$	5.417(2)	5.416	[27]	6.7(8)[56]	$7d_{5/2}$	10.518(4)	
$3d_{3/2}$	0.904(1)	0.904	[27]		$7f_{5/2}$	23.60(1)	23.49
$3d_{5/2}$	0.901(1)	0.905	[27]	0.92(6)[57]	$7f_{7/2}$	23.60(1)	
$4s_{1/2}$	4.174(1)	4.131	[27]	4.4(3)[58]	$8s_{1/2}$	26.17(1)	26.22
$4p_{1/2}$	8.072(3)	8.030	[37]	8.5(9)[56]	$8p_{1/2}$	42.47(5)	41.57
$4p_{3/2}$	8.086(1)				$8p_{3/2}$	42.66(4)	
$4d_{3/2}$	2.067(1)	2.081	[37]	2.3(2)[58]	$8d_{3/2}$	15.58(1)	15.71
$4d_{5/2}$	2.066(1)				$8d_{5/2}$	15.58(1)	
$4f_{5/2}$	4.531(1)	4.522	[37]	4.9(2)[57]	$8f_{5/2}$	35.01(1)	34.77
$4f_{7/2}$	4.525(1)				$8f_{7/2}$	35.03(1)	
$5s_{1/2}$	7.194(2)	7.213	[37]		$9s_{1/2}$	36.78(2)	36.81
$5p_{1/2}$	12.935(6)	12.76	[37]		$9p_{1/2}$	58.86(14)	57.25
$5p_{3/2}$	12.918(4)				$9p_{3/2}$	58.86(7)	
$5d_{3/2}$	3.950(1)	3.971	[37]	3.5(4)[56]	$9d_{3/2}$	22.05(1)	22.22
$5d_{5/2}$	3.938(2)				$9d_{5/2}$	22.01(1)	
$5f_{5/2}$	8.739(2)	8.739	[37]	9.0(8)[56]	$9f_{5/2}$	49.71(2)	49.18
$5f_{7/2}$	8.734(1)				$9f_{7/2}$	49.73(2)	
$6s_{1/2}$	11.673(2)	11.70	[37]		$10s_{1/2}$	49.89(7)	50.02
$6p_{1/2}$	20.04(2)	19.71	[37]		$10p_{1/2}$	78.9(7)	76.66
$6p_{3/2}$	20.05(1)				$10p_{3/2}$	78.6(2)	
$6d_{3/2}$	6.701(2)	6.754	[37]	7.3(8)[56]			
$6d_{5/2}$	6.700(2)						
$6f_{5/2}$	14.959(6)	14.93	[37]				
$6f_{7/2}$	14.948(6)						

correlation corrections. Our final results and their uncertainties given in Table II are used to calculate the recommended values of the transition rates, oscillator strengths, and lifetimes as well as evaluate the uncertainties of these results.

### B. Transition rates, oscillator strengths, and line strengths

We combine recommended NIST energies [73] and our final values of the matrix elements listed in Table II to calculate transition rates  $A_r$  and oscillator strengths  $f$ . The transition rates are calculated using

$$A_{ab} = \frac{2.02613 \times 10^{18}}{\lambda^3} \frac{S}{2j_a + 1} \text{s}^{-1}, \quad (1)$$

where the wavelength  $\lambda$  is in  $\text{\AA}$  and the line strength  $S = (Z^{(\text{final})})^2$  is in atomic units.

Most of the previous results presented for the transition rates, oscillator strengths, and line strengths in  $\text{Be}^+$  were obtained in non-relativistic approximation [14, 18, 24–27, 29, 37, 38, 48, 49, 53, 54, 57, 62]. A fraction of those results were used in recently published compi-

lation [63]. In order to compare our results with recommended NIST values of the transition rates, oscillator strengths, and line strengths for  $\text{Be}^+$ , we average over  $j$  and  $j'$  our results  $A_r(nlj, n'l'j')$ ,  $f(nlj, n'l'j')$ , and  $S(nlj, n'l'j')$  obtained in relativistic approximation. We obtain the 190 averaged transitions instead of 489 transitions with fixed  $j$ . The average over  $j$  transition rates, oscillator strengths, and line strengths are listed in Table III. In this table, we display the same transitions that were listed in the NIST compilation [63]. The relative uncertainties in the values of transition rates, oscillator strengths, and line strengths are the same, since all of these properties have the same dependence on the E1 matrix elements. The uncertainties in percent are given in column “Unc.” of Table III. The values of the relative uncertainties are less than 0.1% for all transitions displayed in Table III. Wavelengths listed in Table III for references are taken from Table 7 of NIST compilation [63].

We do not incorporate the recommended value of transition rates, oscillator strengths, and line strengths from [63] in Table III to save space. Comparison of those results with our results given in Table III shows excellent agreement. The difference is about 0.01% - 0.1% for half of the transitions displayed in Table III. The difference

TABLE VI: Contributions to multipole polarizabilities of the  $2s$  state of Li-like  $\text{Be}^+$  in  $a_0^3$ . Uncertainties are given in parenthesis. <sup>(a)</sup> Includes estimate of relativistic effects.

Contr.	$\alpha^{E1}$
$2p_{1/2}$	7.847(2)
$2p_{3/2}$	15.692(3)
$(3-26)p_j$	0.889
Tail	0.003
Core	0.052
Total	24.483(4)
Ref. [9] <sup>(a)</sup>	24.489(4)
Ref. [8]	24.4966(1)
Contr.	$\alpha^{E2}$
$3d_{3/2}$	18.374(4)
$4d_{3/2}$	1.744(1)
$(5-26)d_{3/2}$	1.362
$3d_{5/2}$	27.561(6)
$4d_{5/2}$	2.616(1)
$(5-26)d_{5/2}$	2.044
Tail	0.025
Core	0.015
Total	53.741(7)
Ref. [8]	53.7659(2)
Contr.	$\alpha^{E3}$
$4f_{5/2}$	80.963(16)
$5f_{5/2}$	29.633(6)
$6f_{5/2}$	13.872(3)
$(7-19)f_{5/2}$	25.899(3)
$(20-26)f_{5/2}$	45.578
$(27-30)f_{5/2}$	3.483
$4f_{7/2}$	107.952(22)
$5f_{7/2}$	39.512(8)
$6f_{7/2}$	18.497(4)
$(7-19)f_{7/2}$	36.612(4)
$(20-26)f_{7/2}$	59.691
$(27-30)f_{7/2}$	3.651
Tail	0.010
Core	0.011
Total	465.36(3)
Ref. [8]	465.7621(1)

is larger than 2% for three transitions ( $2s-7p$ ,  $2s-9p$ , and  $3d-9f$ ) which have the smallest values of the line strengths.

Oscillator strengths for transitions in  $\text{Be}^+$  calculated using Hylleraas bases functions [8] are compared with our results in Table IV. Our results of oscillator strengths are calculated using the recommended values of reduced electric-dipole matrix elements  $Z^{(\text{final})}$  and their uncertainties given in Table II. Our relativistic values  $f(nlj, n'l'j')$  are averaged over  $j$  and  $j'$  to make comparison with results from Ref. [8]. The smallest difference is 0.0002% for the  $3d-4f$  transition, while the largest difference (0.14%) is for the  $2s-3p$  transition. Less than 0.01% differences are observed for the  $2p-3d$  and  $2p-4d$  transitions. The differences are about 0.03% - 0.07% for

the  $2s-2p$ ,  $2p-3s$ ,  $3s-3p$ ,  $3p-3d$ , and  $3p-4s$  transitions. These differences are in part explained by relativistic effects omitted in Ref. [8].

### C. Lifetimes in $\text{Be}^+$

We calculated lifetimes of the  $ns$  ( $n = 3-10$ ),  $np_j$  ( $n = 2-10$ ),  $nd_j$  ( $n = 3-9$ ), and  $nf_j$  ( $n = 4-9$ ) states in  $\text{Be}^+$  using out final values of the transition rates listed in Table III. The uncertainties in the lifetime values are obtained from the uncertainties in the transition rates listed in Table III. We list the lifetimes of the 52 levels in Table V. We also evaluate the lowest-order DF lifetimes to estimate the size of the correlation effects. The difference between the lowest-order values and our final lifetimes are 3% - 5%.

The present values displayed in Table V are compared with beam-foil experimental measurements by Andersen *et al.* [58], Bromander [57], and Hontzas *et al.* [56]. The accuracy of the measurements was about 5% - 10%.

Our lifetime values are also compared with theoretical lifetimes obtained by multiconfiguration Breit - Pauli (BP) approach by Froese Fisher *et al.* [27]. In the MCHF method, the radial functions were used to construct the CSFs (configuration state functions). Once radial functions were determined, a configuration interaction calculation can be performed over the set of configuration states, where the interaction matrix was evaluated with respect to the BP Hamiltonian. New, efficient programs based on the combination of second quantization in coupled tensorial form, and a generalized graphical technique were used for performing angular integrations for the evaluation of matrix elements [27]. Numerical values of the lifetimes evaluated in [27] for eight levels are listed in column “Theory” of Table V. We find excellent agreement (about 0.03% difference) between our results and results from [27]. The disagreement is larger (1%-3%) between our lifetime values and theoretical results given by Theodosiou [37]. Lifetimes in [37] were calculated using the Coulomb approximation with a Hartree-Slater core (CAHS) approach. Since those results are non-relativistic lifetime values, we placed in column “Theory” of Table V only one number for  $nlj$  level with smaller value of  $j$ . The contribution of relativistic effects leads to the 0.05% - 0.2% difference between the  $nlj$  lifetime values with different  $j$  for fixed  $nl$  states.

## IV. STATIC MULTIPOLE POLARIZABILITIES OF THE $2s$ STATE

The static multipole polarizability  $\alpha^{Ek}$  of Li-like  $\text{Be}^+$  in its ground state can be separated into two terms; a dominant first term from intermediate valence-excited states, and a smaller second term from intermediate core-excited states. The later term is smaller than the former one by several orders of magnitude and is evaluated

TABLE VII: The  $\alpha_0$  scalar and  $\alpha_2$  tensor polarizabilities for  $\text{Be}^+$  ion in  $a_0^3$ . Uncertainties are given in parenthesis.  $X(a)[b]$  means the  $X \times 10^b$  with uncertainty “a” in the last digit of X.

Scalar polarizabilities $\alpha_0$							
$2s$	$3s$	$4s$	$5s$	$6s$	$7s$	$8s$	$9s$
24.483(4)	588.7(1)	5002(1)	25400(4)	94411(14)	284420(40)	736200(100)	1698300(360)
$2p_{1/2}$	$3p_{1/2}$	$4p_{1/2}$	$5p_{1/2}$	$6p_{1/2}$	$7p_{1/2}$	$8p_{1/2}$	$9p_{1/2}$
2.025(2)	1491.3(3)	14816(3)	78545(17)	296710(70)	899600(200)	2333800(500)	5387800(1200)
$2p_{3/2}$	$3p_{3/2}$	$4p_{3/2}$	$5p_{3/2}$	$6p_{3/2}$	$7p_{3/2}$	$8p_{3/2}$	$9p_{3/2}$
2.029(2)	1492.9(3)	14832(3)	78630(16)	297120(60)	900900(200)	2337100(500)	5396900(1100)
	$3d_{3/2}$	$4d_{3/2}$	$5d_{3/2}$	$6d_{3/2}$	$7d_{3/2}$	$8d_{3/2}$	$9d_{3/2}$
	-8.469(2)[2]	2.090[5]	1.392(1)[6]	5.778(4)[6]	1.826(2)[7]	4.763(7)[7]	1.118(2)[8]
	$3d_{5/2}$	$4d_{5/2}$	$5d_{5/2}$	$6d_{5/2}$	$7d_{5/2}$	$8d_{5/2}$	$9d_{5/2}$
	-8.476(2)[2]	2.100[5]	1.397(1)[6]	5.757(4)[6]	1.826(2)[7]	4.762(7)[7]	1.118(2)[8]
Tensor polarizabilities $\alpha_2$							
$2p_{3/2}$	$3p_{3/2}$	$4p_{3/2}$	$5p_{3/2}$	$6p_{3/2}$	$7p_{3/2}$	$8p_{3/2}$	$9p_{3/2}$
5.848(2)	8.540(1)	-105.3(7)	-760(4)	-3050(14)	-9166(43)	-23050(100)	-51420(400)
	$3d_{3/2}$	$4d_{3/2}$	$5d_{3/2}$	$6d_{3/2}$	$7d_{3/2}$	$8d_{3/2}$	$9d_{3/2}$
	6.523(2)[2]	-3.696(1)[4]	-2.526(2)[5]	-1.058(1)[6]	-3.358(4)[6]	-8.759(14)[6]	-2.058(6)[7]
	$3d_{5/2}$	$4d_{5/2}$	$5d_{5/2}$	$6d_{5/2}$	$7d_{5/2}$	$8d_{5/2}$	$9d_{5/2}$
	9.330(2)[2]	-5.300(2)[4]	-3.620(2)[5]	-1.504(1)[6]	-4.796(6)[6]	-1.251(2)[7]	-2.940(8)[7]

here in the random-phase approximation [80]. The dominant valence contribution is calculated using the sum-over-state approach

$$\alpha_v^{Ek} = \frac{1}{2k+1} \sum_n \frac{|\langle nl_j || r^k C_{kq} || 2s \rangle|^2}{E_{nl_j} - E_{2s}}, \quad (2)$$

where  $C_{kq}(\hat{r})$  is a normalized spherical harmonic and where  $nl_j$  is  $np_j$ ,  $nd_j$ , and  $nf_j$  for  $k = 1, 2$ , and  $3$ , respectively [81]. The reduced matrix elements in the dominant contributions to the above sum are evaluated using out final values of the dipole matrix elements and NIST energies [73]. The uncertainties in the polarizability contributions are obtained from the uncertainties in the matrix elements. The final values for the quadrupole and octupole matrix elements and their uncertainties are determined using the procedure that was described above for the dipole matrix elements.

We use recommended energies from [73] and our final matrix elements to evaluate terms in the sum with  $n \leq 10$ , and we use theoretical SD energies and wave functions to evaluate terms with  $10 \leq n \leq 26$ . The remaining contributions to  $\alpha^{Ek}$  from orbitals with  $27 \leq n \leq 70$  are evaluated in the RPA approximation since the contributions from these terms are smaller than 0.01% in all cases. These terms are grouped together as “Tail”. In the case of  $\alpha^{E3}$ , we find that the contribution (1.5%) from the  $(27-30)nf_j$  part of sum over  $j$  is substantial, and we use theoretical SD energies and wave functions to evaluate terms with  $10 \leq n \leq 30$ .

We evaluate core contributions in the random-phase approximation [80] for E1, E2, and E3 polarizabilities. Our result for core E1 polarizability is the same as in [80].

The core polarizabilities are small in comparison with the valence ones and their uncertainties are negligible.

Contributions to dipole, quadrupole, and octupole polarizabilities of the  $2s$  ground state are presented in Table VI. The first two terms in the sum-over-states for  $\alpha^{E1}$  contribute 96.4% of the total. The remaining 3.6% of  $\alpha^{E1}$  comes from the  $(3-26)np_j$  states. The first four terms in the sum-over-states for  $\alpha^{E2}$  contribute 93.7% of the totals. The remaining 6.3% of  $\alpha^{E2}$  contribution is from the  $(5-26)nd_j$  states. However, the first six terms in the sum-over-states for  $\alpha^{E3}$  contribute only 62.4% of the totals. The remaining 37.6% of  $\alpha^{E3}$  contribution was divided into three parts:  $(7-19)nf_j$  (13.4%),  $(20-26)nf_j$  (22.6%), and  $(27-30)nf_j$  (1.5%).

Final results for the multipole polarizabilities of the Li-like  $\text{Be}^+$  ground state are compared in Table VI with high-precision calculations given by Tang *et al.* [8]. Calculations were performed using variationally determined wave functions with Hylleraas basis set expansions. Authors underlined that the values reported were the results of calculations close to convergence [8]. We found excellent agreement between our final results and results obtained by Hylleraas basis set: the difference is 0.055%, 0.046%, and 0.086% for the  $\alpha^{E1}$ ,  $\alpha^{E2}$ , and  $\alpha^{E3}$  polarizabilities, respectively.

## V. SCALAR AND TENSOR EXCITED STATE POLARIZABILITIES

The valence scalar  $\alpha_0(v)$  and tensor  $\alpha_2(v)$  polarizabilities of an excited state  $v$  of Li-like  $\text{Be}^+$  are given by

TABLE VIII: Contributions to the  $\alpha_0(nd_{5/2})$  scalar and  $\alpha_2(nd_{5/2})$  tensor polarizabilities for  $\text{Be}^+$  ion in  $a_0^3$ . Uncertainties are given in parenthesis. The dominant contributions to the polarizabilities are listed separately with the corresponding absolute values of electric-dipole reduced matrix elements given in columns labeled  $D^{\text{final}}$ . The experimental NIST transition energies ( $\text{cm}^{-1}$ ) are given in columns  $\Delta E$ . The remaining contributions to valence polarizability are given in the next row after the dominant contribution. X(a)[b] means the  $X \times 10^b$  with uncertainty “a” in the last digit of X value.

Level	Contr.	$\Delta E$	$Z^{\text{final}}$	$\alpha_0(nd_{5/2})$	$\alpha_2(nd_{5/2})$
$3d_{5/2}$	$3d_{5/2} - 3p_{3/2}$	-1557.81	7.853(1)	-9.654(2)[2]	9.654(2)[2]
	$3d_{5/2} - np_{3/2}$			-1.75	1.75
	$3d_{5/2} - 4f_{5/2}$	21391.49	2.1122(1)	5.086(1)	5.812(1)
	$3d_{5/2} - nf_{5/2}$			6.10[-1]	6.98[-1]
	$3d_{5/2} - 4f_{7/2}$	21391.62	9.4461(4)	1.017[2]	-3.633([1]
	$3d_{5/2} - nf_{7/2}$			1.22[1]	-4.36
Total				-8.476(2)[2]	9.330(2)[2]
$4d_{5/2}$	$4d_{5/2} - 4p_{3/2}$	-660.12	16.175(1)	-9.665(2)[3]	9.665(2)[3]
	$4d_{5/2} - np_{3/2}$			-1.65	1.65
	$4d_{5/2} - 4f_{5/2}$	25.15	3.2885(3)	1.049[4]	1.198[4]
	$4d_{5/2} - nf_{5/2}$			2.38[1]	2.72[1]
	$4d_{5/2} - 4f_{7/2}$	25.28	14.707(2)	2.086[5]	-7.451(1)[4]
	$4d_{5/2} - nf_{7/2}$			4.75[2]	-1.70[2]
Total				2.100[5]	-5.300(2)[4]
$5d_{5/2}$	$5d_{5/2} - 5p_{3/2}$	-338.20	26.705(2)	-5.142(1)[4]	5.142(1)[4]
	$5d_{5/2} - np_{3/2}$			2.41[1]	-2.41[1]
	$5d_{5/2} - 5f_{5/2}$	13.60	6.2139(5)	6.924(1)[4]	7.913(2)[4]
	$5d_{5/2} - nf_{5/2}$			7.61[1]	8.70[1]
	$5d_{5/2} - 5f_{7/2}$	13.67	27.790(2)	1.378(1)[6]	-4.920(2)[5]
	$5d_{5/2} - nf_{7/2}$			1.52(0)[3]	-5.44[2]
Total				1.397(1)[6]	-3.620(2)[5]
$6d_{5/2}$	$6d_{5/2} - 6p_{3/2}$	-195.54	39.518(2)	-1.948[5]	1.948[5]
	$6d_{5/2} - np_{3/2}$			1.61[2]	-1.61[2]
	$6d_{5/2} - 6f_{5/2}$	8.05	9.6857(6)	2.842(2)[5]	3.248(1)[5]
	$6d_{5/2} - nf_{5/2}$			2.04[2]	2.33[2]
	$6d_{5/2} - 6f_{7/2}$	8.08	43.316(3)	5.663(4)[6]	-2.022(1)[6]
	$6d_{5/2} - nf_{7/2}$			4.07[3]	-1.45[3]
Total				5.757(4)[6]	-1.504(1)[6]
$7d_{5/2}$	$7d_{5/2} - 7p_{3/2}$	-123.05	54.635(3)	-5.916(1)[5]	5.916(1)[5]
	$7d_{5/2} - np_{3/2}$			6.24[2]	-6.24[2]
	$7d_{5/2} - 7f_{5/2}$	5.14	13.7530(7)	8.974(9)[5]	1.026(1)[6]
	$7d_{5/2} - nf_{5/2}$			4.77[2]	5.45[2]
	$7d_{5/2} - 7f_{7/2}$	5.14	61.506(3)	1.795(2)[7]	-6.410(6)[6]
	$7d_{5/2} - nf_{7/2}$			9.54[3]	-3.41[3]
Total				1.826(2)[7]	-4.796(6)[6]
$8d_{5/2}$	$8d_{5/2} - 8p_{3/2}$	-82.40	72.062(4)	-1.537[6]	1.537[6]
	$8d_{5/2} - np_{3/2}$			1.88[3]	-1.88[3]
	$8d_{5/2} - 8f_{5/2}$	3.54	18.430(1)	2.340(3)[6]	2.674(3)[6]
	$8d_{5/2} - nf_{5/2}$			1.01[3]	1.15[3]
	$8d_{5/2} - 8f_{7/2}$	3.54	82.423(6)	4.680(7)[7]	-1.671(2)[7]
	$8d_{5/2} - nf_{7/2}$			2.02[4]	-7.22[3]
Total				4.762(7)[7]	-1.251(2)[7]
$9d_{5/2}$	$9d_{5/2} - 9p_{3/2}$	-57.84	91.799(6)	-3.553(1)[6]	3.553(1)[6]
	$9d_{5/2} - np_{3/2}$			4.79[3]	-4.79[3]
	$9d_{5/2} - 9f_{5/2}$	2.50	23.722(2)	5.489(11)[6]	6.273(12)[6]
	$9d_{5/2} - nf_{5/2}$			1.97[3]	2.26[3]
	$9d_{5/2} - 9f_{7/2}$	2.50	106.089(7)	1.098(2)[8]	-3.921(8)[7]
	$9d_{5/2} - nf_{7/2}$			3.95[4]	-1.41[4]
Total				1.118(2)[8]	-2.940(8)[7]

TABLE IX: Contributions to the  $2s_{1/2}$  dipole hyperpolarizabilities  $\gamma_0$  of  $\text{Be}^+$  in a.u. Uncertainties are given in parenthesis. Sums in Eqs. (16) and (17) are evaluated for  $n_m = 2-26$ ,  $n_k = 2-26$ , and  $n_n = 3-26$ . Values for ‘Tail’ is a contribution from DF results evaluated with  $n_i = 27-70$ . The  $\gamma_{vc}$  contribution is obtained from including  $1s$  states in the sum in Eq. (16).

Contr	$\gamma_0^{(\text{DF})}(2s)$	$\gamma_0^{(\text{final})}(2s)$
$\frac{1}{18}T(s, p_{1/2}, p_{1/2})$	35.247	32.605(53)
$-\frac{1}{18}T(s, p_{1/2}, p_{3/2})$	70.487	68.886(92)
$-\frac{1}{18}T(s, p_{3/2}, p_{1/2})$	70.487	68.886(92)
$\frac{1}{18}T(s, p_{3/2}, p_{3/2})$	140.965	137.669(109)
$T(spp)$	317.186	308.046(178)
$\gamma_{vc}$	-0.399	-0.399
Tail	-0.096	-0.096
Total	316.691	307.551
$\frac{1}{18}T(d_{3/2}, p_{1/2}, p_{1/2})$	208.678	202.031(121)
$\frac{1}{18\sqrt{10}}T(d_{3/2}, p_{1/2}, p_{3/2})$	41.731	40.403(18)
$\frac{1}{18\sqrt{10}}T(d_{3/2}, p_{3/2}, p_{1/2})$	41.731	40.403(18)
$\frac{1}{180}T(d_{3/2}, p_{3/2}, p_{3/2})$	8.345	8.080(3)
$\frac{1}{30}T(d_{5/2}, p_{3/2}, p_{3/2})$	450.761	438.434(148)
$T(dpp)$	751.246	729.351(192)
$\gamma_{vc}$	0.0	0.0
Tail	1.800	1.800
Total	753.042	730.151(192)
$\alpha_0 \times \beta$	2041.637	1995.743(382)
Total	-971.904	-958.041(463)
$\gamma_0$	-11663	-11496(6)
Ref. [8]		-11521.30(3)

$$\alpha_0(v) = \frac{2}{3(2j_v + 1)} \sum_{nlj} \frac{|\langle v || rC_1 || nlj \rangle|^2}{E_{nlj} - E_v} \quad (3)$$

$$\alpha_2(v) = (-1)^{j_v} \sqrt{\frac{40j_v(2j_v - 1)}{3(j_v + 1)(2j_v + 1)(2j_v + 3)}} \times \sum_{nlj} (-1)^j \begin{Bmatrix} j_v & 1 & j \\ 1 & j_v & 2 \end{Bmatrix} \frac{|\langle v || rC_1 || nlj \rangle|^2}{E_{nlj} - E_v}. \quad (4)$$

The excited state polarizability calculations are carried out in the same way as the calculations of the multipole polarizabilities discussed in the previous section. We summarize our results for the scalar  $\alpha_0$  and tensor  $\alpha_2$  polarizabilities of  $\text{Be}^+$  in Table VII. In this table, we list our final values for the polarizabilities of the  $ns$ ,  $np_{1/2}$ ,  $np_{3/2}$ ,  $nd_{3/2}$ , and  $nd_{5/2}$  states with  $n < 10$ . The uncertainties of all values are given. If no uncertainty is listed, is it zero for the significant figures that are quoted. We note again that we could only evaluate dominant uncertainties due to missing Coulomb correlation effects.

The polarizability values rapidly increase with increasing  $n$ , but the rate of increase depends on  $l$ . The ratio of

the  $\alpha_0(3l)$  and  $\alpha_0(2l)$  is substantially different for  $l = s$  and  $l = p$ . This difference in ratios decreases with  $n$ . The ratio of the  $\alpha_0(3s)$  and  $\alpha_0(2s)$  is equal to 24, while the ratios of the  $\alpha_0(3p)$  and  $\alpha_0(2p)$  is 740. The ratio of the  $\alpha_0(4s)$  and  $\alpha_0(3s)$  is equal to 8.5, while the ratio of the  $\alpha_0(4p)$  and  $\alpha_0(3p)$  is only slightly different (9.9). The ratios of  $\alpha_0(nl)$  and  $\alpha_0(n-1)l$  for the  $l = s$  and  $l = p$  are equal to 5.1 and 5.3 for  $n = 5$  and 3.7 - 3.8 for  $n = 6$ . There are no differences in the  $\alpha_0(nl)$  and  $\alpha_0((n-1)l)$  ratios for the  $l = s$  and  $l = p$  in the case of  $n = 7, 8$ , and 9. The ratios of the  $\alpha_0(nl)$  and  $\alpha_0((n-1)l)$  are similar for the  $nd$  states; 3.2, 2.6, and 2.3 for  $n = 7, 8$ , and 9, respectively; it is only slightly different for tensor polarizabilities. The values of  $\alpha_2(4l)$  and  $\alpha_2(3l)$  have different sign and their ratios are equal -12 for to  $l = p$  and -57 for  $l = d$ . Significant cancellations among different contributions are observed that leads to similar values for the  $\alpha_2(3p_{3/2})$  and  $\alpha_2(2p_{3/2})$  tensor polarizabilities. These cancellations were previously observed for  $\alpha_2(nl)$  polarizabilities in  $\text{Sr}^+$  [79],  $\text{Rb}$  [77], and  $\text{Ca}^+$  [76].

We illustrate the importance of different contributions and evaluation of uncertainties for the scalar and tensor  $nd_{5/2}$  polarizabilities in Table VIII. Uncertainties are given in parenthesis. The dominant contributions to the polarizabilities are listed separately with the corresponding absolute values of electric-dipole reduced matrix elements given in column labeled  $Z^{\text{final}}$ . The experimental NIST transition energies [73] are given in column  $\Delta E$ . The dominant contributions for the  $\alpha_0(nd_{5/2})$  scalar and  $\alpha_2(nd_{5/2})$  polarizabilities are from the  $nd_{5/2} - np_{3/2}$ ,  $nd_{5/2} - nf_{5/2}$ , and  $nd_{5/2} - nf_{7/2}$  transitions. The remaining contributions to valence polarizability are given in the next row after the dominant contribution. For example, the dominant contribution to the  $\alpha_0(4d_{5/2})$  polarizability are from the three matrix elements:  $4d_{5/2} - 4p_{3/2}$ ,  $4d_{5/2} - 4f_{5/2}$ , and  $4d_{5/2} - 4f_{7/2}$ . These give 99.7% in the final value of the  $\alpha_0(4d_{5/2})$  polarizability. The 0.3% remaining contribution comes from the sum over  $n = 2, 3, 5-26$  for  $4d_{5/2} - np_{3/2}$  contribution and sum over  $n=5-26$  for the  $4d_{5/2} - nf_{5/2}$  and  $4d_{5/2} - nf_{7/2}$  contribution. The contributions from the core and tail ( $n > 26$ ) terms are very small (less than 0.1 in  $\alpha_0^3$ ) and are omitted from the table.

The dominant contribution to the  $nd_{5/2}$  polarizabilities comes from the transitions with the largest values of dipole matrix elements among the 71 matrix elements that are included in evaluation of these polarizabilities. The ratio of the  $Z^{\text{final}}(nd_{5/2} - nf_{7/2})$  and  $Z^{\text{final}}(nd_{5/2} - nf_{5/2})$  is equal to 4.47 for  $n = 3 - 9$ . Therefore, the contribution of the  $nd_{5/2} - nf_{5/2}$  transition is smaller by a factor of 20 in comparison with the contributions from the  $nd_{5/2} - nf_{7/2}$  transition. There are almost no differences in the  $\Delta E(nd_{5/2} - nf_{5/2})$  and  $\Delta E(nd_{5/2} - nf_{7/2})$  energy transitions, while the  $\Delta E(nd_{5/2} - np_{3/2})$  energy transition is larger by a factor of 23-26 than the  $\Delta E(nd_{5/2} - nf_j)$  energy transitions. That leads to the smaller contribution by a factor of 23-26 from the  $nd_{5/2} - np_{3/2}$  transitions in comparison with

the  $nd_{5/2} - nf_{7/2}$  transitions. As a result, the dominant  $nd_{5/2} - nf_{7/2}$  transition is the largest contributor to the values of the  $nd_{5/2}$  polarizabilities. This transition contributes 99.3% - 98.2% to the value of the  $\alpha_0(nd_{5/2})$  ( $n=4-9$ ) polarizabilities. Distribution of contributions to the tensor polarizability is different in comparison with the scalar one due to different angular factors (compare Eq. (3) and Eq. (4)). The  $nd_{5/2} - np_{3/2}$  and  $nd_{5/2} - nd_{5/2}$  contributions have different sign in comparison with the  $nd_{5/2} - nd_{7/2}$  contributions. As a result, the dominant  $nd_{5/2} - nd_{7/2}$  contributions are larger than the final tensor  $\alpha_2(nd_{5/2})$  polarizabilities by a factor of 1.41-1.33 for  $n = 4 - 9$ , respectively.

We find that it is very important to use the accurate values of the energy transitions to evaluate the polarizability values. We use the recommended NIST data [73] that are given for  $\text{Be}^+$  with two significant figures after the decimal point in  $\text{cm}^{-1}$  for the most of the levels.

The transition energy for the dominant  $nd_{5/2} - nd_{7/2}$  transition decreases with  $n$  from  $25.28 \text{ cm}^{-1}$  for  $n = 4$  up  $2.50 \text{ cm}^{-1}$  for  $n = 9$ . Therefore, the uncertainties in the energy values can not longer be assumed to be negligible for these transitions. We take the experimental transition energy uncertainties to be  $0.005 \text{ cm}^{-1}$  based on the number of significant figures given in the NIST database. The uncertainty in these small energy intervals dominates the uncertainty in the polarizabilities for the  $nd$  states with  $n > 4$ . More accurate measurement of the transition energies are needed to improve the precision of these polarizabilities.

## VI. SCALAR HYPERPOLARIZABILITY OF $\text{Be}^+$

Non-relativistic scalar hyperpolarizability  $\gamma_0$  was defined by Tang *et al.* [3]. Using the same procedure, we derive the following equation for the relativistic scalar hyperpolarizability  $\gamma_0$ :

$$\gamma_0(n_0 l_0 j_0) = \frac{24}{\sqrt{(2j_0 + 1)}} \sum_{n_m l_m j_m} \sum_{n_n l_n j_n} \sum_{n_k l_k j_k} \Pi_0(j_0, j_m, j_n, j_k) \times \Upsilon(n_0 l_0 j_0, n_m l_m j_m, n_n l_n j_n, n_k l_k j_k) \quad (5)$$

where

$$\Pi_0(j_0, j_m, j_n, j_k) = \sum_{K_1} (-1)^{j_0 - j_n + 2K_1} (2K_1 + 1) \frac{(2K_1 + 1)}{\sqrt{(2j_0 + 1)}} \begin{pmatrix} 1 & 1 & K_1 \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} 1 & 1 & K_1 \\ j & j_n & j_m \end{Bmatrix} \begin{Bmatrix} 1 & 1 & K_1 \\ J & j_n & j_k \end{Bmatrix} \quad (6)$$

and

$$\begin{aligned} \Upsilon(n_0 l_0 j_0, n_m l_m j_m, n_n l_n j_n, n_k l_k j_k) &= I(n_0 l_0 j_0, n_m l_m j_m, n_n l_n j_n, n_k l_k j_k) - \\ &- (-1)^{2j_0 - j_m - j_k} \delta(j_0, j_n) \frac{\langle n_0 l_0 j_0 | r C_1 | n_m l_m j_m \rangle^2}{(E(n_m l_m j_m) - E(n_0 l_0 j_0))} \frac{\langle n_0 l_0 j_0 | r C_1 | n_k l_k j_k \rangle^2}{(E(n_k l_k j_k) - E(n_0 l_0 j_0))^2}. \end{aligned} \quad (7)$$

The most complicated part in the calculation of  $\gamma_0(n_0 l_0 j_0)$  is in the evaluation of sum over  $I(n_0 l_0 j_0, n_m l_m j_m, n_n l_n j_n, n_k l_k j_k)$ :

$$\begin{aligned} &I(n_0 l_0 j_0, n_m l_m j_m, n_n l_n j_n, n_k l_k j_k) \\ &= \frac{\langle n_0 l_0 j_0 | r C_1 | n_m l_m j_m \rangle \langle n_m l_m j_m | r C_1 | n_n l_n j_n \rangle \langle n_n l_n j_n | r C_1 | n_k l_k j_k \rangle \langle n_k l_k j_k | r C_1 | n_0 l_0 j_0 \rangle}{[E(n_m l_m j_m) - E(n_0 l_0 j_0)] [E(n_n l_n j_n) - E(n_0 l_0 j_0)] [E(n_k l_k j_k) - E(n_0 l_0 j_0)]}. \end{aligned} \quad (8)$$

The angular part of  $\gamma_0(n_0 l_0 j_0)$  is defined as:

$$\Pi_0(j_0, j_m, j_n, j_k) = \sum_{K_1} (-1)^{j_0 - j_n + 2K_1} \frac{(2K_1 + 1)}{\sqrt{(2j_0 + 1)}} \begin{pmatrix} 1 & 1 & K_1 \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} 1 & 1 & K_1 \\ j & j_n & j_m \end{Bmatrix} \begin{Bmatrix} 1 & 1 & K_1 \\ J & j_n & j_k \end{Bmatrix}. \quad (9)$$

The sum over  $K_1$  includes only two terms  $K_1 = 0$  and  $K_1 = 2$ . This allows the following simplification of the  $\Pi_0(j_0, j_m, j_n, j_k)$  equation

$$\begin{aligned}
\Pi_0(j_0, j_m, j_n, j_k) &= (-1)^{j_0-j_n} \frac{1}{\sqrt{(2j_0+1)}} \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} 1 & 1 & 0 \\ j_0 & j_n & j_m \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 0 \\ j_0 & j_n & j_k \end{Bmatrix} \\
&+ (-1)^{j_0-j_n} \frac{5}{\sqrt{(2j_0+1)}} \begin{pmatrix} 1 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} 1 & 1 & 2 \\ j_0 & j_n & j_m \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 2 \\ j_0 & j_n & j_k \end{Bmatrix} \\
&= \frac{1}{3} (-1)^{2j_n+j_m+j_k} \frac{1}{3} \frac{1}{(2j_0+1)^{3/2}} \delta(j_0, j_n) + (-1)^{j_0-j_n} \frac{2}{3} \frac{1}{\sqrt{(2j_0+1)}} \begin{Bmatrix} 1 & 1 & 2 \\ j_0 & j_n & j_m \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 2 \\ j_0 & j_n & j_k \end{Bmatrix}.
\end{aligned} \tag{10}$$

Finally, we obtain:

$$\Pi_0^{K_1=0}(j_0, j_m, j_n, j_k) = (-1)^{j_m-j_k} \frac{1}{9} \frac{1}{(2j_0+1)^{3/2}} \delta(j_0, j_n) \tag{11}$$

$$\Pi_0^{K_1=2}(j_0, j_m, j_n, j_k) = (-1)^{j_0-j_n} \frac{2}{3} \frac{1}{\sqrt{(2j_0+1)}} \begin{Bmatrix} 1 & 1 & 2 \\ j_0 & j_n & j_m \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 2 \\ j_0 & j_n & j_k \end{Bmatrix} \tag{12}$$

Let us consider the most important case for the alkali-metal atomic systems  $n_0 l_0 j_0 = n_0 s_{1/2}$ . We can rewrite Eq. (5) in the following way:

$$\gamma_0(n_0 s_{1/2}) = 12 \times T(spp) + 12 \times T(dpp) - 12 \times \alpha_0(n_0 l_0 j_0) \times \beta_0(n_0 l_0 j_0), \tag{13}$$

where  $\alpha_0(n_0 l_0 j_0)$  is scalar dipole polarizability and  $\beta_0(n_0 l_0 j_0)$  is the first order nonadiabatic correction to dipole polarizability [8]:

$$\alpha_0(n_0 l_0 j_0) = \frac{1}{3} \sum_{nlj} \frac{\langle n_0 l_0 j_0 | r C_1 | nlj \rangle^2}{E(nlj) - E(n_0 l_0 j_0)} \tag{14}$$

$$\beta_0(n_0 l_0 j_0) = \frac{1}{6} \sum_{nlj} \frac{\langle n_0 l_0 j_0 | r C_1 | nlj \rangle^2}{(E(nlj) - E(n_0 l_0 j_0))^2} \tag{15}$$

The values of the  $T(spp)$  and  $T(dpp)$  are defined as

$$T(s, p_j, p_{j'}) = \sum_{n_m} \sum_{n_n} \sum_{n_k} \frac{\langle n_0 s_{1/2} | r C_1 | n_m p_j \rangle \langle n_m p_j | r C_1 | n_n s_{1/2} \rangle \langle n_n s_{1/2} | r C_1 | n_k p_{j'} \rangle \langle n_k p_{j'} | r C_1 | n_0 s_{1/2} \rangle}{[E(n_m p_j) - E(n_0 s_{1/2})] [E(n_n s_{1/2}) - E(n_0 s_{1/2})] [E(n_k p_{j'}) - E(n_0 s_{1/2})]} \tag{16}$$

and

$$T(d_{j''}, p_j, p_{j'}) = \sum_{n_m} \sum_{n_n} \sum_{n_k} \frac{\langle n_0 s_{1/2} | r C_1 | n_m p_j \rangle \langle n_m p_j | r C_1 | n_n d_{j''} \rangle \langle n_n d_{j''} | r C_1 | n_k p_{j'} \rangle \langle n_k p_{j'} | r C_1 | n_0 s_{1/2} \rangle}{[E(n_m p_j) - E(n_0 s_{1/2})] [E(n_n s_{1/2}) - E(n_0 s_{1/2})] [E(n_k p_{j'}) - E(n_0 s_{1/2})]}. \tag{17}$$

Numerical results for Li-like  $\text{Be}^+$  are given in Table IX. Sums in Eqs. (16) and (17) are evaluated for  $n_m = 2-26$ ,  $n_k = 2-26$ , and  $n_n = 3-26$ . The ‘Tail’ contribution from  $n_i = 27-70$  is evaluated in the DF approximation. The  $\gamma_{vc}$  contribution is obtained from including  $1s$  states in the sum in Eq. (16). Final result for the  $\gamma_0(2s)$  hyperpolarizability is obtained using Eq. (13) and numerical values given in Table IX.

The difference between  $\gamma_0^{\text{final}}(2s)$  and  $\gamma_0^{(\text{DF})}(2s)$  is about 1.5%, so the overall correlation contribution is small. In the last row of Table IX, we display the  $\gamma_0(2s)$

value evaluated using Hylleraas basis functions [8]. Our  $\gamma_0^{\text{final}}(2s)$  value is in excellent agreement with that result. The difference is about 0.22%.

## VII. CONCLUSION

A systematic study of  $\text{Be}^+$  atomic properties is carried out using high-precision relativistic all-order method where all single, double, and partial triple excitations of the Dirac-Fock wave function are included to all or-

ders of perturbation theory. Energies, multipole matrix elements, line strengths, oscillator strengths, transition rates, lifetimes, scalar and tensor polarizabilities of the  $ns$ ,  $np_j$ ,  $nd_j$ , and  $nf_j$  ( $n \leq 9$ ) states are calculated. Additionally, we evaluated the ground state hyperpolarizability in Li-like  $\text{Be}^+$ . The uncertainties of our calculations are evaluated for most of the values listed in this work. These calculations provide recommended values critically evaluated for their accuracy for a number of  $\text{Be}^+$  atomic

properties useful for a variety of applications.

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- [1] M. S. Safronova and W. R. Johnson, Adv. At. Mol. Opt. Phys. **55**, 191 (2008).
  - [2] M. S. Safronova, U. I. Safronova, and C. W. Clark, Phys. Rev. A **86**, 042505 (2012).
  - [3] Li-Yan Tang, Zong-Chao Yan, Ting-Yun Shi, and James F. Babb, Phys. Rev. A **79**, 062712 (2009).
  - [4] Li-Yan Tang, Zong-Chao Yan, Ting-Yun Shi, and J. Mitroy, Phys. Rev. A **81** (2010).
  - [5] M. Puchalski, D. Kędziera, and K. Puchalski, Phys. Rev. A **84**, 052518 (2011).
  - [6] L.-Y. Tang, J.-Y. Zhang, Z.-C. Yan, T.-Y. Shi, and J. Mitroy, J. Chem. Phys. **133**, 104306 (2010).
  - [7] M. Puchalski, D. Kędziera, and K. Pachucki, Phys. Rev. A **85**, 019910 (2012).
  - [8] L.-Y. Tang, J.-Y. Zhang, Z.-C. Yan, T.-Y. Shi, J. F. Babb, and J. M. Mitroy, Phys. Rev. A **80**, 042511 (2009).
  - [9] L.-Y. Tang, Z.-C. Yan, T.-Y. Shi, and J. M. Mitroy, Phys. Rev. A **81**, 042521 (2010).
  - [10] Z.-C. Yan, H. X. Qiao, and G. W. F. Drake, **85**, 052513 (2012).
  - [11] L. M. Wang, Z.-C. Yan, H. X. Qiao, and G. W. F. Drake, Phys. Rev. A **83**, 034503 (2011).
  - [12] Z.-C. Yan, W. Nörtershäuser, and G. W. F. Drake, Phys. Rev. Lett. **100**, 243002 (2008).
  - [13] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A **61**, 022504 (2000).
  - [14] Z.-C. Yan, M. Tambasco, and G. W. F. Drake, Phys. Rev. A **57**, 1652 (1998).
  - [15] Z.-C. Yan and G. W. F. Drake, Phys. Rev. Lett. **79**, 1646 (1997).
  - [16] Z.-C. Yan, D. K. McKenzie, and G. W. F. Drake, Phys. Rev. A **54**, 1322 (1996).
  - [17] Z.-C. Yan, J. F. Baab, A. Dalgarno, and G. W. F. Drake, Phys. Rev. A **54**, 2824 (1996).
  - [18] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A **52**, R4316 (1995).
  - [19] Z.-C. Yan and G. W. F. Drake, Phys. Rev. A **52**, 3711 (1995).
  - [20] G. W. F. Drake and Z.-C. Yan, Phys. Rev. A **52**, 3681 (1995).
  - [21] D. K. McKenzie and G. W. F. Drake, Phys. Rev. A **44**, R6973 (1991).
  - [22] J. Mitroy, M. S. Safronova, and C. W. Clark, J. Phys. B **43**, 202001 (2010).
  - [23] M. Godefroid, C. F. Fischer, and P. Jönsson, J. Phys. B **34**, 1079 (2001).
  - [24] L.-H. Qu, Z.-W. Wang, and B.-W. Li, Opt. Commun. **162**, 223 (1999).
  - [25] L. Qu, Z. Wang, and B. Li, Eur. Phys. J. D **5**, 173 (1999).
  - [26] L. Qu, Z. Wang, and B. Li, J. Phys. B **31**, 3601 (1998).
  - [27] C. F. Fischer, M. Saporov, G. Gaigalas, and M. Godefroid, At. Data Nucl. Data Tables **70**, 119 (1998).
  - [28] A. E. Kramida, Phys. Scr. **57**, 66 (1998).
  - [29] P. Villorosi, P. Bidoli, and P. Nicolosi, J. Quant. Spectrosc. Radiat. Transfer **57**, 847 (1997).
  - [30] S. H. Patil and K. T. Tang, J. Chem. Phys. **106**, 2298 (1997).
  - [31] A. Bharadvaja and K. L. Baluja, Z. Phys. D **38**, 1 (1996).
  - [32] L. J. Curtis, D. G. Ellis, and I. Martinson, Phys. Rev. A **51**, 251 (1995).
  - [33] Z.-W. Wang and K. T. Chung, J. Phys. B **27**, 855 (1994).
  - [34] K. T. Chung, in *6th International Conference on the Physics of Highly Charged Ions, Manhattan, KS, USA, 28 Sept.-2 Oct. 1992, AIP Conf. Proc. Vol. 274*, edited by P. Richard, M. Stöckli, C. L. Cocke, and C. D. Lin (AIP Press, New York, NY, 1993).
  - [35] Z.-W. Wang, X.-W. Zhu, and K. T. Chung, Phys. Rev. A **46**, 6914 (1992).
  - [36] Z.-W. Wang, X.-W. Zhu, and K. T. Chung, J. Phys. B **25**, 3915 (1992).
  - [37] C. E. Theodosiou, Phys. Scr. **45**, 450 (1992).
  - [38] C. E. Theodosiou, L. J. Curtis, and M. El-Mekki, Phys. Rev. A **44**, 7144 (1991).
  - [39] S. A. Blundell, W. R. Johnson, Z. W. Liu, and J. Sapirstein, Phys. Rev. A **40**, 2233 (1989).
  - [40] G. Peach, H. E. Saraph, and M. J. Seaton, J. Phys. B **21**, 3669 (1988).
  - [41] J. Pipin and W. Woznicki, Chem. Phys. Lett. **95**, 392 (1983).
  - [42] C. F. Fischer, Phys. Rev. A **26**, 2627 (1982).
  - [43] K. T. Cheng, Y.-K. Kim, and J. P. Desclaux, At. Data Nucl. Data Tables **24**, 111 (1979).
  - [44] A. Lindgård and S. E. Nielsen, At. Data Nucl. Data Tables **19**, 533 (1977).
  - [45] A. W. Weiss, J. Quant. Spectrosc. Radiat. Transfer **18**, 481 (1977).
  - [46] Y.-K. Kim and J. P. Desclaux, Phys. Rev. Lett. **36**, 139 (1976).
  - [47] L. Armstrong Jr., W. R. Fielder, and D. L. Lin, Phys. Rev. A **14**, 1114 (1976).
  - [48] G. A. Martin and W. L. Wiese, Phys. Rev. A **13**, 699 (1976).
  - [49] S. Lunell, Phys. Scr. **12**, 63 (1975).
  - [50] U. I. Safronova, Opt. Spectrosc. **38**, 477 (1975).
  - [51] U. I. Safronova, J. Quant. Spectrosc. Radiat. Transfer **15**, 231 (1975).
  - [52] U. I. Safronova, J. Quant. Spectrosc. Radiat. Transfer **14**, 251 (1974).

- [53] S. A. Adelman and A. Szabo, *J. Chem. Phys.* **58**, 687 (1973).
- [54] C. Laughlin, M. N. Lewis, and Z. J. Horak, *J. Phys. B* **6**, 1953 (1973).
- [55] G. W. F. Drake, *Can. J. Phys.* **50**, 1896 (1972).
- [56] S. Hontzeas, I. Martinson, P. Erman, and R. Buchta, *Phys. Scr.* **6**, 55 (1972).
- [57] J. Bromander, *Phys. Scr.* **4**, 61 (1971).
- [58] T. Andersen, K. A. Jessen, and G. Sørensen, *Phys. Rev.* **188**, 76 (1969).
- [59] T. Andersen, K. A. Jessen, and G. Sørensen, *Phys. Lett. A* **29**, 384 (1969).
- [60] I. Bergström, J. Bromander, R. Buchta, L. Lundin, and I. Martinson, *Phys. Lett. A* **28**, 721 (1969).
- [61] J. Bromander, R. Buchta, and L. Lundin, *Phys. Lett. A* **29**, 523 (1969).
- [62] A. W. Weiss, *Astrophys. J.* **138**, 1262 (1963).
- [63] J. R. Fuhr and W. L. Wiese, *J. Phys. Chem. Ref. Data* **39**, 013101 (2010).
- [64] E. Träbert and L. J. Curtis, *Phys. Scr.* **74**, C46 (2006).
- [65] C. Chen and Z. W. Wang, *J. Chem. Phys.* **121**, 4171 (2004).
- [66] W. R. Johnson, S. A. Blundell, and J. Sapirstein, *Phys. Rev. A* **37**, 307 (1988).
- [67] W. R. Johnson, U. I. Safronova, A. Derevianko, and M. S. Safronova, *Phys. Rev. A* **77**, 022510 (2008).
- [68] J. Sapirstein and K. T. Cheng, *Phys. Rev. A* **66**, 042501 (2002).
- [69] Z.-C. Yan and G. W. F. Drake, *Phys. Rev. Lett.* **81**, 774 (1998).
- [70] L. Labzowsky, I. Goidenko, M. Tokman, and P. Pyykk, *Phys. Rev. A* **59**, 2707 (1999).
- [71] M. S. Safronova, W. R. Johnson, and U. I. Safronova, *Phys. Rev. A* **53**, 4036 (1996).
- [72] M. S. Safronova, W. R. Johnson, and U. I. Safronova, *J. Phys. B* **30**, 2375 (1997).
- [73] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team (2012). NIST Atomic Spectra Database (version 5.0), [Online]. Available: <http://physics.nist.gov/asd> [2012, December 11]. National Institute of Standards and Technology, Gaithersburg, MD.
- [74] S. A. Blundell, W. R. Johnson, M. S. Safronova, and U. I. Safronova, *Phys. Rev. A* **77**, 032507 (2008).
- [75] W. R. Johnson, Z. W. Liu, and J. Sapirstein, *At. Data and Nucl. Data Tables* **64**, 279 (1996).
- [76] M. S. Safronova and U. I. Safronova, *Phys. Rev. A* **83**, 012503 (2011).
- [77] M. S. Safronova and U. I. Safronova, *Phys. Rev. A* **83**, 052508 (2011).
- [78] M. S. Safronova and U. I. Safronova, *Phys. Rev. A* **85**, 022504 (2012).
- [79] U. I. Safronova, *Phys. Rev. A* **82**, 022504 (2010).
- [80] W. R. Johnson, D. Kolb, and K.-N. Huang, *At. Data Nucl. Data Tables* **28**, 333 (1983).
- [81] W. R. Johnson, D. R. Plante, and J. Sapirstein, *Adv. Atom. Mol. Opt. Phys.* **35**, 255 (1995).