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Relativistic configuration-interaction calculation of energy levels of core-excited states in lithiumlike ions: Argon through krypton

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Large-scale relativistic configuration-interaction calculation of energy levels of core-excited states of lithium-like ions is presented. Quantum electrodynamic, nuclear recoil, and frequency-dependent Breit corrections are included in the calculation. The approach is consistently applied for calculating all $n = 2$ core-excited states for all lithium-like ions starting from argon ($Z = 18$) and ending with krypton ($Z = 36$). The results obtained are supplemented with systematical estimations of calculation errors and omitted effects.

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I. INTRODUCTION

Spectroscopy of lithium-like ions has received remarkable attention over the past two decades. To a large extent, this attention was triggered by the famous experiment by Schweppe *et al.* [1], which demonstrated that the $1s^22p$–$1s^22s$ energy difference in lithium-like ions can be measured with an accuracy of better than 0.1% of the QED contribution. This result, recapitulated and surpassed in the following experiments (Refs. [2–6], to name a few), made lithium-like ions arguably the best playground for testing QED effects in the region of strong nuclear binding field.

A large number of sophisticated *ab initio* QED calculations have been accomplished during the past years in order to advance theory up to the experimental level of accuracy. In particular, the two-electron self-energy, two-electron vacuum-polarization, and the two-photon exchange corrections were calculated [7–13]. As a result, the $1s^22p_J$–$1s^22s$ transition energies in lithium-like ions are presently among the most precise in the medium- and high-Z region. This is not the case, however, for the higher excited states of lithium-like ions, which received much less attention from theorists. In the present work, we aim to correct this drawback.

The object of our present study is the energy levels of the $n = 2$ core-excited states of medium-Z lithium-like ions. Their precise knowledge is required for interpretation of astrophysical spectra, as these states contribute to the most prominent K-shell emission lines, observable in spectra of nearly all classes of cosmic x-ray sources (see, e.g., the review in Ref. [14]). Another important motivation for studying the K-shell emission [15,16] is that it is used for the diagnostics of hot laboratory plasmas, particularly those produced in magnetically confined fusion research.

Accurate theoretical description of transitions involving the core-excited states is complicated by two main issues. The first is a large contribution of the QED effects. Indeed, the QED effects are strongest for the K-shell electrons and, therefore, for the K-shell transitions. The second problem is that the core-excited states are mostly autoionizing states. This means that one might expect a strong mixing of the reference state with the closely lying continuum of single excited states (i.e., a closed core + an electron in continuum). This interaction with the continuum is very difficult to treat accurately in theoretical calculations.

Accurate theoretical data on the core-excited states of lithium-like ions were first obtained by Vainstein and Safronova within the $1/Z$ expansion method [17]. Later, these states were addressed within the multiconfigurational Dirac-Fock approach [18–20] and, more recently, within the relativistic many-body perturbation theory [21]. In the present work, we employ the configuration-interaction (CI) method to obtain accurate values for the Dirac-Coulomb-Breit energies, including the nuclear recoil contribution and the frequency-dependent Breit correction. The CI energies are supplemented with the QED correction calculated separately in the one-electron approximation with a local screening potential. This approach is much simpler (and, consequently, less accurate) than the full-scale QED calculations reported in Refs. [9–13] for the $1s^22p_J$–$1s^22s$ transitions, but it reproduces the results of those more complete calculations remarkably well. Our present approach is similar to the one applied previously by Chen *et al.* [22] for calculating the lowest lying $n = 2$ energy levels of lithium-like ions.

The developed approach is applied for a systematic calculation of energy levels of all $n = 2$ core-excited states for all lithium-like ions starting from argon ($Z = 18$) and ending with krypton ($Z = 36$). For some of these ions, no data on the core-excited states were previously available in the literature.

An important feature of the present investigation is a systematic estimation of uncertainties of the calculated results. For each particular state and each nuclear charge, we perform our CI calculations with a large number (typically, 20–30) of different sets of configuration-state functions. By analyzing the successive increments of the results obtained with the set of configuration-state functions, which is increased in all possible directions, we obtain a realistic estimate of how well our CI results have converged. Beside the uncertainty of the Dirac-Coulomb-Breit energy, we also estimate the uncertainty due to the omitted higher-order QED effects. This is done by performing the QED calculations with three different screening potentials and analyzing the dependence of the results on the choice of the potential.

The remaining paper is organized as follows. In the following section, we give a brief outline of our implementation of the CI method. The evaluation of the QED correction is discussed in Sec. III. Section IV presents the numerical details of the calculations. Finally, in Sec. V, we report the results of our calculations and compare them with data available in the literature. Relativistic units $\hbar = c = 1$ and charge units $e^2/4\pi = \alpha$ are used throughout this paper.

II. CONFIGURATION INTERACTION METHOD

A. DCB Hamiltonian

Relativistic Dirac-Coulomb-Breit (DCB) Hamiltonian of an N-electron atom with an infinitely heavy nucleus is given by

$$H_{\rm DCB} = \sum_i h_D(i) + \sum_{i<j} [V_C(i,j) + V_B(i,j)]\,, \tag{1}$$

where indices $i,j = 1,\ldots,N$ numerate the electrons, h_D is the one-particle Dirac Hamiltonian,

$$h_D(i) = \boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + (\beta - 1)\, m + V_{\rm nuc}(r_i), \tag{2}$$

$\boldsymbol{\alpha}$ and β are the Dirac matrices, $\boldsymbol{p}$ is the momentum operator, $V_{\rm nuc}$ is the binding potential of the nucleus, V_C and V_B are the Coulomb and the (frequency-independent) Breit parts of the electron-electron interaction,

$$V_C(i,j) = \frac{\alpha}{r_{ij}}, \tag{3}$$

$$V_B(i,j) = -\frac{\alpha}{2\,r_{ij}}\,[\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j + (\boldsymbol{\alpha}_i \cdot \hat{\boldsymbol{r}}_{ij})(\boldsymbol{\alpha}_j \cdot \hat{\boldsymbol{r}}_{ij})], \tag{4}$$

with $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$ and $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$. The operator $H_{\rm DCB}$ acts in the space of the positive-energy eigenfunctions of some one-particle Dirac Hamiltonian $\tilde{h}_D$, which does not necessarily coincides with (2). It is usually convenient to include a part of the electron-electron interaction already in the one-electron orbitals by introducing a screening potential $V_{\rm scr}(r)$ and defining $\tilde{h}_D$ as

$$\tilde{h}_D(i) = \boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + (\beta - 1)\, m + V_{\rm nuc}(r_i) + V_{\rm scr}(r_i). \tag{5}$$

The N-electron wave function of the system with parity P, angular momentum quantum number J, and its projection M is represented as a linear combination of configuration-state functions (CSFs)

$$\Psi(PJM) = \sum_{r=1}^{N_{\rm CSF}} c_r\, \Phi(\gamma_r PJM), \tag{6}$$

where γ_r denotes the set of additional quantum numbers that determine the CSF. The CSFs are constructed as antisymmetrized products of one-electron orbitals ψ_n of the form

$$\psi_n(\boldsymbol{r}) = \frac{1}{r}\begin{bmatrix} G_n(r)\, \chi_{\kappa_n m_n}(\hat{\boldsymbol{r}}) \\ i\,F_n(r)\, \chi_{-\kappa_n m_n}(\hat{\boldsymbol{r}}) \end{bmatrix}, \tag{7}$$

where $\chi_{\kappa m}$ the spin-angular spinor [23], $\kappa = (-1)^{j+l+1/2}(j + 1/2)$ is the relativistic angular parameter, and m is the angular momentum projection. In the present work, we chose the one-electron orbitals ψ_n to be the (positive-energy) eigenfunctions of the one-electron Dirac Hamiltonian (5) with the screening potential being the frozen-core Dirac-Fock potential $V_{\rm DF}$, defined by its action on a wave function as

$$V_{\rm DF}(\boldsymbol{r}_1)\,\psi(\boldsymbol{r}_1) = \sum_c \int d\boldsymbol{r}_2\, \psi_c^+(\boldsymbol{r}_2)\, \frac{\alpha}{r_{12}} \times [\psi_c(\boldsymbol{r}_2)\,\psi(\boldsymbol{r}_1) - \psi_c(\boldsymbol{r}_1)\,\psi(\boldsymbol{r}_2)], \tag{8}$$

where the index c runs over the core orbitals.

In the CI method, the energy levels of the system and the mixing coefficients c_r in Eq. (6) are obtained by solving the secular equation

$$\det\{\langle \gamma_r PJM | H_{\rm DCB} | \gamma_s PJM\rangle - E_r\, \delta_{rs}\} = 0. \tag{9}$$

The matrix elements of the Hamiltonian between the CSFs can be represented as linear combinations of the one- and two-particle radial integrals [24],

$$\langle \gamma_r PJM | H_{\rm DCB} | \gamma_s PJM\rangle = \sum_{ab} d_{rs}(ab)\, I(ab) + \alpha \sum_k \sum_{abcd} v_{rs}^{(k)}(abcd) R_k(abcd). \tag{10}$$

Here, a, b, c, and d specify the one-electron orbitals, d_{rs} and $v_{rs}^{(k)}$ are the angular coefficients, $I(ab)$ are the one-electron radial integrals, and $R_k(abcd)$ are the relativistic generalization of Slater radial integrals. Further details of our implementation of the CI method can be found in our previous study [25].

B. Corrections to DCB energies

In the present work, we include two corrections to the DCB Hamiltonian (1), namely the nuclear recoil and the frequency-dependent Breit corrections. The nuclear recoil correction is small and will be treated nonrelativistically. It is conveniently separated into two parts, the normal mass shift (NMS) and the specific mass shift (SMS). The NMS part can be easily factorized out and accounted for by multiplying the eigenvalues of the DCB Hamiltonian (1) by the reduced mass prefactor

$$E_{\rm DCB} \to \frac{\mu}{m}\, E_{\rm DCB}, \tag{11}$$

where $\mu/m = 1/(1 + m/M)$ and m and M are masses of the electron and the nucleus, respectively. The SMS part of the recoil effect is accounted for by adding an additional term to the DCB Hamiltonian,

$$\delta H_{\rm SMS} = \frac{m}{M} \sum_{i<j} \boldsymbol{p}_i \cdot \boldsymbol{p}_j. \tag{12}$$

The frequency-dependent Breit correction comes from the QED theory. It can be obtained by substituting the Coulomb V_C and the standard Breit V_B interactions by the full QED electron-electron interaction operator, when calculating the matrix elements of the DCB Hamiltonian (1) with the reference-state wave function(s). Note that in our work, contrary to the approach sometimes used in the literature (e.g., in Ref. [22]), we do not construct the whole DCB Hamiltonian matrix with the frequency-dependent Breit interaction but apply the frequency-dependent Breit interaction for the reference CSFs only. The reason is that the DCB Hamiltonian (1) was derived [26] for the standard (frequency-independent) Breit interaction only, and inclusion of the frequency dependency for highly excited CSFs can lead to sizable spurious effects.

The QED electron-electron interaction operator $I(\omega)$ depends on the energy of the virtual photon ω and has different forms in different gauges. In the Feynman gauge, it is given by

$$I_{\text{Feyn}}(\omega,r_{ij}) = \alpha(1-\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j)\frac{e^{i\,|\omega|\,r_{ij}}}{r_{ij}}, \tag{13}$$

whereas in the Coulomb gauge, it reads

$$I_{\text{Coul}}(\omega,r_{ij}) = I_{\text{Feyn}}(\omega,r_{ij}) - \alpha\left[1+\frac{(\boldsymbol{\alpha}_i\cdot\nabla_i)(\boldsymbol{\alpha}_j\cdot\nabla_j)}{\omega^2}\right]\frac{e^{i\,|\omega|\,r_{ij}}-1}{r_{ij}}. \tag{14}$$

General QED expressions for the one-photon exchange correction for a given reference state [27] involve two kind of matrix elements, the direct ones of the form $\langle ab|I|ab\rangle$ and the exchange ones of the form $\langle ba|I|ab\rangle$. The energy of the virtual photon is fixed by $\omega = 0$ in the direct terms and by $\omega = \varepsilon_a - \varepsilon_b$ in the exchange terms. In the case of several equivalent reference CSFs, there are also nondiagonal terms and, consequently, matrix elements of a general form $\langle ab|I|cd\rangle$. For them, we used an energy symmetrized expression [28],

$$\langle ab|I|cd\rangle \to \tfrac{1}{2}[\langle ab|I(\varepsilon_a-\varepsilon_c)|cd\rangle + \langle ab|I(\varepsilon_b-\varepsilon_d)|cd\rangle]. \tag{15}$$

It can be easily verified that, for a single reference state, the matrix elements of the operator I are gauge independent. In the case of several reference-state configurations, gauge invariance is not exact, but we checked that the residual is completely negligible in each particular case.

III. RADIATIVE QED CORRECTIONS

In this section, we deal with corrections to the DCB energies due to QED effects. For the purpose of the present investigation, it will be sufficient to take into account only the dominant part of the radiative QED effects, given by the one-electron self-energy and the vacuum polarization calculated in a local screening potential.

The total QED contribution for a given many-electron reference state is obtained by summing the QED contributions from the one-electron orbitals, weighted by their fractional occupation numbers as obtained from the eigenvectors of the CI calculation,

$$\delta E_{\text{QED}} = \sum_a q_a[\langle a|\Sigma_{\text{SE}}(\varepsilon_a)|a\rangle + \langle a|V_{\text{VP}}|a\rangle], \tag{16}$$

where index a runs over all one-electron orbitals contributing to the given many-electron state, q_a is the occupation number of the one-electron orbital, Σ_{SE} is the self-energy operator, ε_a is the Dirac energy of the one-electron state a, and V_{VP} is the vacuum polarization potential.

The one-electron self-energy correction in a general local potential is calculated rigorously to all orders in the nuclear binding strength parameter $Z\alpha$. The method used in the present work is quite close to the one developed by Blundell and Snyderman [29]. We, however, introduced several improvements to their original calculation scheme. First, we used the dually kinetically balanced B-spline basis set [30], which yielded significantly better convergence than the original B-spline method by Johnson *et al.* [31]. Second, we evaluated the many-potential electron propagator $G^{(2+)}$ by forming the difference

$$G^{(2+)} = G - G^{(0)} - G^{(1)}, \tag{17}$$

where G, $G^{(0)}$, and $G^{(1)}$ are the full electron propagator, the free propagator, and the one-potential propagator, respectively. The one-potential propagator was calculated by taking a numerical derivative of the B-spline basis set with respect to the nuclear charge Z,

$$G^{(1)} = Z\left(\frac{d}{dZ}G\right)_{Z=0}. \tag{18}$$

We found that this approach yields results equivalent to those obtained by the direct (triple) summation over the spectrum but is much faster in actual computations.

The one-electron vacuum-polarization contribution was straightforwardly calculated as an expectation value of the Uehling and Wichmann-Kroll potentials with the one-electron orbitals. The Wichmann-Kroll potential was evaluated by the approximate formulas tabulated in Ref. [32].

In our calculations of the one-electron self-energy and vacuum-polarization corrections, we assume that the initial state and all intermediate states in the electron propagator are the eigenstates of the Dirac Hamiltonian (5) with a screening potential V_{scr}. The screening potential allows us to account for the dominant part of the electron-electron interaction and should be chosen with care. It would be natural to use the same screening potential as in the CI part of our calculations, but this is not possible since the Dirac-Fock potential (8) is nonlocal. Because of this, we introduce three different local screening potentials, whose eigenstates and eigenvalues are quite close to the Dirack-Fock ones.

Each potential is constructed into two steps. First, we solve the Dirac-Fock problem (for the center of gravity of all equivalent relativistic configurations) and find the Dirac-Fock wave functions. Second, we use these wave function to set up our local screening potentials.

The simplest choice is the potential induced by the charge density of all other electron orbitals except the reference one. This is the core-Hartree (CH) potential defined, for a given one-electron state a, as

$$V_{\text{CH},a}(r) = \alpha\int_0^\infty dr'\,\frac{1}{\max(r,r')}\,\rho_a(r'), \tag{19}$$

where ρ_a is the density of all one-electron orbitals excluding a,

$$\rho_a(r) = \sum_{b\neq a} q_b\left[G_b^2(r) + F_b^2(r)\right], \tag{20}$$

with G_b and F_b being the upper and the lower components of the Dirac-Fock solution. Note that the CH potential defined in this way differs from the one frequently encountered in the literature because we do not require self-consistency for $V_{\text{CH},a}$.

The second choice of the screening potential is a variant of the Kohn-Sham potential [33,34], defined as

$$V_{\rm KS}(r) = \alpha \int_0^\infty dr' \frac{1}{\max(r,r')}\,\rho(r') - \frac{2}{3}\frac{\alpha}{r}\left[\frac{81}{32\pi^2}\, r\,\rho(r)\right]^{1/3} - \frac{\alpha}{r}\left[1-e^{-(Ar)^2}\right], \quad (21)$$

where $\rho(r)$ is the *total* Dirac-Fock charge density,

$$\rho(r) = \sum_b q_b \left[G_b^2(r) + F_b^2(r)\right]. \quad (22)$$

The second term in the right-hand side Eq. (21) is the exchange correction derived from density functional theory, whereas the third term is a kind of the Latter correction [35], which restores the physical asymptotical behavior of the KS potential at large distances. The parameter A in the Latter correction was chosen to be about $Z\alpha/10$. Again, the KS potential (21) differs from the one encountered in the literature because we do not require self-consistency in its definition.

The third screening potential employed in this work is referred to as the localized Dirac-Fock (LDF) potential. For a given state a, the LDF potential $V_{{\rm LDF},a}$ is obtained by inverting the Dirac-Fock equations with the known solutions G_a and F_a and then smoothing out the result in the vicinity of zeros of G_a. The LDF potential was first introduced for calculations of the QED corrections to the parity-nonconserving transition amplitudes in cesium [36,37]. In the present work, we employ the variant of the LDF potential described in detail in Ref. [12].

According to our experience and comparison with the results of more complete calculations, the LDF potential yields better results in calculations of the QED effects than the KS and CH potentials. Therefore, we will use this potential for obtaining the final results for the QED correction in our present calculation.

IV. NUMERICAL DETAILS

In the present work, we use our implementation of the CI method employed previously in Refs. [25,38] for the evaluation of the hyperfine splitting in Li and Be$^+$. The one-electron basis was constructed with help of the dual-kinetic-balance B-spline method [30]. The screening potential in the one-electron Hamiltonian (5) was taken to be the frozen-core DF potential (8), with the $1s^2$ core in the case of the ground and valence-excited states and the $1s$ core in the case of the core-excited states. The standard Fermi model of the nuclear charge distribution was used to represent the nuclear potential.

For a given number of B splines n_a, all Dirac eigenstates were taken with the energy $0 < \varepsilon_n \leqslant mc^2(1+Z\alpha\,\epsilon)$ and the orbital quantum number $l \leqslant L_{\rm max}$, where the value of the energy cutoff parameter ϵ was varied between 4 and 16 and $L_{\rm max}$, between 1 and 7. In order to check convergence of our CI results with respect to the number of partial waves included and the size of the basis, we perform a set of calculations with a different number of basis functions and analyze the successive increments as the size of the basis is enlarged. In our analysis, we study the dependence of the results obtained on the parameters n_a, ϵ, and $L_{\rm max}$ and the type of virtual excitations included. In all cases relevant for the present study, the contribution of triple excitations was found to be very small. We thus perform our calculations first with including single and double excitations only and then adding the contribution of the triples calculated separately with a smaller basis. The analysis of the convergence of the partial-wave expansion is supplemented with an estimation of the omitted tail, which is obtained by a polynomial least-squares fitting of the increments in $1/l$.

An example of our CI calculations is presented in Table I for the Dirac-Coulomb energy and in Table II for the Breit correction. The results reported in these tables are obtained by performing calculations with 27 different sets of basis functions. Each set is characterized by parameters n_a, ϵ, and $L_{\rm max}$. For example, for $n_a = 30$, $\epsilon = 4$, and $L_{\rm max} = 7$, the one-electron basis reads $17s\ 16p\ 16d\ 15f\ 15g\ 15h\ 14i\ 14k$, where $16p$ means 16 lowest-lying orbitals of the $p_{1/2}$ symmetry *and* 16 lowest-lying orbitals of the $p_{3/2}$ symmetry, and so on. Generating all possible single- and double-excited CSF's with this set of one-electron orbitals leads to a basis of about $N_{\rm CSF} = 30\,000$ functions. As another example, for $n_a = 50$, $\epsilon = 16$, and $L_{\rm max} = 2$, the set of one-electron orbitals is $29s\ 29p\ 28d$, leading to the basis of about $N_{\rm CSF} = 25\,000$ functions.

TABLE I. Contributions to the Coulomb energy (in a.u.) for the $1s2s2p\ {}^4P^o_{1/2}$ state of lithium-like iron ($Z = 26$), for the infinitely heavy nucleus. The values listed after the first row are the increments obtained on successively adding configurations while increasing the maximal value of the orbital quantum number $L_{\rm max}$ and enlarging the size of the one-electron basis. Label SD denotes single and double excitations, T denotes the triple excitations, n_a is the number of B splines in the one-electron basis set, and ϵ is the energy cutoff parameter; see text for the details.

$L_{\rm max}$	δ E
SD, $n_a = 30$, $\epsilon = 4$	
1	−497.762 342 48
2	−0.008 719 04
3	−0.000 662 72
4	−0.000 124 13
5	−0.000 034 81
6	−0.000 012 45
7	−0.000 005 18
$\geqslant 8$	−0.000 005 55
SD, $n_a = 40$, $\epsilon = 8$	
1	−0.000 173 23
2	−0.000 001 34
3	−0.000 001 13
$\geqslant 4$	−0.000 001 07
SD, $n_a = 50$, $\epsilon = 16$	
1	−0.000 006 46
2	−0.000 000 43
T, $n_a = 25$, $\epsilon = 4$	
1	−0.000 000 22
2	−0.000 000 77
3	−0.000 000 09
$\geqslant 4$	−0.000 000 04
Final result	**−497.772 091(7)**

TABLE II. Contributions to the frequency-independent Breit energy (in a.u.) for the $1s2s2p\,{}^4P^o_{1/2}$ state of lithium-like iron ($Z = 26$) for the infinitely heavy nucleus. Notations are the same as in Table I.

$L_{\max}$	δ E
SD, $n_a = 30$, $\epsilon = 4$	
1	0.065 471 70
2	−0.000 330 01
3	−0.000 050 23
4	−0.000 014 47
5	−0.000 005 98
$\geqslant 6$	−0.000 009 15
SD, $n_a = 40$, $\epsilon = 8$	
1	−0.000 001 76
2	−0.000 000 43
3	−0.000 000 25
SD, $n_a = 50$, $\epsilon = 16$	
1	0.000 004 49
Final result	**0.065 064(9)**

Analysis of data presented in Tables I and II allows us to give a reliable estimate of the uncertainty of our CI calculations. In the case shown in these tables, the dominant error comes from the omitted tail of the partial-wave expansion. For higher core-excited states, however, the dominant error often comes from the convergence of the one-electron basis of *np* and *nd* symmetries, which is explained by strong mixing of the reference (autoionizing, core-excited) states with the closely lying continuum of single-excited $1s^2np$ and $1s^2nd$ virtual states. In some cases (particularly, for the ${}^2D$ states), we had to employ large one-electron basis sets, up to $40s\,39p\,39d$ ($N_{\rm CSF} = 47\,000$ functions) in order to ensure the convergence of CI results.

We now discuss our calculations of the radiative QED corrections. Table III presents a detailed breakdown of individual QED contributions for the $1s2s2p\,{}^4P^o_{1/2}$- $1s^22s\,{}^2S_{1/2}$ transition in lithium-like iron. The calculation is performed for the LDF, KS, and CH potentials. All three results for the transition energy agree very well with each other. Remarkably, the agreement is much better for the energy difference than for each energy level separately. The same situation occurs for the other transitions from the core excited states to the ground state.

As a final result for the QED contribution, we take the value obtained with the LDF potential (since this potential yields the best agreement with the results of more complete calculations). The uncertainty of the QED contribution was estimated as the maximal deviation of the KS and CH values from the LDF one. We checked that such estimation of uncertainty is consistent with the results of more sophisticated QED calculations available for the $1s^22p_J$ states [7,8,13]. The set of calculations presented in Table III takes about 30 h of processor time on a modern workstation.

V. RESULTS

Table IV presents our calculation results for the energy levels of the $1s^22s$, $1s^22p$, and $1s\,2l\,2l'$ states of lithium-like ions, from argon ($Z = 18$) to krypton ($Z = 36$). The total energies are listed in the table for the ground state, whereas for all other states, relative energies with respect to the ground state are given. Note that for the $1s^22p_J$-$1s^22s$ energy differences, much more accurate theoretical

TABLE III. QED contributions (in a.u.) for the $1s2s2p\,{}^4P^o_{1/2}$–$1s^22s\,{}^2S_{1/2}$ transition in lithium-like iron ($Z = 26$) for different screening potentials. q denotes the occupation number of the single electron orbitals as obtained from the CI calculations. SE, VP, and QED denote the self-energy, the vacuum-polarization, and the total QED contribution, respectively.

	${}^4P^o_{1/2}$				${}^2S_{1/2}$				
State	q	SE	VP	QED	q	SE	VP	QED	${}^4P^o_{1/2}$–${}^2S_{1/2}$
LDF potential									
$1s$	1.000	0.15688	−0.01337	0.14350	2.000	0.30432	−0.02610	0.27822	−0.13472
$2s$	1.000	0.01974	−0.00158	0.01816	1.000	0.01894	−0.00153	0.01741	0.00075
$2p_{1/2}$	0.943	−0.00052	−0.00001	−0.00053					−0.00053
$2p_{3/2}$	0.057	0.00005	0.00000	0.00005					0.00005
Sum									−0.13445
KS potential									
$1s$	1.000	0.15512	−0.01326	0.14186	2.000	0.30287	−0.02600	0.27687	−0.13501
$2s$	1.000	0.01991	−0.00159	0.01832	1.000	0.01922	−0.00154	0.01768	0.00064
$2p_{1/2}$	0.943	−0.00053	−0.00001	−0.00054					−0.00054
$2p_{3/2}$	0.057	0.00005	0.00000	0.00005					0.00005
Sum									−0.13487
CH potential									
$1s$	1.000	0.15674	−0.01337	0.14338	2.000	0.30384	−0.02607	0.27778	−0.13440
$2s$	1.000	0.01956	−0.00157	0.01799	1.000	0.01894	−0.00153	0.01741	0.00058
$2p_{1/2}$	0.943	−0.00051	−0.00001	−0.00052					−0.00052
$2p_{3/2}$	0.057	0.00005	0.00000	0.00005					0.00005
Sum									−0.13429
Final result									**−0.13445 (43)**

TABLE IV. Energy levels of lithium-like ions from argon through krypton in Rydbergs, 1 Ry = 109 737.315 685 39 (55) cm^{-1}. Separately listed are the Dirac-Coulomb energy, the frequency-independent Breit correction, the QED correction, the specific mass-shift (SMS) correction, and the frequency-dependent Breit (Breit′) correction. The total energies are presented for the ground state, whereas for all other states, the energies relative to the ground state are given. μ/m is the reduced mass prefactor and R is the nuclear root-mean-square charge radius.

Term		J	Coulomb	Breit	QED	SMS	Breit′	Total
Ar ($Z = 18$), $1 - \mu/m = 0.00001373$, $R = 3.427$ fm								
$1s^22s$	^2S	1/2	−696.0032	0.1504	0.1676	0.0001	−0.0001	−695.6852(4)
$1s^22p$	$^2P^o$	1/2	2.3412	0.0113	−0.0098	−0.0006	−0.0003	2.3417(6)
		3/2	2.5867	−0.0015	−0.0092	−0.0006	−0.0004	2.5749(8)
$1s2s^2$	^2S	1/2	226.5266	−0.1362	−0.0669	−0.0001	0.0001	226.3234(17)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	227.0887	−0.1094	−0.0753	−0.0007	−0.0002	226.9032(4)
		3/2	227.1777	−0.1359	−0.0751	−0.0007	−0.0003	226.9658(4)
		5/2	227.3442	−0.1469	−0.0747	−0.0007	−0.0003	227.1215(3)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	228.9723	−0.1355	−0.0751	0.0003	0.0004	228.7624(9)
		3/2	229.0991	−0.1400	−0.0748	0.0005	0.0005	228.8852(4)
$1s(^2S)2p^2(^3P)$	^4P	1/2	229.6458	−0.1074	−0.0852	−0.0013	−0.0005	229.4514(6)
		3/2	229.7494	−0.1074	−0.0850	−0.0013	−0.0005	229.5553(6)
		5/2	229.8938	−0.1384	−0.0847	−0.0013	−0.0006	229.6689(6)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	229.8117	−0.1136	−0.0749	−0.0005	−0.0001	229.6226(39)
		3/2	229.8798	−0.1322	−0.0748	−0.0006	−0.0002	229.6720(43)
$1s(^2S)2p^2(^1D)$	^2D	3/2	230.9327	−0.1099	−0.0849	−0.0006	−0.0001	230.7372(33)
		5/2	230.9812	−0.1507	−0.0847	−0.0007	−0.0003	230.7449(35)
$1s(^2S)2p^2(^3P)$	^2P	1/2	231.2057	−0.1479	−0.0845	0.0005	0.0005	230.9743(12)
		3/2	231.4382	−0.1464	−0.0845	0.0004	0.0004	231.2081(7)
$1s(^2S)2p^2(^1S)$	^2S	1/2	232.5676	−0.1241	−0.0823	−0.0006	−0.0002	232.3605(133)
K ($Z = 19$), $1 - \mu/m = 0.00001408$, $R = 3.435$ fm								
$1s^22s$	^2S	1/2	−777.9530	0.1782	0.2021	0.0001	−0.0001	−777.5727(5)
$1s^22p$	$^2P^o$	1/2	2.4910	0.0137	−0.0119	−0.0007	−0.0004	2.4918(7)
		3/2	2.8025	−0.0018	−0.0112	−0.0006	−0.0005	2.7882(7)
$1s2s^2$	^2S	1/2	253.5172	−0.1614	−0.0808	−0.0001	0.0001	253.2750(17)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	254.1116	−0.1296	−0.0910	−0.0008	−0.0003	253.8901(4)
		3/2	254.2222	−0.1612	−0.0907	−0.0008	−0.0003	253.9691(4)
		5/2	254.4336	−0.1742	−0.0902	−0.0008	−0.0004	254.1681(4)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	256.1274	−0.1593	−0.0908	0.0003	0.0005	255.8781(9)
		3/2	256.2908	−0.1663	−0.0904	0.0005	0.0005	256.0351(4)
$1s(^2S)2p^2(^3P)$	^4P	1/2	256.8569	−0.1273	−0.1031	−0.0015	−0.0006	256.6246(7)
		3/2	256.9900	−0.1272	−0.1027	−0.0015	−0.0006	256.7579(7)
		5/2	257.1686	−0.1642	−0.1024	−0.0014	−0.0007	256.8999(7)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	257.0338	−0.1357	−0.0906	−0.0005	−0.0001	256.8070(36)
		3/2	257.1170	−0.1559	−0.0904	−0.0007	−0.0002	256.8698(40)
$1s(^2S)2p^2(^1D)$	^2D	3/2	258.2528	−0.1309	−0.1027	−0.0006	−0.0001	258.0184(21)
		5/2	258.3223	−0.1784	−0.1024	−0.0008	−0.0003	258.0404(22)
$1s(^2S)2p^2(^3P)$	^2P	1/2	258.5281	−0.1750	−0.1029	0.0006	0.0006	258.2514(7)
		3/2	258.8289	−0.1726	−0.1022	0.0005	0.0005	258.5551(8)
$1s(^2S)2p^2(^1S)$	^2S	1/2	260.0040	−0.1472	−0.1003	−0.0007	−0.0002	259.7557(40)
Ca ($Z = 20$), $1 - \mu/m = 0.00001373$, $R = 3.476$ fm								
$1s^22s$	^2S	1/2	−864.5349	0.2094	0.2412	0.0001	−0.0002	−864.0843(6)
$1s^22p$	$^2P^o$	1/2	2.6419	0.0163	−0.0143	−0.0007	−0.0004	2.6426(8)
		3/2	3.0317	−0.0021	−0.0135	−0.0007	−0.0006	3.0148(8)
$1s2s^2$	^2S	1/2	282.0476	−0.1895	−0.0965	−0.0001	0.0001	281.7615(17)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	282.6744	−0.1522	−0.1088	−0.0008	−0.0003	282.4123(4)
		3/2	282.8100	−0.1897	−0.1085	−0.0008	−0.0004	282.5106(5)
		5/2	283.0754	−0.2046	−0.1079	−0.0008	−0.0005	282.7617(4)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	284.8243	−0.1855	−0.1086	0.0003	0.0005	284.5311(9)
		3/2	285.0324	−0.1958	−0.1081	0.0006	0.0006	284.7297(5)
$1s(^2S)2p^2(^3P)$	^4P	1/2	285.6153	−0.1494	−0.1233	−0.0016	−0.0007	285.3403(8)
		3/2	285.7844	−0.1494	−0.1229	−0.0016	−0.0008	285.5098(8)
		5/2	286.0022	−0.1931	−0.1225	−0.0016	−0.0008	285.6842(8)

TABLE IV. (*Continued.*)

Term		J	Coulomb	Breit	QED	SMS	Breit′	Total
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	285.8054	−0.1608	−0.1083	−0.0005	−0.0001	285.5357(33)
		3/2	285.9054	−0.1822	−0.1081	−0.0008	−0.0003	285.6141(38)
$1s(^2S)2p^2(^1D)$	^2D	3/2	287.1271	−0.1547	−0.1228	−0.0007	−0.0001	286.8488(15)
		5/2	287.2249	−0.2093	−0.1224	−0.0009	−0.0004	286.8919(15)
$1s(^2S)2p^2(^3P)$	^2P	1/2	287.4004	−0.2050	−0.1231	0.0006	0.0007	287.0736(8)
		3/2	287.7846	−0.2015	−0.1221	0.0005	0.0005	287.4620(8)
$1s(^2S)2p^2(^1S)$	^2S	1/2	289.0017	−0.1730	−0.1200	−0.0007	−0.0003	288.7077(25)
Sc ($Z = 21$), $1 - \mu/m = 0.00001221$, $R = 3.544$ fm								
$1s^22s$	^2S	1/2	−955.7643	0.2440	0.2853	0.0001	−0.0002	−955.2351(6)
$1s^22p$	$^2P^o$	1/2	2.7937	0.0190	−0.0171	−0.0007	−0.0005	2.7944(9)
		3/2	3.2760	−0.0026	−0.0160	−0.0007	−0.0007	3.2560(9)
$1s2s^2$	^2S	1/2	312.1222	−0.2208	−0.1142	−0.0001	0.0001	311.7872(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	312.7818	−0.1773	−0.1289	−0.0008	−0.0003	312.4744(5)
		3/2	312.9458	−0.2214	−0.1286	−0.0008	−0.0004	312.5946(5)
		5/2	313.2757	−0.2384	−0.1278	−0.0008	−0.0006	312.9081(5)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	315.0672	−0.2140	−0.1287	0.0003	0.0006	314.7254(10)
		3/2	315.3299	−0.2287	−0.1280	0.0006	0.0007	314.9745(5)
$1s(^2S)2p^2(^3P)$	^4P	1/2	315.9258	−0.1741	−0.1462	−0.0016	−0.0008	315.6032(9)
		3/2	316.1389	−0.1740	−0.1456	−0.0016	−0.0009	315.8168(9)
		5/2	316.4006	−0.2254	−0.1452	−0.0015	−0.0010	316.0276(9)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	316.1327	−0.1893	−0.1282	−0.0005	−0.0001	315.8146(32)
		3/2	316.2512	−0.2112	−0.1280	−0.0008	−0.0004	315.9109(38)
$1s(^2S)2p^2(^1D)$	^2D	3/2	317.5616	−0.1815	−0.1456	−0.0006	−0.0001	317.2338(13)
		5/2	317.6965	−0.2434	−0.1451	−0.0008	−0.0005	317.3067(13)
$1s(^2S)2p^2(^3P)$	^2P	1/2	317.8285	−0.2383	−0.1459	0.0006	0.0008	317.4456(9)
		3/2	318.3134	−0.2333	−0.1447	0.0005	0.0006	317.9364(9)
$1s(^2S)2p^2(^1S)$	^2S	1/2	319.5686	−0.2019	−0.1423	−0.0007	−0.0003	319.2234(20)
Ti ($Z = 22$), $1 - \mu/m = 0.00001144$, $R = 3.591$ fm								
$1s^22s$	^2S	1/2	−1051.6554	0.2823	0.3347	0.0001	−0.0002	−1051.0386(7)
$1s^22p$	$^2P^o$	1/2	2.9466	0.0222	−0.0202	−0.0007	−0.0006	2.9473(10)
		3/2	3.5371	−0.0030	−0.0189	−0.0007	−0.0008	3.5136(10)
$1s2s^2$	^2S	1/2	343.7454	−0.2553	−0.1341	−0.0001	0.0001	343.3559(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	344.4377	−0.2051	−0.1514	−0.0009	−0.0004	344.0800(6)
		3/2	344.6340	−0.2566	−0.1511	−0.0008	−0.0005	344.2250(5)
		5/2	345.0404	−0.2758	−0.1501	−0.0008	−0.0007	344.6130(5)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	346.8601	−0.2450	−0.1512	0.0003	0.0007	346.4649(11)
		3/2	347.1888	−0.2651	−0.1504	0.0006	0.0008	346.7748(6)
$1s(^2S)2p^2(^3P)$	^4P	1/2	347.7928	−0.2014	−0.1716	−0.0016	−0.0009	347.4173(10)
		3/2	348.0593	−0.2013	−0.1711	−0.0016	−0.0010	347.6843(10)
		5/2	348.3697	−0.2612	−0.1706	−0.0016	−0.0012	347.9351(10)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	348.0211	−0.2212	−0.1506	−0.0005	−0.0001	347.6489(32)
		3/2	348.1601	−0.2430	−0.1503	−0.0008	−0.0005	347.7656(38)
$1s(^2S)2p^2(^1D)$	^2D	3/2	349.5619	−0.2113	−0.1711	−0.0006	−0.0001	349.1787(12)
		5/2	349.7449	−0.2810	−0.1704	−0.0009	−0.0006	349.2920(13)
$1s(^2S)2p^2(^3P)$	^2P	1/2	349.8177	−0.2749	−0.1715	0.0006	0.0009	349.3729(10)
		3/2	350.4228	−0.2681	−0.1700	0.0004	0.0007	349.9858(11)
$1s(^2S)2p^2(^1S)$	^2S	1/2	351.7122	−0.2338	−0.1673	−0.0007	−0.0004	351.3099(18)
V ($Z = 23$), $1 - \mu/m = 0.00001077$, $R = 3.599$ fm								
$1s^22s$	^2S	1/2	−1152.2254	0.3244	0.3896	0.0001	−0.0002	−1151.5115(8)
$1s^22p$	$^2P^o$	1/2	3.1007	0.0257	−0.0237	−0.0008	−0.0006	3.1014(11)
		3/2	3.8166	−0.0034	−0.0221	−0.0008	−0.0010	3.7894(12)
$1s2s^2$	^2S	1/2	376.9220	−0.2932	−0.1562	−0.0001	0.0002	376.4727(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	377.6474	−0.2356	−0.1766	−0.0009	−0.0004	377.2340(6)
		3/2	377.8797	−0.2954	−0.1761	−0.0009	−0.0006	377.4067(6)
		5/2	378.3762	−0.3169	−0.1750	−0.0009	−0.0008	377.8827(5)

TABLE IV. (*Continued.*)

Term		J	Coulomb	Breit	QED	SMS	Breit′	Total
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	380.2073	−0.2783	−0.1763	0.0003	0.0007	379.7537(13)
		3/2	380.6974	−0.3053	−0.1753	0.0007	0.0010	380.2185(408)
$1s(^2S)2p^2(^3P)$	^4P	1/2	381.2215	−0.2314	−0.2001	−0.0016	−0.0010	380.7873(11)
		3/2	381.5525	−0.2312	−0.1995	−0.0017	−0.0012	381.1189(12)
		5/2	381.9158	−0.3008	−0.1990	−0.0016	−0.0014	381.4130(12)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	381.4789	−0.2569	−0.1755	−0.0004	0.0000	381.0461(32)
		3/2	381.6291	−0.2776	−0.1752	−0.0009	−0.0006	381.1749(68)
$1s(^2S)2p^2(^1D)$	^2D	3/2	383.1346	−0.2444	−0.1995	−0.0006	0.0000	382.6900(13)
		5/2	383.3790	−0.3221	−0.1986	−0.0009	−0.0008	382.8565(13)
$1s(^2S)2p^2(^3P)$	^2P	1/2	383.3748	−0.3148	−0.2000	0.0007	0.0011	382.8617(12)
		3/2	384.1218	−0.3061	−0.1981	0.0004	0.0007	383.6187(12)
$1s(^2S)2p^2(^1S)$	^2S	1/2	385.4416	−0.2691	−0.1951	−0.0007	−0.0005	384.9760(18)
Cr ($Z = 24$), $1 - \mu/m = 0.00001056$, $R = 3.642$ fm								
$1s^22s$	^2S	1/2	−1257.4911	0.3705	0.4505	0.0001	−0.0002	−1256.6703(9)
$1s^22p$	$^2P^o$	1/2	3.2560	0.0296	−0.0275	−0.0008	−0.0007	3.2566(13)
		3/2	4.1165	−0.0038	−0.0257	−0.0008	−0.0011	4.0851(13)
$1s2s^2$	^2S	1/2	411.6571	−0.3348	−0.1806	−0.0001	0.0001	411.1417(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	412.4160	−0.2691	−0.2044	−0.0009	−0.0005	411.9411(7)
		3/2	412.6880	−0.3382	−0.2039	−0.0009	−0.0007	412.1443(7)
		5/2	413.2899	−0.3619	−0.2025	−0.0009	−0.0010	412.7237(6)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	415.1158	−0.3143	−0.2042	0.0002	0.0008	414.5985(14)
		3/2	415.6178	−0.3494	−0.2029	0.0007	0.0011	415.0673(7)
$1s(^2S)2p^2(^3P)$	^4P	1/2	416.2168	−0.2645	−0.2317	−0.0018	−0.0012	415.7176(12)
		3/2	416.6254	−0.2641	−0.2311	−0.0018	−0.0014	416.1270(13)
		5/2	417.0454	−0.3445	−0.2304	−0.0017	−0.0016	416.4672(13)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	416.5140	−0.2966	−0.2030	−0.0004	0.0000	416.0140(32)
		3/2	416.6968	−0.3153	−0.2027	−0.0009	−0.0007	416.1772(41)
$1s(^2S)2p^2(^1D)$	^2D	3/2	418.2864	−0.2809	−0.2311	−0.0006	0.0000	417.7738(14)
		5/2	418.6077	−0.3669	−0.2299	−0.0010	−0.0010	418.0090(14)
$1s(^2S)2p^2(^3P)$	^2P	1/2	418.5063	−0.3583	−0.2316	0.0007	0.0012	417.9183(13)
		3/2	419.4190	−0.3474	−0.2293	0.0004	0.0008	418.8435(13)
$1s(^2S)2p^2(^1S)$	^2S	1/2	420.7657	−0.3079	−0.2261	−0.0008	−0.0006	420.2303(18)
Mn ($Z = 25$), $1 - \mu/m = 0.00000999$, $R = 3.706$ fm								
$1s^22s$	^2S	1/2	−1367.4718	0.4208	0.5176	0.0001	−0.0002	−1366.5336(10)
$1s^22p$	$^2P^o$	1/2	3.4126	0.0339	−0.0318	−0.0009	−0.0008	3.4130(14)
		3/2	4.4388	−0.0043	−0.0296	−0.0008	−0.0013	4.4027(14)
$1s2s^2$	^2S	1/2	447.9563	−0.3801	−0.2076	−0.0001	0.0002	447.3687(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	448.7489	−0.3056	−0.2352	−0.0010	−0.0006	448.2066(8)
		3/2	449.0646	−0.3851	−0.2346	−0.0009	−0.0007	448.4432(7)
		5/2	449.7894	−0.4110	−0.2329	−0.0010	−0.0011	449.1434(7)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	451.5885	−0.3528	−0.2349	0.0002	0.0009	451.0019(16)
		3/2	452.2021	−0.3976	−0.2333	0.0008	0.0013	451.5732(7)
$1s(^2S)2p^2(^3P)$	^4P	1/2	452.7841	−0.3008	−0.2666	−0.0018	−0.0014	452.2136(14)
		3/2	453.2856	−0.3000	−0.2659	−0.0018	−0.0016	452.7162(14)
		5/2	453.7655	−0.3924	−0.2652	−0.0017	−0.0018	453.1043(14)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	453.1323	−0.3405	−0.2334	−0.0004	0.0000	452.5580(33)
		3/2	453.3390	−0.3562	−0.2331	−0.0010	−0.0008	452.7480(43)
$1s(^2S)2p^2(^1D)$	^2D	3/2	455.0249	−0.3209	−0.2659	−0.0006	0.0000	454.4375(15)
		5/2	455.4416	−0.4155	−0.2644	−0.0011	−0.0012	454.7595(15)
$1s(^2S)2p^2(^3P)$	^2P	1/2	455.2200	−0.4054	−0.2665	0.0007	0.0014	454.5501(14)
		3/2	456.3245	−0.3921	−0.2638	0.0004	0.0008	455.6698(15)
$1s(^2S)2p^2(^1S)$	^2S	1/2	457.6948	−0.3504	−0.2602	−0.0008	−0.0007	457.0825(18)
Fe ($Z = 26$), $1 - \mu/m = 0.00000981$, $R = 3.737$ fm								
$1s^22s$	^2S	1/2	−1482.1862	0.4755	0.5913	0.0001	−0.0002	−1481.1195(11)
$1s^22p$	$^2P^o$	1/2	3.5705	0.0386	−0.0366	−0.0009	−0.0009	3.5708(15)
		3/2	4.7855	−0.0048	−0.0340	−0.0009	−0.0015	4.7442(16)

TABLE IV. (*Continued.*)

Term		J	Coulomb	Breit	QED	SMS	Breit′	Total
$1s2s^2$	^2S	1/2	485.8251	−0.4293	−0.2371	−0.0002	0.0002	485.1587(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	486.6518	−0.3454	−0.2689	−0.0010	−0.0006	486.0358(8)
		3/2	487.0147	−0.4363	−0.2683	−0.0010	−0.0008	486.3082(8)
		5/2	487.8821	−0.4645	−0.2662	−0.0010	−0.0013	487.1491(7)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	489.6315	−0.3940	−0.2686	0.0002	0.0010	488.9700(18)
		3/2	490.3763	−0.4500	−0.2667	0.0008	0.0014	489.6618(8)
$1s(^2S)2p^2(^3P)$	^4P	1/2	490.9284	−0.3404	−0.3049	−0.0019	−0.0015	490.2797(15)
		3/2	491.5408	−0.3392	−0.3041	−0.0019	−0.0019	490.8937(16)
		5/2	492.0829	−0.4449	−0.3034	−0.0018	−0.0021	491.3308(16)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	491.3424	−0.3889	−0.2667	−0.0004	0.0001	490.6865(34)
		3/2	491.5741	−0.4003	−0.2664	−0.0010	−0.0010	490.9054(45)
$1s(^2S)2p^2(^1D)$	^2D	3/2	493.3577	−0.3646	−0.3041	−0.0006	0.0001	492.6885(17)
		5/2	493.8912	−0.4680	−0.3022	−0.0012	−0.0014	493.1184(16)
$1s(^2S)2p^2(^3P)$	^2P	1/2	493.5237	−0.4563	−0.3047	0.0007	0.0015	492.7648(16)
		3/2	494.8479	−0.4406	−0.3016	0.0004	0.0009	494.1071(16)
$1s(^2S)2p^2(^1S)$	^2S	1/2	496.2388	−0.3968	−0.2978	−0.0009	−0.0009	495.5424(19)
Co ($Z = 27$), $1 - \mu/m = 0.00000931$, $R = 3.788$ fm								
$1s^22s$	^2S	1/2	−1601.6551	0.5349	0.6719	0.0001	−0.0003	−1600.4485(12)
$1s^22p$	$^2P^o$	1/2	3.7298	0.0437	−0.0418	−0.0010	−0.0010	3.7298(17)
		3/2	5.1587	−0.0054	−0.0388	−0.0009	−0.0018	5.1118(17)
$1s2s^2$	^2S	1/2	525.2695	−0.4826	−0.2694	−0.0002	0.0002	524.5175(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	526.1306	−0.3886	−0.3059	−0.0011	−0.0007	525.4344(9)
		3/2	526.5444	−0.4921	−0.3052	−0.0010	−0.0010	525.7451(9)
		5/2	527.5765	−0.5224	−0.3027	−0.0011	−0.0016	526.7487(8)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	529.2508	−0.4380	−0.3055	0.0001	0.0010	528.5084(19)
		3/2	530.1487	−0.5068	−0.3033	0.0008	0.0016	529.3411(9)
$1s(^2S)2p^2(^3P)$	^4P	1/2	530.6553	−0.3836	−0.3468	−0.0019	−0.0017	529.9213(16)
		3/2	531.3992	−0.3816	−0.3459	−0.0020	−0.0022	530.6675(17)
		5/2	532.0052	−0.5021	−0.3452	−0.0019	−0.0024	531.1537(17)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	531.1531	−0.4418	−0.3031	−0.0003	0.0001	530.4080(33)
		3/2	531.4106	−0.4478	−0.3028	−0.0011	−0.0012	530.6577(46)
$1s(^2S)2p^2(^1D)$	^2D	3/2	533.2932	−0.4121	−0.3460	−0.0006	0.0001	532.5346(18)
		5/2	533.9678	−0.5246	−0.3436	−0.0012	−0.0018	533.0966(18)
$1s(^2S)2p^2(^3P)$	^2P	1/2	533.4260	−0.5111	−0.3462	0.0007	0.0017	532.5710(17)
		3/2	534.9999	−0.4928	−0.3430	0.0004	0.0010	534.1654(18)
$1s(^2S)2p^2(^1S)$	^2S	1/2	536.4087	−0.4472	−0.3389	−0.0009	−0.0011	535.6206(20)
Ni ($Z = 28$), $1 - \mu/m = 0.00000947$, $R = 3.775$ fm								
$1s^22s$	^2S	1/2	−1725.8987	0.5990	0.7598	0.0001	−0.0003	−1724.5401(13)
$1s^22p$	$^2P^o$	1/2	3.8906	0.0493	−0.0475	−0.0011	−0.0011	3.8902(18)
		3/2	5.5609	−0.0060	−0.0440	−0.0010	−0.0021	5.5078(19)
$1s2s^2$	^2S	1/2	566.2956	−0.5402	−0.3046	−0.0002	0.0002	565.4508(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	567.1915	−0.4353	−0.3462	−0.0012	−0.0008	566.4081(10)
		3/2	567.6594	−0.5527	−0.3455	−0.0011	−0.0011	566.7590(10)
		5/2	568.8807	−0.5850	−0.3425	−0.0012	−0.0018	567.9502(9)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	570.4521	−0.4851	−0.3456	0.0001	0.0011	569.6226(19)
		3/2	571.5279	−0.5681	−0.3431	0.0009	0.0018	570.6193(9)
$1s(^2S)2p^2(^3P)$	^4P	1/2	571.9701	−0.4306	−0.3926	−0.0021	−0.0019	571.1430(18)
		3/2	572.8692	−0.4275	−0.3916	−0.0022	−0.0025	572.0454(19)
		5/2	573.5400	−0.5642	−0.3909	−0.0020	−0.0027	572.5801(19)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	572.5730	−0.4995	−0.3425	−0.0003	0.0002	571.7309(32)
		3/2	572.8572	−0.4990	−0.3423	−0.0012	−0.0014	572.0134(45)
$1s(^2S)2p^2(^1D)$	^2D	3/2	574.8396	−0.4636	−0.3916	−0.0006	0.0002	573.9840(20)
		5/2	575.6830	−0.5854	−0.3887	−0.0014	−0.0021	574.7053(19)
$1s(^2S)2p^2(^3P)$	^2P	1/2	574.9358	−0.5699	−0.3923	0.0007	0.0019	573.9762(19)
		3/2	576.7913	−0.5491	−0.3881	0.0004	0.0010	575.8555(19)
$1s(^2S)2p^2(^1S)$	^2S	1/2	578.2157	−0.5017	−0.3839	−0.0010	−0.0013	577.3278(21)

TABLE IV. (*Continued.*)

Term		J	Coulomb	Breit	QED	SMS	Breit′	Total
Cu ($Z = 29$), $1 - \mu/m = 0.00000872$, $R = 3.882$ fm								
$1s^22s$	^2S	1/2	−1854.9408	0.6681	0.8552	0.0001	−0.0003	−1853.4176(14)
$1s^22p$	$^2P^o$	1/2	4.0529	0.0552	−0.0537	−0.0011	−0.0012	4.0521(20)
		3/2	5.9944	−0.0068	−0.0497	−0.0010	−0.0024	5.9345(21)
$1s2s^2$	^2S	1/2	608.9100	−0.6022	−0.3428	−0.0002	0.0002	607.9650(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	609.8413	−0.4857	−0.3900	−0.0011	−0.0009	608.9636(11)
		3/2	610.3663	−0.6184	−0.3892	−0.0010	−0.0012	609.3564(11)
		5/2	611.8041	−0.6525	−0.3858	−0.0011	−0.0021	610.7626(10)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	613.2423	−0.5352	−0.3897	0.0000	0.0012	612.3185(12)
		3/2	614.5230	−0.6340	−0.3864	0.0009	0.0020	613.5055(10)
$1s(^2S)2p^2(^3P)$	^4P	1/2	614.8788	−0.4816	−0.4422	−0.0020	−0.0021	613.9508(19)
		3/2	615.9600	−0.4771	−0.4412	−0.0022	−0.0029	615.0367(21)
		5/2	616.6956	−0.6315	−0.4405	−0.0020	−0.0031	615.6185(21)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	615.6116	−0.5620	−0.3864	−0.0002	0.0003	614.6632(22)
		3/2	615.9231	−0.5540	−0.3861	−0.0011	−0.0016	614.9802(32)
$1s(^2S)2p^2(^1D)$	^2D	3/2	618.0060	−0.5191	−0.4413	−0.0006	0.0003	617.0454(22)
		5/2	619.0488	−0.6506	−0.4378	−0.0014	−0.0026	617.9565(21)
$1s(^2S)2p^2(^3P)$	^2P	1/2	618.0629	−0.6327	−0.4420	0.0007	0.0021	616.9909(20)
		3/2	620.2337	−0.6096	−0.4372	0.0003	0.0011	619.1884(21)
$1s(^2S)2p^2(^1S)$	^2S	1/2	621.6716	−0.5606	−0.4327	−0.0010	−0.0015	620.6759(22)
Zn ($Z = 30$), $1 - \mu/m = 0.00000858$, $R = 3.929$ fm								
$1s^22s$	^2S	1/2	−1988.8028	0.7424	0.9586	0.0001	−0.0003	−1987.1019(15)
$1s^22p$	$^2P^o$	1/2	4.2169	0.0617	−0.0605	−0.0011	−0.0013	4.2157(22)
		3/2	6.4617	−0.0075	−0.0559	−0.0011	−0.0027	6.3945(23)
$1s2s^2$	^2S	1/2	653.1192	−0.6689	−0.3841	−0.0002	0.0002	652.0663(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	654.0862	−0.5399	−0.4374	−0.0012	−0.0010	653.1067(12)
		3/2	654.6712	−0.6893	−0.4363	−0.0011	−0.0013	653.5432(14)
		5/2	656.3556	−0.7250	−0.4325	−0.0012	−0.0025	655.1944(10)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	657.6277	−0.5888	−0.4362	0.0000	0.0012	656.6039(42)
		3/2	659.1435	−0.7048	−0.4333	0.0009	0.0022	658.0086(11)
$1s(^2S)2p^2(^3P)$	^4P	1/2	659.3869	−0.5369	−0.4961	−0.0021	−0.0023	658.3496(21)
		3/2	660.6806	−0.5304	−0.4949	−0.0023	−0.0033	659.6496(22)
		5/2	661.4806	−0.7042	−0.4943	−0.0020	−0.0035	660.2766(22)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	660.2779	−0.6297	−0.4327	−0.0002	0.0004	659.2157(14)
		3/2	660.6180	−0.6126	−0.4301	−0.0012	−0.0019	659.5722(15)
$1s(^2S)2p^2(^1D)$	^2D	3/2	662.8018	−0.5789	−0.4950	−0.0006	0.0004	661.7277(24)
		5/2	664.0779	−0.7205	−0.4909	−0.0015	−0.0031	662.8620(23)
$1s(^2S)2p^2(^3P)$	^2P	1/2	662.8170	−0.6998	−0.4958	0.0007	0.0023	661.6244(22)
		3/2	665.3388	−0.6745	−0.4903	0.0003	0.0012	664.1755(23)
$1s(^2S)2p^2(^1S)$	^2S	1/2	666.7886	−0.6239	−0.4856	−0.0010	−0.0018	665.6762(23)
Ga ($Z = 31$), $1 - \mu/m = 0.00000796$, $R = 3.997$ fm								
$1s^22s$	^2S	1/2	−2127.5105	0.8221	1.0703	0.0001	−0.0003	−2125.6182(17)
$1s^22p$	$^2P^o$	1/2	4.3826	0.0687	−0.0679	−0.0011	−0.0014	4.3809(23)
		3/2	6.9654	−0.0083	−0.0626	−0.0011	−0.0031	6.8903(25)
$1s2s^2$	^2S	1/2	698.9307	−0.7403	−0.4288	−0.0002	0.0002	697.7617(16)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	699.9339	−0.5982	−0.4887	−0.0012	−0.0011	698.8448(14)
		3/2	700.5811	−0.7658	−0.4879	−0.0011	−0.0015	699.3250(20)
		5/2	702.5455	−0.8029	−0.4831	−0.0012	−0.0028	701.2554(11)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	703.6159	−0.6458	−0.4882	−0.0001	0.0013	702.4831(218)
		3/2	705.3997	−0.7805	−0.4839	0.0009	0.0024	704.1386(13)
$1s(^2S)2p^2(^3P)$	^4P	1/2	705.5012	−0.5966	−0.5542	−0.0020	−0.0025	704.3458(22)
		3/2	707.0412	−0.5877	−0.5531	−0.0023	−0.0038	705.8943(24)
		5/2	707.9046	−0.7823	−0.5524	−0.0020	−0.0039	706.5640(24)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	706.5825	−0.7024	−0.4837	−0.0001	0.0005	705.3967(83)
		3/2	706.9519	−0.6755	−0.4830	−0.0012	−0.0022	705.7900(131)
$1s(^2S)2p^2(^1D)$	^2D	3/2	709.2370	−0.6430	−0.5531	−0.0006	0.0005	708.0407(30)
		5/2	710.7834	−0.7952	−0.5483	−0.0015	−0.0037	709.4348(26)

TABLE IV. (*Continued.*)

Term		J	Coulomb	Breit	QED	SMS	Breit′	Total
$1s(^2S)2p^2(^3P)$	^2P	1/2	709.2091	−0.7712	−0.5539	0.0006	0.0025	707.8871(24)
		3/2	712.1194	−0.7439	−0.5477	0.0003	0.0012	710.8294(26)
$1s(^2S)2p^2(^1S)$	^2S	1/2	713.5797	−0.6919	−0.5429	−0.0010	−0.0021	712.3418(24)
Ge ($Z = 32$), $1 - \mu/m = 0.00000742$, $R = 4.074$ fm								
$1s^22s$	^2S	1/2	−2271.0881	0.9075	1.1906	0.0001	−0.0003	−2268.9901(18)
$1s^22p$	$^2P^o$	1/2	4.5501	0.0762	−0.0758	−0.0011	−0.0015	4.5478(25)
		3/2	7.5083	−0.0092	−0.0698	−0.0011	−0.0035	7.4247(27)
$1s2s^2$	^2S	1/2	746.3513	−0.8168	−0.4768	−0.0002	0.0003	745.0578(17)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	747.3914	−0.6606	−0.5439	−0.0012	−0.0012	746.1846(15)
		3/2	748.1030	−0.8480	−0.5430	−0.0010	−0.0016	746.7093(21)
		5/2	750.3834	−0.8862	−0.5376	−0.0012	−0.0033	748.9552(12)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	751.2140	−0.7065	−0.5435	−0.0001	0.0014	749.9652(531)
		3/2	753.3017	−0.8612	−0.5384	0.0008	0.0027	751.9056(13)
$1s(^2S)2p^2(^3P)$	^4P	1/2	753.2278	−0.6610	−0.6169	−0.0020	−0.0027	751.9452(24)
		3/2	755.0515	−0.6492	−0.6156	−0.0022	−0.0043	753.7802(27)
		5/2	755.9772	−0.8662	−0.6151	−0.0019	−0.0044	754.4897(27)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	754.5352	−0.7805	−0.5382	−0.0001	0.0007	753.2170(186)
		3/2	754.9348	−0.7427	−0.5377	−0.0012	−0.0025	753.6507(364)
$1s(^2S)2p^2(^1D)$	^2D	3/2	757.3212	−0.7116	−0.6157	−0.0006	0.0006	755.9938(62)
		5/2	759.1781	−0.8749	−0.6101	−0.0015	−0.0043	757.6872(46)
$1s(^2S)2p^2(^3P)$	^2P	1/2	757.2496	−0.8474	−0.6165	0.0006	0.0027	755.7891(26)
		3/2	760.5881	−0.8182	−0.6095	0.0003	0.0013	759.1619(56)
$1s(^2S)2p^2(^1S)$	^2S	1/2	762.0579	−0.7639	−0.6046	−0.0010	−0.0025	760.6860(37)
As ($Z = 33$), $1 - \mu/m = 0.00000732$, $R = 4.097$ fm								
$1s^22s$	^2S	1/2	−2419.5616	0.9986	1.3200	0.0001	−0.0003	−2417.2431(19)
$1s^22p$	$^2P^o$	1/2	4.7194	0.0843	−0.0845	−0.0012	−0.0017	4.7164(27)
		3/2	8.0933	−0.0101	−0.0776	−0.0011	−0.0040	8.0004(29)
$1s2s^2$	^2S	1/2	795.3885	−0.8983	−0.5284	−0.0002	0.0003	793.9619(19)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	796.4664	−0.7274	−0.6033	−0.0012	−0.0013	795.1332(20)
		3/2	797.2441	−0.9362	−0.6024	−0.0011	−0.0018	795.7026(29)
		5/2	799.8803	−0.9752	−0.5961	−0.0012	−0.0038	798.3039(13)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	800.4294	−0.7710	−0.6030	−0.0002	0.0014	799.0566(550)
		3/2	802.8605	−0.9472	−0.5970	0.0008	0.0029	801.3201(14)
$1s(^2S)2p^2(^3P)$	^4P	1/2	802.5739	−0.7302	−0.6843	−0.0020	−0.0029	801.1544(25)
		3/2	804.7224	−0.7149	−0.6830	−0.0023	−0.0049	803.3173(37)
		5/2	805.7087	−0.9559	−0.6825	−0.0020	−0.0049	804.0634(67)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	804.1468	−0.8640	−0.5968	−0.0001	0.0008	802.6867(218)
		3/2	804.5775	−0.8143	−0.5963	−0.0012	−0.0029	803.1627(488)
$1s(^2S)2p^2(^1D)$	^2D	3/2	807.0554	−0.7862	−0.6831	−0.0006	0.0007	805.5863(998)
		5/2	809.2657	−0.9609	−0.6765	−0.0017	−0.0051	807.6216(1014)
$1s(^2S)2p^2(^3P)$	^2P	1/2	806.9501	−0.9282	−0.6838	0.0006	0.0030	805.3416(28)
		3/2	810.7578	−0.8977	−0.6760	0.0003	0.0014	809.1858(195)
$1s(^2S)2p^2(^1S)$	^2S	1/2	812.2371	−0.8408	−0.6710	−0.0010	−0.0029	810.7213(106)
Se ($Z = 34$), $1 - \mu/m = 0.00000687$, $R = 4.140$ fm								
$1s^22s$	^2S	1/2	−2572.9594	1.0958	1.4588	0.0001	−0.0002	−2570.4050(21)
$1s^22p$	$^2P^o$	1/2	4.8906	0.0929	−0.0937	−0.0012	−0.0018	4.8867(29)
		3/2	8.7233	−0.0112	−0.0860	−0.0011	−0.0046	8.6205(31)
$1s2s^2$	^2S	1/2	846.0488	−0.9853	−0.5837	−0.0002	0.0003	844.4799(29)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	847.1672	−0.7987	−0.6669	−0.0012	−0.0014	845.6989(20)
		3/2	848.0123	−1.0307	−0.6661	−0.0010	−0.0019	846.3125(119)
		5/2	851.0472	−1.0702	−0.6589	−0.0012	−0.0043	849.3126(13)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	851.2706	−0.8397	−0.6667	−0.0002	0.0015	849.7654(405)
		3/2	854.0877	−1.0387	−0.6597	0.0008	0.0032	852.3932(15)
$1s(^2S)2p^2(^3P)$	^4P	1/2	853.5469	−0.8045	−0.7565	−0.0020	−0.0031	851.9808(27)
		3/2	856.0652	−0.7851	−0.7552	−0.0023	−0.0056	854.5169(35)
		5/2	857.1102	−1.0518	−0.7547	−0.0020	−0.0056	855.2962(234)

TABLE IV. (*Continued.*)

Term		J	Coulomb	Breit	QED	SMS	Breit′	Total
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	855.4287	−0.9531	−0.6596	0.0000	0.0010	853.8170(198)
		3/2	855.8914	−0.8906	−0.6591	−0.0012	−0.0033	854.3372(459)
$1s(^2S)2p^2(^1D)$	^2D	3/2	858.4816	−0.8631	−0.7553	−0.0006	0.0008	856.8635(52)
		5/2	861.0919	−1.0507	−0.7478	−0.0017	−0.0060	859.2857(80)
$1s(^2S)2p^2(^3P)$	^2P	1/2	858.3216	−1.0140	−0.7560	0.0005	0.0032	856.5553(30)
		3/2	862.6461	−0.9817	−0.7473	0.0002	0.0015	860.9187(31)
$1s(^2S)2p^2(^1S)$	^2S	1/2	864.1319	−0.9252	−0.7423	−0.0010	−0.0034	862.4600(55)
Br ($Z = 35$), $1 - \mu/m = 0.00000695$, $R = 4.163$ fm								
$1s^22s$	^2S	1/2	−2731.3084	1.1992	1.6072	0.0001	−0.0002	−2728.5021(22)
$1s^22p$	$^2P^o$	1/2	5.0639	0.1021	−0.1038	−0.0013	−0.0020	5.0589(31)
		3/2	9.4015	−0.0122	−0.0950	−0.0012	−0.0052	9.2879(33)
$1s2s^2$	^2S	1/2	898.3291	−1.0778	−0.6428	−0.0002	0.0003	896.6087(104)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	899.5015	−0.8747	−0.7351	−0.0013	−0.0016	897.8889(18)
		3/2	900.4152	−1.1315	−0.7342	−0.0011	−0.0021	898.5463(73)
		5/2	903.8953	−1.1711	−0.7260	−0.0013	−0.0049	901.9918(14)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	903.7457	−0.9124	−0.7349	−0.0003	0.0015	902.0997(321)
		3/2	906.9946	−1.1357	−0.7269	0.0008	0.0034	905.1362(16)
$1s(^2S)2p^2(^3P)$	^4P	1/2	906.1546	−0.8838	−0.8338	−0.0021	−0.0033	904.4315(29)
		3/2	909.0908	−0.8599	−0.8325	−0.0025	−0.0063	907.3896(33)
		5/2	910.1947	−1.1536	−0.8320	−0.0021	−0.0062	908.2007(40)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	908.3921	−1.0480	−0.7267	0.0000	0.0012	906.6186(171)
		3/2	908.8879	−0.9717	−0.7263	−0.0013	−0.0038	907.1849(396)
$1s(^2S)2p^2(^1D)$	^2D	3/2	911.5806	−0.9460	−0.8326	−0.0006	0.0010	909.8023(33)
		5/2	914.6402	−1.1469	−0.8241	−0.0019	−0.0070	912.6604(39)
$1s(^2S)2p^2(^3P)$	^2P	1/2	911.3776	−1.1048	−0.8333	0.0005	0.0034	909.4434(32)
		3/2	916.2637	−1.0713	−0.8236	0.0002	0.0016	914.3705(34)
$1s(^2S)2p^2(^1S)$	^2S	1/2	917.7570	−1.0135	−0.8185	−0.0011	−0.0039	915.9200(53)
Kr ($Z = 36$), $1 - \mu/m = 0.00000654$, $R = 4.188$ fm								
$1s^22s$	^2S	1/2	−2894.6404	1.3090	1.7657	0.0001	−0.0002	−2891.5659(24)
$1s^22p$	$^2P^o$	1/2	5.2393	0.1120	−0.1143	−0.0013	−0.0022	5.2334(33)
		3/2	10.1312	−0.0134	−0.1046	−0.0012	−0.0059	10.0061(36)
$1s2s^2$	^2S	1/2	952.2849	−1.1759	−0.7058	−0.0002	0.0003	950.4035(25)
$1s(^2S)2s2p(^3P^o)$	$^4P^o$	1/2	953.4789	−0.9554	−0.8078	−0.0013	−0.0017	951.7127(19)
		3/2	954.4617	−1.2389	−0.8069	−0.0011	−0.0023	952.4125(37)
		5/2	958.4372	−1.2784	−0.7977	−0.0013	−0.0056	956.3541(15)
$1s(^2S)2s2p(^3P^o)$	$^2P^o$	1/2	957.8644	−0.9895	−0.8076	−0.0003	0.0016	956.0686(268)
		3/2	961.5943	−1.2385	−0.7985	0.0008	0.0037	959.5618(17)
$1s(^2S)2p^2(^3P)$	^4P	1/2	960.4056	−0.9684	−0.9164	−0.0020	−0.0036	958.5153(30)
		3/2	963.8120	−0.9394	−0.9150	−0.0025	−0.0071	961.9480(35)
		5/2	964.9725	−1.2619	−0.9146	−0.0021	−0.0070	962.7869(36)
$1s(^2S)2s2p(^1P^o)$	$^2P^o$	1/2	963.0497	−1.1487	−0.7983	0.0000	0.0015	961.1041(147)
		3/2	963.5798	−1.0577	−0.7979	−0.0013	−0.0043	961.7186(338)
$1s(^2S)2p^2(^1D)$	^2D	3/2	966.3745	−1.0340	−0.9151	−0.0006	0.0012	964.4259(36)
		5/2	969.9362	−1.2492	−0.9055	−0.0019	−0.0081	967.7716(37)
$1s(^2S)2p^2(^3P)$	^2P	1/2	966.1294	−1.2011	−0.9158	0.0004	0.0037	964.0167(34)
		3/2	971.6277	−1.1665	−0.9051	0.0002	0.0017	969.5580(36)
$1s(^2S)2p^2(^1S)$	^2S	1/2	973.1282	−1.1071	−0.8999	−0.0011	−0.0045	971.1155(57)

results are available in the literature [11,13]. We nevertheless present our own results for the $1s^22p_J$ states in the table since they (i) provide us with an independent check of accuracy of our calculations and (ii) allow us to deduce the transition energies between the core excited and the $1s^22p_J$ states.

The third and fourth columns of Table IV present our results for the Dirac-Coulomb and Breit energies (multiplied by the reduced mass prefactor). For each value of the nuclear charge Z and each state, the CI calculation was performed with 20–30 different basis sets. After that, an extrapolation of the partial-wave expansion to $L_{\max} = \infty$ was performed and an estimation of the uncertainty was made by analyzing the results as illustrated by Tables I and II. The procedure for the error estimation is fully automatized and done consistently in the same way for all Z and all states. Each set of CI calculations for

TABLE V. Theoretical wavelengths of the $1s2l2l' \rightarrow 1s^22l'$ transitions in lithlium-like ions, in Å. Transitions are labeled as by Gabriel [39].

Key	Transition	$Z = 18$	$Z = 19$	$Z = 20$	$Z = 21$	$Z = 22$	$Z = 23$	$Z = 24$
a	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	3.985716(12)	3.562881(7)	3.203642(6)	2.895849(6)	2.630130(5)	2.399149(5)	2.197103(4)
b	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	3.981655(8)	3.558756(6)	3.199456(6)	2.891608(5)	2.625838(4)	2.394811(4)	2.192723(4)
c	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	3.989796(22)	3.567118(7)	3.208023(7)	2.900372(6)	2.634791(6)	2.403940(5)	2.202015(5)
d	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	3.985727(20)	3.562983(7)	3.203826(6)	2.896118(5)	2.630484(5)	2.399585(4)	2.197616(4)
e	$1s(^2S)2p^2(^3P)\,^4P_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	4.012732(12)	3.586089(7)	3.223791(6)	2.913522(6)	2.645790(5)	2.413162(5)	2.209764(4)
f	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	4.014740(11)	3.588094(7)	3.225781(6)	2.915487(6)	2.647719(5)	2.415043(5)	2.211588(4)
g	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	4.010620(7)	3.583910(6)	3.221537(6)	2.911188(5)	2.643369(5)	2.410648(4)	2.207150(4)
h	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	4.016579(12)	3.589979(7)	3.227718(7)	2.917481(6)	2.649774(6)	2.417167(5)	2.213788(5)
i	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	4.012454(7)	3.585791(6)	3.223469(6)	2.913176(5)	2.645418(5)	2.412764(4)	2.209341(4)
j	$1s(^2S)2p^2(^1D)\,^2D_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	3.993809(61)	3.570066(29)	3.210076(16)	2.901656(10)	2.635408(7)	2.403973(6)	2.201533(5)
k	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	3.989864(58)	3.566231(28)	3.206360(15)	2.898069(9)	2.631959(7)	2.400670(6)	2.198382(5)
l	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	3.993942(59)	3.570374(28)	3.210564(16)	2.902330(10)	2.636271(7)	2.405029(6)	2.202784(5)
m	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	3.965728(230)	3.546235(55)	3.189673(27)	2.884054(17)	2.620117(13)	2.390606(10)	2.189781(8)
n	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	3.961707(229)	3.542148(54)	3.185524(27)	2.879847(17)	2.615858(13)	2.386299(10)	2.185430(8)
o	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	4.072729(35)	3.637985(27)	3.269158(22)	2.953565(18)	2.681441(15)	2.445151(13)	2.238674(11)
p	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	4.068489(33)	3.633684(26)	3.264800(21)	2.949154(18)	2.676980(15)	2.440646(12)	2.234127(11)
q	$1s(^2S)2s2p(^3P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	3.981328(7)	3.559148(6)	3.200463(5)	2.893146(5)	2.627836(4)	2.396693(257)	2.195468(3)
r	$1s(^2S)2s2p(^3P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	3.983465(15)	3.561332(12)	3.202698(11)	2.895435(9)	2.630186(9)	2.399627(9)	2.197951(8)
s	$1s(^2S)2s2p(^1P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	3.967689(75)	3.547584(56)	3.190554(43)	2.884570(34)	2.620349(29)	2.390680(42)	2.189613(21)
t	$1s(^2S)2s2p(^1P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	3.968543(68)	3.548452(50)	3.191430(37)	2.885449(29)	2.621228(24)	2.391488(20)	2.190472(17)
u	$1s(^2S)2s2p(^3P^o)\,^4P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	4.014997(6)	3.588101(6)	3.225603(5)	2.915172(5)	2.647301(4)	2.414549(4)	2.211039(4)
v	$1s(^2S)2s2p(^3P^o)\,^4P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	4.016105(6)	3.589219(6)	3.226725(5)	2.916294(5)	2.648416(4)	2.415655(4)	2.212130(4)
Key	Transition	$Z = 25$	$Z = 26$	$Z = 27$	$Z = 28$	$Z = 29$	$Z = 30$	$Z = 31$
a	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.019352(4)	1.862150(4)	1.722447(3)	1.597740(3)	1.485954(3)	1.385365(3)	1.294526(3)
b	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	2.014933(3)	1.857696(3)	1.717960(3)	1.593221(2)	1.481407(2)	1.380792(2)	1.289927(2)
c	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.024374(4)	1.867272(4)	1.727654(4)	1.603022(4)	1.491298(3)	1.390759(3)	1.299959(3)
d	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	2.019934(4)	1.862793(3)	1.723139(3)	1.598473(3)	1.486718(3)	1.386150(3)	1.295322(2)
e	$1s(^2S)2p^2(^3P)\,^4P_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.030897(4)	1.872775(4)	1.732309(4)	1.606968(3)	1.494655(3)	1.393626(3)	1.302417(3)
f	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.032655(4)	1.874458(4)	1.733912(4)	1.608485(3)	1.496082(3)	1.394963(3)	1.303665(3)
g	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	2.028178(4)	1.869945(3)	1.729364(3)	1.603905(3)	1.491473(3)	1.390326(2)	1.299002(2)
h	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.034937(4)	1.876829(4)	1.736377(4)	1.611051(4)	1.498754(4)	1.397745(3)	1.306559(3)
i	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	2.030450(4)	1.872304(4)	1.731816(3)	1.606457(3)	1.494129(3)	1.393089(3)	1.301875(3)
j	$1s(^2S)2p^2(^1D)\,^2D_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.023433(4)	1.865920(4)	1.725934(4)	1.600968(3)	1.488945(3)	1.388137(3)	1.297095(3)
k	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	2.020438(4)	1.863083(4)	1.723258(4)	1.598451(3)	1.486586(3)	1.385932(3)	1.295039(4)
l	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.024881(5)	1.867564(4)	1.727773(4)	1.603000(4)	1.491165(4)	1.390540(4)	1.299674(4)
m	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.013050(7)	1.856704(6)	1.717723(5)	1.593626(4)	1.482358(4)	1.382212(3)	1.291750(3)
n	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	2.008658(6)	1.852275(5)	1.713259(5)	1.589130(4)	1.477833(3)	1.377659(3)	1.287171(2)
o	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	2.057194(9)	1.896835(8)	1.754442(7)	1.627428(7)	1.513656(6)	1.411347(6)	1.319011(5)
p	$1s2s^2\,^2S_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	2.052608(9)	1.892213(8)	1.749786(7)	1.622741(7)	1.508938(6)	1.406601(5)	1.314238(5)
q	$1s(^2S)2s2p(^3P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	2.017983(3)	1.861013(3)	1.721512(3)	1.596979(3)	1.485345(2)	1.384886(2)	1.294159(2)
r	$1s(^2S)2s2p(^3P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	2.020539(7)	1.863646(7)	1.724224(6)	1.599773(5)	1.488224(3)	1.387849(9)	1.297208(40)
s	$1s(^2S)2s2p(^1P^o)\,^2P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	2.012747(19)	1.856299(17)	1.717241(15)	1.593087(12)	1.481783(8)	1.381603(3)	1.291131(24)
t	$1s(^2S)2s2p(^1P^o)\,^2P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	2.013592(15)	1.857127(13)	1.718049(11)	1.593874(9)	1.482547(5)	1.382350(3)	1.291850(15)
u	$1s(^2S)2s2p(^3P^o)\,^4P^o_{3/2} \rightarrow 1s^22s\,^2S_{1/2}$	2.032068(3)	1.873847(3)	1.733287(3)	1.607856(3)	1.495458(3)	1.394349(3)	1.303067(4)
v	$1s(^2S)2s2p(^3P^o)\,^4P^o_{1/2} \rightarrow 1s^22s\,^2S_{1/2}$	2.033141(3)	1.874897(3)	1.734312(3)	1.608852(3)	1.496423(3)	1.395280(3)	1.303962(3)
Key	Transition	$Z = 32$	$Z = 33$	$Z = 34$	$Z = 35$	$Z = 36$		
a	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	1.212215(8)	1.137399(27)	1.069188(2)	1.006833(2)	0.949680(2)		
b	$1s(^2S)2p^2(^3P)\,^2P_{3/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	1.207593(8)	1.132755(27)	1.064525(2)	1.002151(1)	0.944980(1)		
c	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	1.217678(3)	1.142882(3)	1.074690(3)	1.012344(2)	0.955196(2)		
d	$1s(^2S)2p^2(^3P)\,^2P_{1/2} \rightarrow 1s^22p\,^2P^o_{1/2}$	1.213015(2)	1.138194(2)	1.069978(2)	1.007610(2)	0.950441(2)		
e	$1s(^2S)2p^2(^3P)\,^4P_{5/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	1.219796(3)	1.144717(9)	1.076288(30)	1.013744(4)	0.956429(2)		
f	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \rightarrow 1s^22p\,^2P^o_{3/2}$	1.220956(3)	1.145791(4)	1.077280(3)	1.014659(3)	0.957272(2)		

TABLE V. (*Continued.*)

Key	Transition	$Z = 32$	$Z = 33$	$Z = 34$	$Z = 35$	$Z = 36$
g	$1s(^2S)2p^2(^3P)\,^4P_{3/2} \to 1s^22p\,^2P^o_{1/2}$	1.216268(2)	1.141079(4)	1.072546(3)	1.009904(2)	0.952496(2)
h	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \to 1s^22p\,^2P^o_{3/2}$	1.223965(3)	1.148916(3)	1.080519(3)	1.018012(3)	0.960736(3)
i	$1s(^2S)2p^2(^3P)\,^4P_{1/2} \to 1s^22p\,^2P^o_{1/2}$	1.219254(2)	1.144178(2)	1.075757(2)	1.013225(2)	0.955926(2)
j	$1s(^2S)2p^2(^1D)\,^2D_{5/2} \to 1s^22p\,^2P^o_{3/2}$	1.214598(7)	1.139624(144)	1.071240(9)	1.008739(3)	0.951451(2)
k	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \to 1s^22p\,^2P^o_{1/2}$	1.212685(9)	1.137847(142)	1.069591(6)	1.007211(2)	0.950036(2)
l	$1s(^2S)2p^2(^1D)\,^2D_{3/2} \to 1s^22p\,^2P^o_{3/2}$	1.217345(10)	1.142532(143)	1.074300(6)	1.011941(3)	0.954786(2)
m	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \to 1s^22p\,^2P^o_{3/2}$	1.209762(5)	1.135223(15)	1.067258(6)	1.005112(5)	0.948141(5)
n	$1s(^2S)2p^2(^1S)\,^2S_{1/2} \to 1s^22p\,^2P^o_{1/2}$	1.205159(5)	1.130597(15)	1.062611(6)	1.000446(5)	0.943456(5)
o	$1s2s^2\,^2S_{1/2} \to 1s^22p\,^2P^o_{3/2}$	1.235393(5)	1.159430(5)	1.090216(5)	1.026987(13)	0.969023(4)
p	$1s2s^2\,^2S_{1/2} \to 1s^22p\,^2P^o_{1/2}$	1.230594(5)	1.154605(4)	1.085367(5)	1.022116(12)	0.964130(4)
q	$1s(^2S)2s2p(^3P^o)\,^2P^o_{3/2} \to 1s^22s\,^2S_{1/2}$	1.211943(2)	1.137207(2)	1.069069(2)	1.006773(2)	0.949670(2)
r	$1s(^2S)2s2p(^3P^o)\,^2P^o_{1/2} \to 1s^22s\,^2S_{1/2}$	1.215079(86)	1.140429(79)	1.072375(51)	1.010162(36)	0.953140(27)
s	$1s(^2S)2s2p(^1P^o)\,^2P^o_{3/2} \to 1s^22s\,^2S_{1/2}$	1.209137(58)	1.134598(69)	1.066636(57)	1.004500(44)	0.947540(33)
t	$1s(^2S)2s2p(^1P^o)\,^2P^o_{1/2} \to 1s^22s\,^2S_{1/2}$	1.209833(30)	1.135271(31)	1.067286(25)	1.005127(19)	0.948146(15)
u	$1s(^2S)2s2p(^3P^o)\,^4P^o_{3/2} \to 1s^22s\,^2S_{1/2}$	1.220377(3)	1.145236(4)	1.076750(15)	1.014157(8)	0.956799(4)
v	$1s(^2S)2s2p(^3P^o)\,^4P^o_{1/2} \to 1s^22s\,^2S_{1/2}$	1.221235(2)	1.146056(3)	1.077531(3)	1.014900(2)	0.957502(2)

one value of Z and one state takes about 20–50 h of processor time on a modern workstation.

The fifth column of Table IV presents our calculation results for the QED correction. For each value of Z and each state, the calculation was performed with three screening potentials. The results listed in the table are obtained with the LDF potential. The maximal deviation of the KS and CH results from the LDF one was taken as the uncertainty of the QED correction. Small additional contributions to the energy levels from the specific mass shift and the frequency-dependent Breit correction are listed in the sixth and seventh columns of Table IV, respectively.

One may note that the uncertainties of our calculation results presented in Table IV have some irregularities along the Z sequence. For some values of Z the estimated uncertainty turns out to be much larger than for the neighboring ones. This is caused by a nonuniform convergence of the results with respect to the size of the basis set, which is due to the interaction of the reference autoionizing state with the continuum of single-excited states. In the CI calculations, the continuum is discretized and, if a continuum state in the basis happens to be nearly degenerate in energy with the reference state, a sizable nonphysical contribution may arise. (It is nonphysical since the true Green function $G(\varepsilon)$ is known to be regular at energies $\varepsilon > m$.) When this occurs, we observe irregularity in the convergence of our results and have to increase the uncertainty accordingly. Note that for a given state, we use exactly the same basis for all values of Z listed in Table IV and estimate the uncertainty exactly in the same way, without any smoothing of energies or uncertainties along the Z sequence.

Our final theoretical results for the wavelengths of the 22 strongest $1s2l2l' \to 1s^22l'$ transitions in lithium-like ions are summarized in Table V. The transitions are labeled from "a" to "v," following the standard notations from Gabriel [39].

We now turn to the comparison of our calculation results for the three most important elements, namely argon, iron, and krypton, with data previously reported in the literature. Since the amount of the experimental and theoretical data available for these ions is rather voluminous, we decided to restrict ourselves to a comparison with the relativistic many-body perturbation calculation by Safronova and Safronova [21] and with the extensive compilations of the theoretical and experimental world data [40–42]. The calculation by Safronova and Safronova is apparently the best of the previous theoretical studies of the core-excited states and the compilations [40–42] are the primary sources for the NIST recommended spectral data for these ions [43]. In the case of argon, the values reported in the compilation by Saloman [40] include the results by Safronova and Safronova but in addition provide estimations of uncertainties, so we compare only with Saloman's compilation.

TABLE VI. Energy levels of Ar XVI($Z = 18$), relative to the ground state. Comparison is made with the recent compilation of theoretical and experimental world data by Saloman [40]. Units are Rydbergs.

State	J	Present work	Saloman [40]
$1s^22p\,^2P^o$	1/2	2.3417(6)	2.342 193(36)
	3/2	2.5749(8)	2.575 268(36)
$1s(^2S)2s^2\,^2S$	1/2	226.3234(17)	226.324(12)
$1s(^2S)2s2p(^3P^o)\,^4P^o$	1/2	226.9032(4)	226.915(17)
	3/2	226.9658(4)	226.977(17)
	5/2	227.1215(3)	
$1s(^2S)2s2p(^3P^o)\,^2P^o$	1/2	228.7624(9)	228.766(17)
	3/2	228.8852(4)	228.887(17)
$1s(^2S)2p^2(^3P)\,^4P$	1/2	229.4514(6)	229.467(12)
	3/2	229.5553(6)	229.569(12)
	5/2	229.6689(6)	229.682(17)
$1s(^2S)2s2p(^1P^o)\,^2P^o$	1/2	229.6226(39)	229.625(17)
	3/2	229.6720(43)	229.678(17)
$1s(^2S)2p^2(^1D)\,^2D$	3/2	230.7372(33)	230.741(12)
	5/2	230.7449(35)	230.746(17)
$1s(^2S)2p^2(^3P)\,^2P$	1/2	230.9743(12)	230.975(12)
	3/2	231.2081(7)	231.208(12)
$1s(^2S)2p^2(^1S)\,^2S$	1/2	232.361(13)	232.368(13)

TABLE VII. Energy levels of Fe XXIV($Z = 26$), relative to the ground state. Comparison is made with the compilation of theoretical and experimental world data by Shirai *et al*. [41] and with recent calculation by Safronova and Safronova [21]. Units are Rydbergs.

State	J	Present work	Shirai [41]	Safronova [21]
$1s^2 2p\,^2P^o$	1/2	3.5708(15)	3.572 01	3.575
	3/2	4.7442(16)	4.745 49	4.749
$1s(^2S)2s^2\,^2S$	1/2	485.1587(16)	485.120	485.165
$1s(^2S)2s2p(^3P^o)\,^4P^o$	1/2	486.0358(8)	486.097	486.053
	3/2	486.3082(8)	486.316	486.326
	5/2	487.1491(7)		487.165
$1s(^2S)2s2p(^3P^o)\,^2P^o$	1/2	488.9700(18)	489.021	488.980
	3/2	489.6618(8)	489.644	489.668
$1s(^2S)2p^2(^3P)\,^4P$	1/2	490.2797(15)	490.307	490.305
	3/2	490.8937(16)	490.918	490.919
	5/2	491.3308(16)	491.337	491.358
$1s(^2S)2s2p(^1P^o)\,^2P^o$	1/2	490.6865(34)	490.709	490.695
	3/2	490.9054(45)	490.909	490.915
$1s(^2S)2p^2(^1D)\,^2D$	3/2	492.6885(17)	492.638	492.708
	5/2	493.1184(16)	493.104	493.130
$1s(^2S)2p^2(^3P)\,^2P$	1/2	492.7648(16)	492.777	492.772
	3/2	494.1071(16)	494.084	494.112
$1s(^2S)2p^2(^1S)\,^2S$	1/2	495.5424(19)	495.489	495.559

The comparison for argon, iron, and krypton is presented in Tables VI, VII, and VIII, respectively. In the case of argon, the compilation [40] includes estimations of uncertainties. The agreement is nearly always within the given error bars but our results are significantly more accurate. For iron and krypton, there are no estimations of uncertainty given in previous works, but probable errors might be guessed from the differences between different results. Agreement of our results with results by Safronova and Safronova is in most cases better than that with the NIST compilation data, especially in the case of krypton.

Comparison of our calculation results for other ions with the NIST spectral data [43] looks similar to what can be seen in Tables VI, VII, and VIII. The root-mean-square deviation of energies of core-excited states varies from 0.002 Ry for argon to 0.05 Ry for krypton and grows smoothly with the increase of the nuclear charge. The only large deviation is found for the $1s2s2p\,^2P^o_{1/2}$ state of copper, for which the NIST database reports 615.26 Ry, whereas our result is 612.319 (1) Ry. This deviation is most probably due to a misprint in the NIST database. No data on energies of core-excited states is available in the database for $Z = 30$ and $Z = 32$–35 and only a few levels are available for $Z = 20$ and 21.

In summary, we performed a large-scale relativistic CI calculation of the energy levels of all $n = 2$ core-excited states of lithium-like ions from argon to krypton. The CI results include the nuclear recoil contribution and the frequency-dependent Breit correction. The QED correction was calculated separately in the one-electron approximation with a local screening potential. The calculation results are

TABLE VIII. Energy levels of Kr XXXIV($Z = 36$), relative to the ground state. Comparison is made with the compilation of theoretical and experimental world data by Saloman [42] and with recent calculation by Safronova and Safronova [21]. Units are Rydbergs.

State	J	Present work	Saloman [42]	Safronova [21]
$1s^2 2p\,^2P^o$	1/2	5.2334(33)	5.23598	5.242
	3/2	10.0061(36)	10.00839	10.02
$1s(^2S)2s^2\,^2S$	1/2	950.4035(25)	950.49	950.42
$1s(^2S)2s2p(^3P^o)\,^4P^o$	1/2	951.7127(19)	951.96	951.75
	3/2	952.4125(37)	952.69	952.44
	5/2	956.3541(15)		956.38
$1s(^2S)2s2p(^3P^o)\,^2P^o$	1/2	956.069(27)	956.33	956.09
	3/2	959.5618(17)	959.62	959.58
$1s(^2S)2p^2(^3P)\,^4P$	1/2	958.5153(30)	958.88	958.56
	3/2	961.9480(35)	962.13	962.00
	5/2	962.7869(36)	962.97	962.83
$1s(^2S)2s2p(^1P^o)\,^2P^o$	1/2	961.104(15)	961.21	961.12
	3/2	961.719(34)	961.80	961.74
$1s(^2S)2p^2(^1D)\,^2D$	3/2	964.4259(36)	964.61	964.45
	5/2	967.7716(37)	967.76	967.80
$1s(^2S)2p^2(^3P)\,^2P$	1/2	964.0167(34)	964.21	964.03
	3/2	969.5580(36)	969.52	969.57
$1s(^2S)2p^2(^1S)\,^2S$	1/2	971.1155(57)	971.08	971.14

supplemented with a systematic estimation of uncertainties. The uncertainties of the CI values were evaluated by analyzing the successive increments of the results obtained with the set of configuration-state functions increased in all possible directions. The uncertainty of the QED corrections were evaluated by performing the QED calculations with three different screening potentials and analyzing the dependence of the results on the choice of the potential.

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