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# Resonance transition energies of Li-, Na-, and Cu-like ions

Y.-K. Kim, D. H. Baik,* and P. Indelicato†
*National Institute of Standards and Technology, Gaithersburg, Maryland 20899*

J. P. Desclaux
*Département de Recherche Fondamentale/Service de Physique Atomique, Centre d'Etudes Nucléaires de Grenoble, Boîte Postale 85X, F-38041 Grenoble CEDEX, France*
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Relativistic correlation energies are determined by taking the difference between the energies derived from the relativistic many-body perturbation method and those from the Dirac-Fock method for the resonance transitions of Li-, Na-, and Cu-like ions. These correlation energies are combined with the Dirac-Fock energies and "screened" QED corrections based on approximate methods. The resulting theoretical transition energies are compared with available experimental data along isoelectronic sequences to identify irregularities in the data and to predict transition energies of ions whose values are unknown or uncertain.

## I. INTRODUCTION

Reliable theoretical predictions of atomic energy levels require methods that account for electron correlation, relativistic, and quantum-electrodynamic (QED) corrections. At present, we do not have a comprehensive and practical method that accounts for all three corrections on equal footing.

For an atom with a low nuclear charge $Z$, electron correlation far exceeds both relativistic and QED corrections, and *ab initio* calculations must take this into consideration. The relativistic multiconfiguration Hartree-Fock method, usually referred to as the multiconfiguration Dirac-Fock (MCDF) method,[1–4] is one of the most flexible computational schemes to produce self-consistent-field (SCF) wave functions that incorporate major parts of electron correlation and relativistic corrections for atoms with both simple and complex valence-shell configurations, but the method is not precise enough for detailed comparison with experiment unless a very large number of "correlation" configurations are included. MCDF calculations with large-scale configuration mixing are successful for atoms with a few bound electrons,[5] but such calculations become increasingly difficult for atoms with a large number of bound electrons, such as Cu-like ions.

As the nuclear charge increases, electron correlation remans insensitive to $Z$ while relativistic and QED corrections grow rapidly as high powers of $Z$ ($Z^2$–$Z^4$). Since major relativistic corrections that arise from the Dirac Hamiltonian and the Breit interaction are included in the MCDF method, reliable theoretical predictions depend on the theoretical capability to accurately evaluate correlation and QED corrections.

Traditionally, the correlation energy was defined as the difference between the exact nonrelativistic, many-electron energy eigenvalue of a level and the corresponding theoretical energy derived from a (nonrelativistic) single-configuration Hartree-Fock (HF) wave function. Since it is a routine procedure now to obtain Dirac-Fock (DF) wave functions that are equivalent to the single-configuration HF wave functions mentioned above, it is more sensible instead to define relativistic correlation energy $E_{\rm rcor}$ as

$$E_{\rm rcor}=E_{\rm rtot}-E_{\rm DF}\ , \qquad (1)$$

where $E_{\rm rtot}$ is the relativistic total energy without QED corrections and $E_{\rm DF}$ is the total energy obtained from a DF wave function with the minimum number of relativistic configurations (also without QED corrections). The relativistic counterpart of a single-configuration HF wave function is not necessarily a single-configuration wave function. For instance, the (nonrelativistic) $2s2p$ configuration of Be is matched by two relativistic configurations, $2s_{1/2}2p_{1/2}$ and $2s_{1/2}2p_{3/2}$. Hence, the definition of $E_{\rm rcor}$ for the $2s2p\ {}^1P_1$ and ${}^3P_1$ levels requires $E_{\rm DF}$ calculated with linear combinations of the two relativistic configurations, while that for the $2s2p\ {}^3P_0$ level involves only $2s_{1/2}2p_{1/2}$ and the $2s2p\ {}^3P_2$ level involves only $2s_{1/2}2p_{3/2}$.

Using a relativistic version of the many-body perturbation theory (MBPT), Johnson, Blundel, and Sapirstein[6–8] have calculated relativistic ionization energies of low-lying levels of Li-, Na-, and Cu-like ions ($ns_{1/2}$, $np_{1/2}$, and $np_{3/2}$). Their values accurately represent the usual relativistic effects as well as the electron correlation. However, quantum-electrodynamic corrections must be added to their values for detailed comparisons with experiment.

The comparison of MBPT and DF results is not straightforward because of their difference in the starting point. In the DF method, all orbitals are made self-consistent for each level, thus producing slightly different core orbitals for the ground and excited states. In this version of the MBPT, a common closed-shell core is used to generate all real and virtual orbitals for the ground and excited states.

For instance, in the Li sequence, a $1s$ orbital is generated for the He-like core, and the $2s$, $2p_{1/2}$, $2p_{3/2}$, and other excited-state orbitals needed in the MBPT are generated in the field of the $1s^2$ core, while the $1s$ orbital is kept frozen. Thus, in the MBPT, the core contribution to the total energies of the ground and excited states cancels exactly, but not in the DF method.

In the MBPT, any change in the total energy due to the "relaxation" of the $1s$ orbital is attributed to higher-order corrections to the valence electron energy, i.e., it is counted as part of the "correlation" energy of the valence electron. However, the core relaxation in a minimum-configuration DF calculation will not be considered as part of "electron correlation."

The core relaxation affects both the nonrelativistic Coulomb interaction and the Breit interaction between bound electrons. The difference in the definition of the "zeroth-order" energy is amplified in the Breit interaction, since it is more sensitive to the details of core orbitals than the Coulomb interaction is. One can avoid these differences and draw meaningful conclusions by using transition energies in Eq. (1) rather than total energies for each level. We have determined the $Z$ dependence of the correlation energy by comparing the MBPT transition energies with the corresponding DF results for the alkali-metal-like ions (Sec. II). Polynomials in $Z$ were fitted to the correlation correction to obtain correlation energies for ions whose MBPT values were not available.

There are two major components in the QED correction. The dominant one is the self-energy. The self-energy for a hydrogenic ion with a point nucleus, which is precisely known,[9–11] must be corrected for the mutual screening of bound electrons in a many-electron atom. One can attempt to establish upper and lower limits of the self-energy screening by taking the hydrogenic self-energy values with no screening (i.e., use the bare nuclear charge value $Z$) and with complete screening (use an effective nuclear charge, $Z'=Z-N+1$, $N$ being the number of bound electrons). Such limits, however, are too far apart to be of any practical value unless $N$ is small and $Z$ is large.

The leading term of a less-dominant QED correction, the vacuum polarization, can be evaluated with the Uehling potential,[12] which can be used with DF wave functions, thus indirectly allowing for the mutual screening. A combination of the fact that the vacuum polarization is much smaller in magnitude than the self-energy and the possibility of using SCF wave functions makes the "screening" of the vacuum polarization less problematic than the screening of the self-energy.

In order to provide reasonable estimates of the screening of the self-energy, three approximate methods (Sec. III), none of which is based on a rigorous QED procedure, have been used in the MCDF computer codes commonly available. By combining DF energy levels, supplemented by correlation corrections determined from the results of Johnson *et al.*, and these "screened" QED corrections, one can study the $Z$ dependence of the difference between theoretical and experimental values of transition energies and predict energies for ions whose experimental values are unknown or uncertain.

Since the $Z$ dependence of all theoretical terms is expected to vary smoothly along an isoelectronic sequence, the difference between theoretical results and experiment can be used to identify experimental irregularities and to extrapolate the difference to predict transition energies. This type of comparison was successfully used by Edlén, who used earlier MCDF results to smooth and extrapolate experimental values.[13] Dirac-Fock results that are available now are more refined than those used by Edlén, mostly in estimating QED corrections. Analyses based on current DF results yield more reliable predictions of expected energy levels, since all leading $Z$-dependent terms are accounted for in the theory and hence the difference between theory and experiment is smaller and less sensitive to $Z$.

Experimental wavelengths for highly charged ions of heavy elements of interest here have been measured using tokamaks, laser-generated plasmas, and ion beams and traps as light sources. As will be seen in Sec. IV, some of these experimental results for $Z>50$ exhibit irregular behavior when compared to theory, indicating much larger uncertainties than those seen in experimental data on lighter elements.

In this paper, we discuss qualitative features in the $Z$ dependence of relativistic correlation energy and QED corrections of Li-, Na-, and Cu-like ions, and present interpolated and extrapolated transition energies for the resonance transitions ($ns_{1/2}\rightarrow np_{1/2}$ and $ns_{1/2}\rightarrow np_{3/2}$), which can be used as guidelines for future experiments (Sec. IV). Similar predictions were made by Seely *et al.* on the same transitions,[14–17] but the QED corrections we used have smaller systematic deviations from experiment than those used by Seely *et al.* There are also new experimental data on heavy Cu-like ions ($Z>50$) that were not available to Seely *et al.* The new data remove some confusion in the $Z$ dependence of the difference between theory and experiment in Cu-like ions for $50<Z<70$, allowing us to draw more definite conclusions about the experimental data above $Z=70$ (Sec. IV). Our conclusions and suggestions for future experiments are presented in Sec. V.

## II. RELATIVISTIC CORRELATION ENERGY

The relativistic Hamiltonian $H_0$ we have used to derive our Dirac-Fock wave functions consists of the Dirac Hamiltonian and the Coulomb repulsion:

$$H_0=\sum_j (\boldsymbol{\alpha}_j\cdot\mathbf{p}_j c+\beta_j mc^2-Ze^2/r_j)+\sum_{j>k} e^2/r_{jk} \ , \tag{2}$$

where $\alpha$ and $\beta$ are $4\times4$ Dirac matrices, $\mathbf{p}_j$ is the momentum operator of the $j$th electron, $c$ is the speed of light, $m$ is the electron rest mass, $e$ is the electronic charge, $r_j$ is the distance between the nucleus and the $j$th electron, $r_{jk}$ is the distance between the $j$th and $k$th electrons, and the summations extends over all bound electrons.

The standard practice is to use $H_0$ with Slater determinants of four-component, one-electron wave functions. For the states of interest in this article, the DF wave functions consist of single determinants, with one electron outside a closed shell. The correlation not well represented by the DF method is the correlation among the core electrons and between the core and valence electrons. The latter is often referred to as the core polarization.

Unlike the HF method, however, the DF method involves some numerical alternatives that must be specified beyond $H_0$ to make the comparison with other methods meaningful.

### A. Nuclear-size parameters

Using a point nucleus, which is common in nonrelativistic calculations, is unsatisfactory because the effect of using an extended nucleus—be it a uniform charge or a Fermi distribution—leads to one of the largest corrections in the binding energies of individual electrons, known as the nuclear-size correction. The nuclear-size correction can be determined simply by solving the SCF equations with an extended nucleus, e.g., with a Fermi distribution of the nuclear charge. However, this correction is sensitive to the choice of nuclear-size parameters, and we must be consistent in choosing these parameters. Johnson and Soff[18] showed that one could choose an appropriate root-mean-square (rms) radius for a uniformly charged nucleus that reproduces the same result as a nucleus with a Fermi distribution. To maintain consistency with the MBPT results, we used Fermi distributions that agreed with the mean radii used by Johnson, Blundel, and Sapirstein[6–8] to deduce $E_{\rm rcor}$ using Eq. (1).

However, there are more recent nuclear-size parameters for $Z \geq 90$, and we used the new parameters for these ions in calculating $E_{\rm DF}$ and corresponding QED corrections to be combined with the $E_{\rm rcor}$ deduced using the old parameters. The new nuclear-size parameters produce DF results for inner-shell x-ray wavelengths more consistent with experimental data.[19] The nuclear parameters are not smooth functions of $Z$; they may cause some irregularity in the $Z$ dependence of theoretical values, though they are less than the usual errors associated with experiment.

### B. Breit operator

There are three different forms of the Hamiltonian $H_{e\text{-}e}$ to describe the electron-electron interaction (including the nonrelativistic Coulomb repulsion).[20]

(a) In the Lorentz gauge,

$$H_{e\text{-}e} = e^2 \sum_{j>k} (1 - \boldsymbol{\alpha}_j \cdot \boldsymbol{\alpha}_k)/r_{jk} \ . \tag{3}$$

(b) In the Coulomb gauge,

$$H_{e\text{-}e} = e^2 \sum_{j>k} \left[ \frac{1 - \boldsymbol{\alpha}_j \cdot \boldsymbol{\alpha}_k}{r_{jk}} + \frac{(\boldsymbol{\alpha}_j \cdot \boldsymbol{\nabla}_j)(\boldsymbol{\alpha}_k \cdot \boldsymbol{\nabla}_k) r_{jk}}{2} \right] . \tag{4}$$

(c) With the energy-dependent retardation,

$$H_{e\text{-}e} = e^2 \sum_{j>k} \left[ \frac{1 - \boldsymbol{\alpha}_j \cdot \boldsymbol{\alpha}_k}{r_{jk}} \right] \cos(\omega_{jk} r_{jk}) \tag{5}$$

in the Lorentz gauge, and

$$H_{e\text{-}e} = e^2 \sum_{j>k} \left[ \frac{1}{r_{jk}} - \frac{\boldsymbol{\alpha}_j \cdot \boldsymbol{\alpha}_k}{r_{jk}} \cos(\omega_{jk} r_{jk}) + \frac{(\boldsymbol{\alpha}_j \cdot \boldsymbol{\nabla}_j)(\boldsymbol{\alpha}_k \cdot \boldsymbol{\nabla}_k)}{\omega_{jk}^2 r_{jk}} [\cos(\omega_{jk} r_{jk}) - 1] \right] , \tag{6}$$

in the Coulomb gauge, where

$$\omega_{jk} = |\varepsilon_j - \varepsilon_k| / c \tag{7}$$

is the difference between one-electron energies $\varepsilon$ of the interacting electrons divided by the speed of light $c$. The $\omega$ in Eqs. (5) and (6) represents the change in the *total* energy of the interacting system in the original derivation of the Breit interaction using QED in which the unperturbed system consists of *noninteracting* electrons. In such a system, each electron has a definite energy associated with it, and the total energy of the system is the sum of such "one-electron" energies.

In a DF as well as an MBPT calculation, it is customary to use orbital energies for $\varepsilon$, although an orbital energy is not really an energy eigenvalue in the usual mathematical sense but is a Lagrange multiplier introduced to enforce the normalization of each orbital. For instance, the $2s$ orbital of a Li-like ion has two Lagrange multipliers, a diagonal one for normalization—normally referred to as the orbital energy—and an off-diagonal one to enforce the orthogonality between the $1s$ and $2s$ orbitals. The total energy of a Li-like ion is not the sum of orbital energies. Moreover, the difference of orbital energies does not represent the change in the total energy of the system caused by the electron-electron interaction in any theoretical method that includes the nonrelativistic Coulomb repulsion in its zeroth-order Hamiltonian. Hence, the use of orbital energies in Eq. (7) already represents a compromise. We used Eq. (6) with orbital energies to define $\omega$, but without the Coulomb repulsion term, which is already included in $H_0$, Eq. (2).

An alternative choice is to start with a set of electrons bound to the nucleus but not interacting with each other, and treat the Coulomb repulsion between them as perturbation. Such a choice may be adequate for highly charged atoms, but it will require extensive perturbation calculations to very high orders for neutral or lightly charged atoms.

### C. Projection operator and unperturbed Hamiltonian

Sucher[21] advocated the use of a projection operator in a relativistic Hamiltonian to exclude negative-energy solutions to avoid difficulties, known as the Brown-Ravenhall disease, arising from the existence of negative-energy solutions in a relativistic formulation. We did not, however, introduce any projection operator, because it is difficult to construct an explicit yet *practical* projection operator suitable for numerical implementation in an iterative scheme. Existing DF codes (a) select positive-energy solutions as the trial solutions, (b) permit only small departures from the trial solutions at each step of iteration, and (c) require all solutions to vanish at a large distance from the nucleus (negative-energy solutions os-

TABLE I. Fitting coefficients for $E_{rcor}$ in the resonance transitions of Li-, Na-, and Cu-like ions. Numbers in square brackets denote powers of 10, e.g., 7.886 28[−1]=7.886 28×10$^{-1}$. See Eqs. (1) and (8).

| | Li sequence | | Na sequence | | Cu sequence | |
|---|---|---|---|---|---|---|
| Coeff. | $2s$-$2p_{1/2}$ | $2s$-$2p_{3/2}$ | $3s$-$3p_{1/2}$ | $3s$-$3p_{3/2}$ | $4s$-$4p_{1/2}$ | $4s$-$4p_{3/2}$ |
| $a_{-4}$ | −1.500 14 | −1.035 15 | | | | |
| $a_{-3}$ | 1.240 69 | 7.886 28[−1] | −1.242 14[2] | −1.095 46[2] | 8.819 62[3] | 9.068 97[3] |
| $a_{-2}$ | −4.040 43[−1] | −2.334 45[−1] | 2.601 09[−1] | 2.190 19[1] | −8.968 62[2] | −9.301 22[2] |
| $a_{-1}$ | 8.823 59[−2] | 5.611 86[−2] | −1.897 84 | −1.447 64 | 3.841 08[1] | 4.032 58[1] |
| $a_0$ | −1.269 90[−2] | −9.450 56[−3] | 7.168 48[−2] | 4.713 13[−2] | −8.498 26[−1] | −9.128 40(−1) |
| $a_1$ | 3.717 92[−4] | 1.875 73[−4] | −1.686 17[−3] | −9.943 63[−4] | 1.108 54[−2] | 1.142 19[−2] |
| $a_2$ | −1.183 07[−5] | −5.125 11[−6] | 1.772 73[−5] | 8.466 83[−6] | −6.369 40[−5] | −7.617 33[−5] |
| $a_3$ | 1.587 19[−7] | 7.779 82[−8] | −8.097 23[−8] | −1.951 42[−8] | 1.570 50[−7] | 2.256 27[−7] |
| $a_4$ | −1.013 25[−9] | −4.255 82[−10] | | | | |

cillate there). However, it is uncertain whether these numerical constraints used in an SCF procedure would automatically satisfy all the properties of a projection operator, as was claimed by Mittleman.[22]

Both Breit[23] and Bethe and Salpeter[24] stated that the Breit operator should not be included in the unperturbed Hamiltonian because the approximations used in deriving the operator is consistent with treating it as a first-order perturbation only. Although Sucher[21] states that such a restriction is unnecessary provided that an appropriate projection operator is used, we have used the Breit operator in the first-order perturbation because we did not explicitly use a projection operator. The unperturbed Hamiltonian we have used consists of a sum of the Dirac Hamiltonian and the nonrelativistic Coulomb repulsion.

### D. Correlation energy

We have compared transition energies calculated by Johnson, Blundel, and Sapirstein[6-8] using the MBPT and our DF results to deduce relativistic correlation energies $E_{rcor}$ according to Eq. (1). The $E_{rcor}$ thus deduced were then fitted to a power series in $Z$:

$$E_{rcor}=a_{-4}/Z^4+a_{-3}/Z^3+a_{-2}/Z^2+a_{-1}/Z +a_0+a_1Z+a_2Z^2+a_3Z^3+a_4Z^4 , \quad (8)$$

where the coefficients $a_i$ were determined by a least-square fitting. The fitted correlation energy agrees with the original data within $5\times10^{-5}$ hartree. Only $E_{rcor}$ for the $ns$-$np_{1/2}$ and $ns$-$np_{3/2}$ transitions in each sequence were fitted and the $E_{rcor}$ for the $np_{1/2}$-$np_{3/2}$ fine-structure splitting was deduced from the other two to avoid conflict among fitted values. The fitted coefficients are listed in Table I.

As is shown in Figs. 1–3, $E_{rcor}$ is less than 0.03 hartree (~0.8 eV) in magnitude for all transitions considered in the present work. In the hydrogenic limit, $ns_{1/2}$ and $np_{1/2}$ are degenerate in energy, and hence we can regard curves I for the $ns$-$np_{1/2}$ transition as representing the Coulomb repulsion between bound electrons and accompanying relativistic corrections, which grow rapidly as $Z$ increases. Curves II for the $ns$-$np_{3/2}$ transition are relatively flat (i.e., $Z$ independent) for intermediate values of $Z$. The flat trend reflects the prediction of the nonrela-

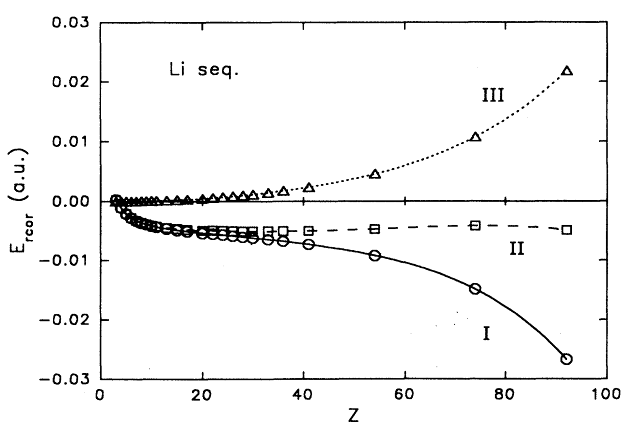


FIG. 1. Relativistic correlation energy, $E_{rcor}$ defined by Eq. (1), of Li-like ions as a function of atomic number $Z$ in atomic units. Curve I: $ns\rightarrow np_{1/2}$ transition. Curve II: $ns\rightarrow np_{3/2}$ transition. Curve III: $np_{1/2}\rightarrow np_{3/2}$ transition. For Li-like ions, $n=2$. Curves are fitted values [Eq. (8) and Table I] and open symbols represents the actual correlation energies calculated from Refs. 6–8.

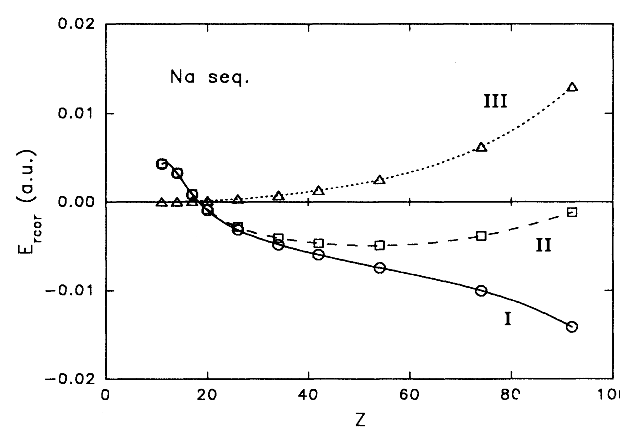


FIG. 2. Relativistic correlation energy of Na-like ions in atomic units. See Fig. 1 caption for legend with $n=3$ for Na-like ions.

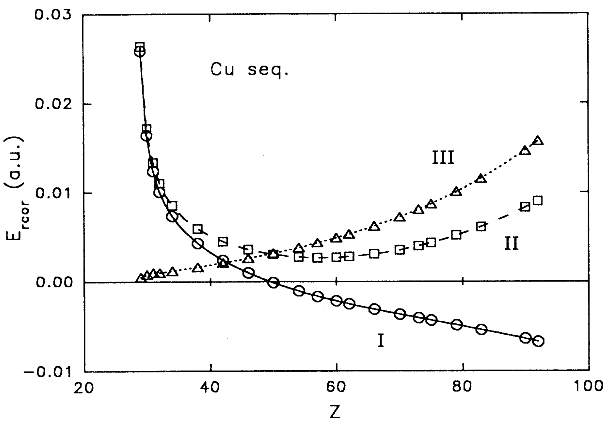


FIG. 3. Relativistic correlation energy of Cu-like ions in atomic units. See Fig. 1 caption for legend with $n=4$ for Cu-like ions.

tivistic $Z$-expansion theory that the leading nonrelativistic correlation energy for such transitions be independent of $Z$. Curves III for the $np_{1/2}$-$np_{3/2}$ transition mainly represent the difference in the correlation energies of the $np_{1/2}$ and $np_{3/2}$ levels.

The DF transition energies without QED corrections are listed in Tables II–VII. We did not include the mass polarization in our calculation, since it is smaller than the uncertainties in the way we estimate QED corrections. Hence, mass polarization, which is included in the MBPT calculation, will appear as part of our correlation energy. The resulting relativistic correlation energies are also listed in Table II–VII. The sum of our DF results (without QED) and $E_{rcor}$ should match the transition energies derived from the MBPT results.[6–8] For Cu-like $U^{63+}$, however, the nuclear parameters used in Ref. 8 were different from those used in Ref. 18 and the present DF calcula-

TABLE II. Energy for the $2s$-$2p_{1/2}$ transition of Li-like ions (in $cm^{-1}$).

| $Z$ | DF no QED | QED $\rho$ | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 6 | 65 118 | −14 | −613 | 64 491 | 64 484±1 | a | 64 483 | 64 484 | a |
| 7 | 81 215 | −27 | −718 | 80 470 | 80 463±1 | a | 80 464 | 80 463 | a |
| 8 | 97 224 | −48 | −797 | 96 379 | 96 375±1 | a | 96 375 | 96 374 | a |
| 9 | 113 199 | −76 | −859 | 112 264 | 112 261±2 | a | 112 262 | 112 261 | a |
| 10 | 129 176 | −116 | −909 | 128 151 | 128 151±2 | a | 128 151 | 128 151 | a |
| 11 | 145 180 | −168 | −951 | 144 061 | 144 062±3 | a | 144 063 | 144 063 | a |
| 12 | 161 229 | −235 | −987 | 160 008 | 160 012±3 | a | 160 012 | 160 012 | a |
| 13 | 177 338 | −318 | −1018 | 176 002 | 176 012±4 | a | 176 008 | 176 008 | a |
| 14 | 193 521 | −421 | −1045 | 192 056 | 192 062±5 | b | 192 064 | 192 063 | a |
| 15 | 209 790 | −544 | −1070 | 208 176 | 208 204±25 | c | 208 185 | 208 184 | a |
| 16 | 226 154 | −691 | −1093 | 224 371 | 224 366±15 | d | 224 381 | 224 380 | a |
| 17 | 242 625 | −864 | −1114 | 240 648 | 240 659±12 | a | 240 659 | 240 657 | a |
| 18 | 259 213 | −1 065 | −1134 | 257 014 | 257 020±7 | a | 257 026 | 257 024 | a |
| 19 | 275 926 | −1 296 | −1153 | 273 476 | 273 500±10 | e | 273 489 | 273 489 | a |
| 20 | 292 774 | −1 560 | −1172 | 290 041 | 290 057±20 | e | 290 055 | 290 057 | a |
| 21 | 309 767 | −1 861 | −1190 | 306 716 | 360 700±300 | e | 306 731 | 306 735 | a |
| 22 | 326 913 | −2 199 | −1209 | 323 506 | 323 541±10 | f | 323 521 | 323 530 | a |
| 23 | 344 224 | −2 578 | −1227 | 340 420 | 340 470±60 | e | 340 435 | 340 451 | a |
| 24 | 361 708 | −3 000 | −1245 | 357 462 | 357 489±30 | g | 357 476 | 357 491 | h |
| 25 | 379 372 | −3 469 | −1263 | 374 640 | 374 700±50 | e | 374 654 | 374 665 | h |
| 26 | 397 230 | −3 987 | −1282 | 391 961 | 392 012±20 | g | 391 975 | 391 986 | h |
| 27 | 415 288 | −4 556 | −1301 | 409 432 | | | 409 445 | 409 454 | h |
| 28 | 433 560 | −5 180 | −1320 | 427 060 | 427 068±20 | g | 427 073 | 427 082 | h |
| 29 | 452 048 | −5 860 | −1339 | 444 848 | 444 850±20 | g | 444 861 | 444 873 | h |
| 30 | 470 769 | −6 602 | −1359 | 462 809 | | | 462 821 | 462 837 | h |
| 31 | 489 733 | −7 406 | −1379 | 480 948 | | | 480 960 | 480 979 | h |
| 32 | 508 946 | −8 276 | −1400 | 499 269 | 499 276±30 | g | 499 281 | 499 307 | h |
| 33 | 528 424 | −9 216 | −1421 | 517 787 | | | 517 798 | 517 828 | h |
| 34 | 548 173 | −10 228 | −1443 | 536 502 | 536 552±45 | g | 536 513 | 536 550 | h |
| 35 | 568 214 | −11 315 | −1465 | 555 434 | | | 555 445 | 555 482 | h |
| 36 | 588 541 | −12 481 | −1488 | 574 572 | 574 594±85 | g | 574 582 | 574 626 | h |
| 37 | 609 182 | −13 729 | −1511 | 593 942 | | | 593 952 | 593 997 | h |
| 38 | 630 146 | −15 062 | −1535 | 613 549 | | | 613 559 | 613 601 | h |
| 39 | 651 441 | −16 483 | −1559 | 633 399 | | | 633 408 | 633 443 | h |
| 40 | 673 075 | −17 994 | −1585 | 653 496 | | | 653 505 | 653 534 | h |
| 41 | 695 061 | −19 603 | −1610 | 673 848 | | | 673 857 | 673 884 | h |
| 42 | 717 399 | −21 310 | −1637 | 694 452 | 694 454±100 | g | 694 460 | 694 499 | h |
| 43 | 740 146 | −23 119 | −1664 | 715 363 | | | 715 371 | 715 393 | h |
| 44 | 763 265 | −25 035 | −1692 | 736 538 | | | 736 546 | 736 570 | h |

TABLE II. (*Continued*).

| $Z$ | DF no QED | QED $\rho$ | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 45 | 786 804 | −27 060 | −1721 | 758 023 | | | 758 030 | 758 041 | h |
| 46 | 810 768 | −29 199 | −1751 | 779 818 | | | 779 825 | 779 820 | h |
| 47 | 835 172 | −31 456 | −1782 | 801 935 | | | 801 942 | 801 916 | h |
| 48 | 859 994 | −33 834 | −1813 | 824 346 | | | 824 352 | 824 338 | h |
| 49 | 885 320 | −36 338 | −1846 | 847 137 | | | 847 143 | 847 100 | h |
| 50 | 911 107 | −38 970 | −1880 | 870 256 | | | 870 262 | 870 213 | h |
| 51 | 937 375 | −41 729 | −1915 | 893 731 | | | 893 736 | 893 688 | h |
| 52 | 964 097 | −44 635 | −1951 | 917 511 | | | 917 516 | 917 538 | h |
| 53 | 991 504 | −47 680 | −1989 | 941 834 | | | 941 839 | 941 779 | h |
| 54 | 1 019 311 | −50 874 | −2028 | 966 409 | 967 590±800 | i | 966 413 | 966 424 | h |
| 55 | 1 047 799 | −54 233 | −2069 | 991 497 | | | 991 501 | | |
| 56 | 1 076 793 | −57 718 | −2111 | 1 016 965 | | | 1 016 969 | | |
| 57 | 1 106 412 | −61 378 | −2155 | 1 042 879 | | | 1 042 882 | | |
| 58 | 1 136 631 | −65 220 | −2200 | 1 069 211 | | | 1 069 214 | | |
| 59 | 1 167 495 | −69 201 | −2248 | 1 096 046 | | | 1 096 048 | | |
| 60 | 1 198 994 | −73 373 | −2297 | 1 123 324 | | | 1 123 326 | | |
| 61 | 1 231 091 | −77 727 | −2349 | 1 151 016 | | | | | |
| 62 | 1 263 789 | −82 267 | −2403 | 1 179 120 | | | | | |
| 63 | 1 297 360 | −86 996 | −2459 | 1 207 905 | | | | | |
| 64 | 1 331 512 | −91 885 | −2518 | 1 237 110 | | | | | |
| 65 | 1 366 541 | −97 009 | −2579 | 1 266 953 | | | | | |
| 66 | 1 402 457 | −102 386 | −2643 | 1 297 429 | | | | | |
| 67 | 1 438 435 | −107 891 | −2710 | 1 327 833 | | | | | |
| 68 | 1 476 326 | −113 650 | −2780 | 1 359 896 | | | | | |
| 69 | 1 514 152 | −119 645 | −2853 | 1 391 654 | | | | | |
| 70 | 1 552 906 | −125 869 | −2930 | 1 424 107 | | | | | |
| 71 | 1 592 744 | −132 329 | −3010 | 1 457 404 | | | | | |
| 72 | 1 633 144 | −139 036 | −3094 | 1 491 014 | | | | | |
| 73 | 1 674 701 | −145 992 | −3182 | 1 525 526 | | | | | |
| 74 | 1 716 605 | −153 212 | −3274 | 1 560 119 | | | | | |
| 75 | 1 760 108 | −160 690 | −3370 | 1 596 048 | | | | | |
| 76 | 1 804 131 | −168 444 | −3471 | 1 632 216 | | | | | |
| 77 | 1 849 030 | −176 478 | −3576 | 1 668 976 | | | | | |
| 78 | 1 894 932 | −184 798 | −3686 | 1 706 448 | | | | | |
| 79 | 1 941 695 | −193 412 | −3801 | 1 744 481 | | | | | |
| 80 | 1 988 967 | −202 332 | −3922 | 1 782 714 | | | | | |
| 81 | 2 037 678 | −211 558 | −4048 | 1 822 072 | | | | | |
| 82 | 2 086 949 | −221 105 | −4179 | 1 861 665 | | | | | |
| 83 | 2 136 921 | −230 979 | −4317 | 1 901 625 | | | | | |
| 84 | 2 188 163 | −241 182 | −4461 | 1 942 520 | | | | | |
| 85 | 2 239 218 | −251 393 | −4611 | 1 983 214 | | | | | |
| 86 | 2 290 295 | −262 271 | −4768 | 2 023 257 | | | | | |
| 87 | 2 343 527 | −273 486 | −4931 | 2 065 109 | | | | | |
| 88 | 2 396 716 | −285 070 | −5102 | 2 106 543 | | | | | |
| 89 | 2 451 049 | −297 017 | −5281 | 2 148 751 | | | | | |
| 90 | 2 499 108 | −309 419 | −5467 | 2 184 222 | | | | | |
| 91 | 2 553 462 | −322 141 | −5661 | 2 225 661 | | | | | |
| 92 | 2 604 989 | −335 311 | −5863 | 2 263 815 | 2 264 100±700 | j | | | |

[a]B. Edlén, Ref. 13.
[b]W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data **12**, 323 (1983).
[c]W. C. Martin, R. Zalubas, and A. Musgrove, J. Phys. Chem. Ref. Data **14**, 751 (1985).
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[e]J. Sugar and C. Corliss, Ref. 41.
[f]J. Sugar (private communication).
[g]E. Hinnov *et al.*, Ref. 51.
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[i]S. Martin *et al.*, Ref. 37.
[j]J. Schweppe *et al.*, Ref. 38.

TABLE III. Energy for the $2s$-$2p_{3/2}$ transition of Li-like ions (in $cm^{-1}$).

| $Z$ | DF no QED | QED $\rho$ | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 6 | 65 220 | −14 | −608 | 64 598 | 64 591±1 | a | 64 591 | 64 591 | a |
| 7 | 81 467 | −27 | −712 | 80 729 | 80 722±1 | a | 80 724 | 80 721 | a |
| 8 | 97 744 | −46 | −787 | 96 911 | 96 906±1 | a | 96 908 | 96 905 | a |
| 9 | 114 158 | −74 | −844 | 113 240 | 113 237±2 | a | 113 239 | 113 236 | a |
| 10 | 130 804 | −112 | −889 | 129 803 | 129 800±2 | a | 129 804 | 129 801 | a |
| 11 | 147 776 | −162 | −925 | 146 689 | 146 693±5 | a | 146 692 | 146 689 | a |
| 12 | 165 169 | −225 | −955 | 163 989 | 163 987±3 | a | 163 994 | 163 992 | a |
| 13 | 183 086 | −304 | −979 | 181 803 | 181 808±5 | a | 181 810 | 181 806 | a |
| 14 | 201 637 | −401 | −999 | 200 236 | 200 238±5 | b | 200 245 | 200 241 | a |
| 15 | 220 938 | −517 | −1017 | 219 404 | 219 430±25 | c | 219 415 | 219 411 | a |
| 16 | 241 115 | −655 | −1031 | 239 428 | 239 429±15 | d | 239 441 | 239 438 | a |
| 17 | 262 303 | −817 | −1044 | 260 442 | 260 429±15 | a | 260 457 | 260 452 | a |
| 18 | 284 646 | −1 005 | −1054 | 282 587 | 282 592±10 | a | 282 603 | 282 598 | a |
| 19 | 308 297 | −1 220 | −1063 | 306 013 | 306 020±9 | e | 306 030 | 306 028 | a |
| 20 | 333 420 | −1 466 | −1071 | 330 883 | 330 918±20 | e | 330 901 | 330 901 | a |
| 21 | 360 189 | −1 745 | −1078 | 357 367 | 357 400±300 | e | 357 386 | 357 389 | a |
| 22 | 388 787 | −2 058 | −1084 | 385 646 | 385 660±10 | f | 385 666 | 385 675 | a |
| 23 | 419 410 | −2 407 | −1089 | 415 914 | 416 020±90 | e | 415 935 | 415 951 | a |
| 24 | 452 261 | −2 797 | −1093 | 448 372 | 448 410±40 | g | 448 394 | 448 404 | h |
| 25 | 487 556 | −3 227 | −1097 | 483 233 | 483 320±50 | e | 483 255 | 483 266 | h |
| 26 | 525 525 | −3 702 | −1099 | 520 724 | 520 800±60 | g | 520 745 | 520 756 | h |
| 27 | 566 404 | −4 223 | −1102 | 561 080 | | | 561 101 | 561 111 | h |
| 28 | 610 447 | −4 792 | −1104 | 604 551 | 604 610±40 | g | 604 572 | 604 582 | h |
| 29 | 657 910 | −5 413 | −1105 | 651 392 | 651 436±90 | g | 651 412 | 651 427 | h |
| 30 | 709 074 | −6 087 | −1106 | 701 881 | | | 701 901 | 701 922 | h |
| 31 | 764 227 | −6 818 | −1107 | 756 302 | | | 756 322 | 756 347 | h |
| 32 | 823 664 | −7 607 | −1107 | 814 949 | 814 963±100 | g | 814 968 | 815 004 | h |
| 33 | 887 706 | −8 458 | −1107 | 878 141 | | | 878 160 | 878 201 | h |
| 34 | 956 674 | −9 373 | −1106 | 946 194 | 946 199±200 | g | 946 213 | 946 267 | h |
| 35 | 1 030 921 | −10 355 | −1105 | 1 019 461 | | | 1 019 479 | 1019 539 | h |
| 36 | 1 110 785 | −11 405 | −1104 | 1 098 276 | 1 098 300±300 | g | 1 098 294 | 1 098 370 | h |
| 37 | 1 196 656 | −12 529 | −1102 | 1 183 025 | | | 1 183 043 | 1 183 126 | h |
| 38 | 1 288 915 | −13 727 | −1100 | 1 274 087 | | | 1 274 104 | 1 274 191 | h |
| 39 | 1 387 962 | −15 004 | −1098 | 1 371 861 | | | 1 371 878 | 1 371 964 | h |
| 40 | 1 494 211 | −16 359 | −1095 | 1 476 756 | | | 1 476 773 | 1 476 858 | h |
| 41 | 1 608 097 | −17 801 | −1092 | 1 589 204 | | | 1 589 220 | 1 589 308 | h |
| 42 | 1 730 061 | −19 330 | −1088 | 1 709 642 | 1 709 400±600 | g | 1 709 658 | 1 709 758 | h |
| 43 | 1 860 619 | −20 949 | −1085 | 1 838 585 | | | 1 838 601 | 1 838 677 | h |
| 44 | 2 000 207 | −22 661 | −1081 | 1 976 465 | | | 1 976 480 | 1 976 549 | h |
| 45 | 2 149 371 | −24 471 | −1076 | 2 123 824 | | | 2 123 839 | 2 123 882 | h |
| 46 | 2 308 629 | −26 381 | −1072 | 2 281 177 | | | 2 281 192 | 2 281 202 | h |
| 47 | 2 478 531 | −28 395 | −1067 | 2 449 070 | | | 2 449 084 | 2 449 052 | h |
| 48 | 2 659 611 | −30 518 | −1061 | 2 628 032 | | | 2 628 046 | 2 628 007 | h |
| 49 | 2 852 533 | −32 751 | −1056 | 2 818 726 | | | 2 818 740 | 2 818 658 | h |
| 50 | 3 057 853 | −35 100 | −1050 | 3 021 703 | | | 3 021 716 | 3 021 624 | h |
| 51 | 3 276 216 | −37 560 | −1044 | 3 237 611 | | | 3 237 624 | 3 237 549 | h |
| 52 | 3 508 241 | −40 152 | −1038 | 3 467 051 | | | 3 467 064 | 3 467 111 | h |
| 53 | 3 754 836 | −42 870 | −1032 | 3 710 934 | | | 3 710 946 | 3 711 009 | h |
| 54 | 4 016 413 | −45 721 | −1025 | 3 969 667 | 3 971 000±5000 | i | 3 969 679 | 3 969 978 | h |
| 55 | 4 293 982 | −48 707 | −1018 | 4 244 256 | | | 4 244 268 | | |
| 56 | 4 588 123 | −51 835 | −1012 | 4 535 276 | | | 4 535 287 | | |
| 57 | 4 899 740 | −55 109 | −1005 | 4 843 626 | | | 4 843 637 | | |
| 58 | 5 229 627 | −58 534 | −998 | 5 170 095 | | | 5 170 106 | | |
| 59 | 5 578 676 | −62 115 | −991 | 5 515 570 | | | 5 515 580 | | |
| 60 | 5 947 762 | −65 857 | −984 | 5 880 921 | | | 5 880 931 | | |
| 61 | 6 337 763 | −69 769 | −977 | 6 267 017 | | | | | |
| 62 | 6 749 637 | −73 852 | −970 | 6 674 814 | | | | | |
| 63 | 7 184 658 | −78 114 | −964 | 7 105 580 | | | | | |

TABLE III. (*Continued*).

| $Z$ | DF no QED | QED $\rho$ | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 64 | 7 643 560 | −82 522 | −957 | 7 560 081 | | | | | |
| 65 | 8 127 725 | −87 155 | −951 | 8 039 619 | | | | | |
| 66 | 8 638 285 | −92 032 | −945 | 8 545 308 | | | | | |
| 67 | 9 175 546 | −97 027 | −939 | 9 077 579 | | | | | |
| 68 | 9 742 660 | −102 269 | −934 | 9 639 458 | | | | | |
| 69 | 10 338 825 | −107 740 | −929 | 10 230 156 | | | | | |
| 70 | 10 966 403 | −113 437 | −924 | 10 852 041 | | | | | |
| 71 | 11 626 934 | −119 369 | −920 | 11 506 645 | | | | | |
| 72 | 12 321 311 | −125 547 | −917 | 12 194 848 | | | | | |
| 73 | 13 051 662 | −131 975 | −914 | 12 918 772 | | | | | |
| 74 | 13 818 698 | −138 673 | −912 | 13 679 114 | | | | | |
| 75 | 14 625 383 | −145 634 | −910 | 14 478 838 | | | | | |
| 76 | 15 472 287 | −152 883 | −910 | 15 318 495 | | | | | |
| 77 | 16 361 577 | −160 425 | −910 | 16 200 243 | | | | | |
| 78 | 17 295 263 | −168 269 | −911 | 17 126 083 | | | | | |
| 79 | 18 275 153 | −176 429 | −914 | 18 097 811 | | | | | |
| 80 | 19 302 927 | −184 921 | −917 | 19 117 089 | | | | | |
| 81 | 20 381 731 | −193 755 | −922 | 20 187 055 | | | | | |
| 82 | 21 512 883 | −202 947 | −927 | 21 309 009 | | | | | |
| 83 | 22 698 898 | −212 508 | −935 | 22 485 455 | | | | | |
| 84 | 23 942 881 | −222 446 | −943 | 23 719 491 | | | | | |
| 85 | 25 245 861 | −232 412 | −953 | 25 012 496 | | | | | |
| 86 | 26 610 810 | −243 141 | −965 | 26 366 703 | | | | | |
| 87 | 28 042 942 | −254 275 | −979 | 27 787 689 | | | | | |
| 88 | 29 542 904 | −265 859 | −994 | 29 276 051 | | | | | |
| 89 | 31 115 207 | −277 894 | −1011 | 30 836 302 | | | | | |
| 90 | 32 755 019 | −290 498 | −1030 | 32 463 490 | | | | | |
| 91 | 34 479 810 | −303 523 | −1051 | 34 175 236 | | | | | |
| 92 | 36 283 247 | −317 112 | −1075 | 35 965 059 | | | | | |

[a]B. Edlén, Ref. 13.
[b]Table II, footnote b.
[c]Table II, footnote c.
[d]Table II, footnote d.
[e]J. Sugar and C. Corliss, Ref. 41.
[f]J. Sugar (private communication).
[g]E. Hinnov *et al.*, Ref. 51.
[h]J. Seely, Ref. 14.
[i]S. Martin, *et al.*, Ref. 37.

TABLE IV. Energy for the $3s$-$3p_{1/2}$ transition of Na-like ions (in $\mathrm{cm}^{-1}$).

| $Z$ | DF no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 14 | 70 618 | −30 | 705 | 71 292 | 71 288 | a | 71 287 | | |
| 15 | 88 201 | −47 | 523 | 88 677 | 88 652±1 | b | 88 652 | | |
| 16 | 105 624 | −69 | 346 | 105 901 | 105 874±2 | c | 105 873 | | |
| 17 | 122 947 | −97 | 182 | 123 032 | 123 001 | d | 123 007 | | |
| 18 | 140 208 | −130 | 33 | 140 110 | 140 093±6 | e | 140 090 | | |
| 19 | 157 437 | −171 | −99 | 157 166 | 157 152±3 | e | 157 152 | | |
| 20 | 174 656 | −219 | −217 | 174 220 | 174 213±3 | e | 174 213 | | |
| 21 | 191 885 | −276 | −321 | 191 288 | 191 288±4 | e | 191 287 | | |
| 22 | 209 136 | −342 | −413 | 208 381 | 208 385±4 | e | 208 385 | | |
| 23 | 226 422 | −417 | −496 | 225 509 | 225 519±5 | e | 225 516 | | |
| 24 | 243 754 | −503 | −570 | 242 681 | 242 688±2 | e | 242 690 | | |
| 25 | 261 140 | −600 | −637 | 259 904 | 259 920±30 | e | 259 914 | | |
| 26 | 278 591 | −709 | −698 | 277 184 | 277 192±3 | e | 277 194 | | |
| 27 | 296 114 | −832 | −754 | 294 528 | 294 540±20 | e | 294 538 | | |
| 28 | 313 715 | −967 | −805 | 311 943 | 311 949±6 | e | 311 953 | | |
| 29 | 331 403 | −1118 | −853 | 329 432 | 329 442±11 | e | 329 442 | | |

TABLE IV. (*Continued*).

| Z | DF no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 349 183 | −1 284 | −898 | 347 002 | 347 008±12 | e | 347 012 | | |
| 31 | 367 064 | −1 465 | −941 | 364 658 | 364 681±13 | e | 364 668 | | |
| 32 | 385 050 | −1 664 | −981 | 382 405 | 382 409±15 | e | 382 415 | | |
| 33 | 403 150 | −1 881 | −1020 | 400 249 | 400 253±16 | e | 400 259 | | |
| 34 | 421 367 | −2 116 | −1056 | 418 194 | 418 195±17 | e | 418 204 | | |
| 35 | 439 711 | −2 371 | −1092 | 436 248 | 436 256±19 | e | 436 258 | | |
| 36 | 458 185 | −2 647 | −1126 | 454 412 | 454 428±20 | e | 454 422 | | |
| 37 | 476 798 | −2 944 | −1159 | 472 695 | | | 472 705 | | |
| 38 | 495 556 | −3 264 | −1191 | 491 101 | | | 491 111 | | |
| 39 | 514 464 | −3 606 | −1223 | 509 635 | 509 645±26 | e | 509 645 | 509 635 | f |
| 40 | 533 528 | −3 973 | −1253 | 528 302 | 528 326±28 | e | 528 312 | 528 307 | f |
| 41 | 552 754 | −4 365 | −1283 | 547 106 | 547 115±30 | e | 547 116 | 547 121 | f |
| 42 | 572 147 | −4 783 | −1313 | 566 051 | 566 040±32 | e | 566 061 | 566 078 | f |
| 43 | 591 722 | −5 229 | −1341 | 585 152 | | | 585 162 | 585 189 | f |
| 44 | 611 476 | −5 702 | −1370 | 604 404 | | | 604 414 | 604 449 | f |
| 45 | 631 423 | −6 205 | −1397 | 623 820 | | | 623 830 | 623 877 | f |
| 46 | 651 567 | −6 738 | −1425 | 643 404 | | | 643 414 | 643 468 | f |
| 47 | 671 916 | −7 303 | −1452 | 663 162 | 663 220±200 | e | 663 172 | 663 240 | f |
| 48 | 692 469 | −7 899 | −1478 | 683 092 | 683 027±70 | f | 683 102 | 683 181 | f |
| 49 | 713 250 | −8 529 | −1504 | 703 217 | | | 703 227 | 703 314 | f |
| 50 | 734 253 | −9 193 | −1530 | 723 529 | 723 856±79 | f | 723 539 | 723 636 | f |
| 51 | 754 486 | −9 893 | −1556 | 744 037 | | | 744 047 | 744 158 | f |
| 52 | 776 947 | −10 629 | −1582 | 764 736 | | | 764 746 | 764 883 | f |
| 53 | 798 695 | −11 403 | −1607 | 785 684 | | | 785 694 | 785 830 | f |
| 54 | 830 667 | −12 217 | −1633 | 806 817 | 806 970±200 | g | 806 827 | 806 985 | f |
| 55 | 842 933 | −13 070 | −1658 | 828 205 | | | | 828 377 | f |
| 56 | 865 457 | −13 965 | −1684 | 849 809 | | | | 849 986 | f |
| 57 | 888 271 | −14 902 | −1709 | 871 660 | | | | 871 847 | f |
| 58 | 911 374 | −15 882 | −1735 | 893 757 | | | | 893 967 | f |
| 59 | 934 782 | −16 908 | −1760 | 916 113 | | | | 916 338 | f |
| 60 | 958 496 | −17 981 | −1786 | 938 730 | | | | 938 958 | f |
| 61 | 982 513 | −19 100 | −1812 | 961 601 | | | | 961 862 | f |
| 62 | 1 006 839 | −20 268 | −1839 | 984 732 | | | | 985 008 | f |
| 63 | 1 031 544 | −21 487 | −1865 | 1 008 192 | | | | 1 008 481 | f |
| 64 | 1 056 563 | −22 756 | −1893 | 1 031 914 | | | | 1 032 205 | f |
| 65 | 1 081 973 | −24 079 | −1920 | 1 055 974 | | | | 1 056 267 | f |
| 66 | 1 107 784 | −25 457 | −1948 | 1 080 379 | | | | 1 080 625 | f |
| 67 | 1 133 794 | −26 887 | −1977 | 1 104 929 | | | | 1 105 314 | f |
| 68 | 1 160 472 | −28 378 | −2007 | 1 130 087 | | | | 1 130 314 | f |
| 69 | 1 187 330 | −29 925 | −2037 | 1 155 367 | | | | 1 155 682 | f |
| 70 | 1 214 620 | −31 532 | −2068 | 1 181 021 | | | | 1 181 335 | f |
| 71 | 1 242 391 | −33 200 | −2100 | 1 207 090 | | | | 1 207 394 | f |
| 72 | 1 270 515 | −34 930 | −2133 | 1 233 452 | | | | 1 233 761 | f |
| 73 | 1 299 150 | −36 725 | −2167 | 1 260 259 | | | | 1 260 525 | f |
| 74 | 1 328 098 | −38 583 | −2202 | 1 287 313 | | | | 1 287 648 | f |
| 75 | 1 357 683 | −40 511 | −2238 | 1 314 934 | | | | 1 315 184 | f |
| 76 | 1 387 639 | −42 506 | −2275 | 1 342 858 | | | | 1 343 021 | f |
| 77 | 1 418 064 | −44 569 | −2314 | 1 371 181 | | | | 1 371 328 | f |
| 78 | 1 448 997 | −46 705 | −2354 | 1 399 938 | | | | 1 399 992 | f |
| 79 | 1 480 411 | −48 913 | −2396 | 1 429 101 | | | | 1 429 123 | f |
| 80 | 1 512 223 | −51 194 | −2439 | 1 458 590 | | | | 1 485 576 | f |
| 81 | 1 544 681 | −53 553 | −2484 | 1 488 643 | | | | 1 488 427 | f |
| 82 | 1 577 568 | −55 988 | −2530 | 1 519 049 | | | | 1 518 695 | f |
| 83 | 1 610 929 | −58 500 | −2579 | 1 549 850 | | | | 1 549 451 | f |
| 84 | 1 644 921 | −61 094 | −2629 | 1 581 197 | | | | 1 580 753 | f |
| 85 | 1 679 178 | −63 765 | −2681 | 1 612 732 | | | | 1 612 383 | f |
| 86 | 1 713 765 | −66 517 | −2736 | 1 644 512 | | | | 1 643 574 | f |
| 87 | 1 749 242 | −69 357 | −2792 | 1 677 093 | | | | 1 675 968 | f |

TABLE IV. (*Continued*).

| Z | DF no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 88 | 1 785 054 | −72 280 | −2851 | 1 709 923 | | | | 1 708 555 | f |
| 89 | 1 821 521 | −75 291 | −2912 | 1 743 318 | | | | 1 741 675 | f |
| 90 | 1 856 731 | −78 365 | −2975 | 1 775 391 | | | | 1 774 717 | f |
| 91 | 1 893 957 | −81 550 | −3041 | 1 809 366 | | | | 1 808 776 | f |
| 92 | 1 930 847 | −84 815 | −3109 | 1 842 923 | | | | 1 842 028 | f |

[a]Table II, footnote b

[b]Table II, footnote c.

[c]Table II, footnote d.

[d]C. E. Moore, *Atomic Energy Levels,* Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 35 (U.S. GPO, Washington, DC, 1971), Vol. 1.

[e]J. Reader, V. Kaufman, J. Sugar, J. O. Ekberg, U. Feldman, C. M. Brown, J. F. Seely, and W. L. Rowan, J. Opt. Soc. Am. B **4**, 1821 (1987).

[f]J. F. Seely *et al.*, Ref. 17.

[g]J. F. Seely and R. A. Wagner, Ref. 15.

TABLE V. Energy for the $3s$-$3p_{3/2}$ transition of Na-like ions (in $\mathrm{cm}^{-1}$).

| Z | DE no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 14 | 71 070 | −29 | 710 | 71 751 | 71 749 | a | 71 750 | | |
| 15 | 88 985 | −45 | 533 | 89 473 | 89 447±1 | b | 89 448 | | |
| 16 | 106 872 | −66 | 360 | 107 166 | 107 138±2 | c | 107 138 | | |
| 17 | 124 818 | −92 | 200 | 124 926 | 124 891 | d | 124 897 | | |
| 18 | 142 894 | −123 | 55 | 142 826 | 142 810±6 | e | 142 804 | | |
| 19 | 161 164 | −161 | −73 | 160 930 | 160 913±3 | e | 160 914 | | |
| 20 | 179 688 | −206 | −186 | 179 296 | 179 288±3 | e | 179 288 | | |
| 21 | 198 523 | −259 | −285 | 197 979 | 197 981±4 | e | 197 979 | | |
| 22 | 217 727 | −320 | −371 | 217 036 | 217 042±5 | e | 217 039 | | |
| 23 | 237 358 | −390 | −448 | 236 521 | 236 525±6 | e | 236 527 | | |
| 24 | 257 476 | −469 | −515 | 256 492 | 256 500±2 | e | 256 501 | | |
| 25 | 278 141 | −559 | −574 | 277 008 | 277 026±8 | e | 277 019 | | |
| 26 | 299 419 | −660 | −626 | 298 133 | 298 143±3 | e | 298 146 | | |
| 27 | 321 376 | −772 | −673 | 319 931 | 319 950±20 | e | 319 945 | | |
| 28 | 344 080 | −896 | −715 | 342 469 | 342 480±20 | e | 342 484 | | |
| 29 | 367 605 | −1034 | −752 | 365 818 | 365 829±13 | e | 365 834 | | |
| 30 | 392 025 | −1185 | −786 | 390 053 | 390 061±15 | e | 390 070 | | |
| 31 | 417 420 | −1351 | −817 | 415 252 | 415 265±17 | e | 415 270 | | |
| 32 | 443 872 | −1532 | −845 | 441 494 | 441 507±19 | e | 441 513 | | |
| 33 | 471 466 | −1729 | −871 | 468 866 | 468 878±22 | e | 468 886 | | |
| 34 | 500 293 | −1943 | −894 | 497 455 | 497 488±25 | e | 497 475 | | |
| 35 | 530 447 | −2175 | −916 | 527 357 | 527 365±28 | e | 527 377 | | |
| 36 | 562 023 | −2424 | −936 | 558 663 | 558 690±31 | e | 558 683 | | |
| 37 | 595 126 | −2693 | −954 | 591 479 | | | 591 499 | | |
| 38 | 629 861 | −2982 | −971 | 625 908 | 625 900±20 | e | 625 928 | | |
| 39 | 666 337 | −3291 | −986 | 662 060 | 662 098±44 | e | 662 080 | 662 107 | f |
| 40 | 704 669 | −3622 | −1001 | 700 047 | 700 089±49 | e | 700 067 | 700 060 | f |
| 41 | 744 977 | −3975 | −1014 | 739 988 | 739 984±55 | e | 740 008 | 740 001 | f |
| 42 | 787 382 | −4352 | −1025 | 782 004 | 782 026±61 | e | 782 024 | 782 026 | f |
| 43 | 832 023 | −4752 | −1036 | 826 234 | | | 826 253 | 826 276 | f |
| 44 | 879 024 | −5178 | −1046 | 872 800 | 872 936±110 | e | 872 818 | 872 859 | f |
| 45 | 928 534 | −5630 | −1054 | 921 849 | 921 880±130 | e | 921 866 | 921 939 | f |
| 46 | 980 696 | −6109 | −1062 | 973 525 | 973 610±140 | e | 973 540 | 973 653 | f |
| 47 | 1 035 661 | −6616 | −1068 | 1 027 977 | 1 028 100±160 | e | 1 027 990 | 1 028 426 | f |

TABLE V. (*Continued*).

| $Z$ | DE no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 48 | 1 093 578 | −7151 | −1074 | 1 085 353 | 1 085 600±180 | f | 1 085 364 | 1 085 564 | f |
| 49 | 1 154 629 | −7716 | −1078 | 1 145 834 | 1 146 000±200 | f | 1 145 842 | 1 146 079 | f |
| 50 | 1 218 969 | −8312 | −1081 | 1 209 575 | 1 209 700±220 | f | 1 209 580 | 1 209 863 | f |
| 51 | 1 286 776 | −8940 | −1084 | 1 276 752 | 1 277 000±400 | g | 1 276 754 | 1 277 090 | f |
| 52 | 1 358 224 | −9601 | −1085 | 1 347 538 | | | 1 347 536 | 1 347 945 | f |
| 53 | 1 433 556 | −10 297 | −1085 | 1 422 174 | 1 423 000±400 | g | 1 422 168 | 1 422 617 | f |
| 54 | 1 512 897 | −11 027 | −1084 | 1 500 786 | 1 502 000±700 | h | 1 500 776 | 1 501 276 | f |
| 55 | 1 596 518 | −11 794 | −1082 | 1 583 641 | 1 584 600±400 | g | 1 583 626 | 1 584 184 | f |
| 56 | 1 684 586 | −12 598 | −1080 | 1 670 908 | | | 1 670 888 | 1 671 514 | f |
| 57 | 1 777 349 | −13 441 | −1075 | 1 762 832 | | | 1 762 807 | 1 763 482 | f |
| 58 | 1 875 028 | −14 325 | −1070 | 1 859 633 | | | 1 859 602 | 1 860 327 | f |
| 59 | 1 977 870 | −15 249 | −1064 | 1 961 556 | | | 1 961 519 | 1 962 323 | f |
| 60 | 2 086 119 | −16 217 | −1057 | 2 068 845 | | | 2 068 802 | 2 069 665 | f |
| 61 | 2 200 021 | −17 228 | −1049 | 2 181 744 | | | 2 181 694 | 2 182 691 | f |
| 62 | 2 319 841 | −18 284 | −1039 | 2 300 518 | | | 2 300 461 | 2 301 496 | f |
| 63 | 2 445 926 | −19 388 | −1029 | 2 425 509 | | | 2 425 445 | 2 426 537 | f |
| 64 | 2 578 490 | −20 540 | −1017 | 2 556 933 | 2 559 200±1300 | f | 2 556 862 | 2 558 003 | f |
| 65 | 2 717 907 | −21 742 | −1004 | 2 695 161 | | | 2 695 083 | 2 696 363 | f |
| 66 | 2 864 493 | −22 996 | −990 | 2 840 507 | | | 2 840 422 | 2 841 636 | f |
| 67 | 3 018 357 | −24 301 | −975 | 2 993 081 | | | 2 992 989 | 2 994 460 | f |
| 68 | 3 180 322 | −25 665 | −959 | 3 153 698 | | | 3 153 599 | 3 154 972 | f |
| 69 | 3 350 222 | −27 082 | −942 | 3 322 198 | | | 3 322 092 | 3 323 695 | f |
| 70 | 3 528 685 | −28 558 | −924 | 3 499 203 | | | 3 499 090 | 3 500 665 | f |
| 71 | 3 716 135 | −30 095 | −905 | 3 685 136 | | | 3 685 016 | 3 686 772 | f |
| 72 | 3 912 834 | −31 692 | −884 | 3 880 258 | | | 3 880 131 | 3 881 988 | f |
| 73 | 4 119 358 | −33 355 | −863 | 4 085 140 | | | 4 085 006 | 4 086 804 | f |
| 74 | 4 335 924 | −35 082 | −840 | 4 300 002 | | | 4 299 861 | 4 302 000 | f |
| 75 | 4 563 325 | −36 880 | −817 | 4 525 628 | | | 4 525 480 | 4 527 550 | f |
| 76 | 4 801 743 | −38 747 | −792 | 4 762 204 | | | 4 762 049 | 4 764 173 | f |
| 77 | 5 051 772 | −40 684 | −766 | 5 010 322 | | | 5 010 160 | 5 012 280 | f |
| 78 | 5 313 965 | −42 698 | −739 | 5 270 528 | 5 270 300±440 | i | 5 270 359 | 5 272 593 | f |
| 79 | 5 588 826 | −44 788 | −711 | 5 543 326 | | | | 5 545 697 | f |
| 80 | 5 876 826 | −46 956 | −682 | 5 829 187 | | | | 5 831 584 | f |
| 81 | 6 178 816 | −49 211 | −652 | 6 128 953 | | | | 6 131 208 | f |
| 82 | 6 495 178 | −51 548 | −621 | 6 443 008 | | | | 6 445 375 | f |
| 83 | 6 826 602 | −53 972 | −589 | 6 772 040 | | | | 6 774 150 | f |
| 84 | 7 173 934 | −56 488 | −556 | 7 116 889 | | | | 7 119 465 | f |
| 85 | 7 537 482 | −59 092 | −522 | 7 477 868 | | | | 7 480 551 | f |
| 86 | 7 918 060 | −61 788 | −487 | 7 855 785 | | | | 7 857 929 | f |
| 87 | 8 317 067 | −64 589 | −451 | 8 252 026 | | | | 8 254 912 | f |
| 88 | 8 734 713 | −67 488 | −414 | 8 666 810 | | | | 8 669 267 | f |
| 89 | 9 172 219 | −70 495 | −376 | 9 101 347 | | | | 9 104 151 | f |
| 90 | 9 628 358 | −73 579 | −337 | 9 554 442 | | | | 9 558 402 | f |
| 91 | 10 107 746 | −76 802 | −298 | 10 030 647 | | | | 10 034 116 | f |
| 92 | 10 608 766 | −80 127 | −257 | 10 528 382 | | | | 10 532 968 | f |

[a]Table II, footnote b.
[b]Table II, footnote c.
[c]Table II, footnote d.
[d]Table IV, footnote d.
[e]Table IV, footnote e.
[f]J. F. Seely *et al.*, Ref. 17.
[g]J. F. Seely, U. Feldman, C. M. Brown, M. C. Richardson, D. D. Dietrich, and W. E. Behring, J. Opt. Soc. Am. B **5**, 785 (1988).
[h]J. F. Seely and R. A. Wagner, Ref. 15.
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TABLE VI. Energy for the $4s$-$4p_{1/2}$ transition of Cu-like ions (in $cm^{-1}$).

| $Z$ | DF no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Preent predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 79 154 | −105 | 2201 | 81 250 | 81 315 | a | 81 320 | | |
| 33 | 95 336 | −141 | 1869 | 97 064 | 97 135 | a | 97 144 | | |
| 34 | 111 255 | −184 | 1610 | 112 681 | 112 762 | a | 112 766 | | |
| 35 | 127 008 | −232 | 1404 | 128 180 | 128 274 | a | 128 268 | | |
| 36 | 142 660 | −286 | 1230 | 143 604 | 143 695±2 | b | 143 694 | | |
| 37 | 158 253 | −346 | 1079 | 158 986 | 159 075±2 | c | 159 077 | | |
| 38 | 173 820 | −414 | 945 | 174 351 | 174 445±2 | d | 174 444 | | |
| 39 | 189 383 | −488 | 826 | 189 721 | 189 811±3 | e | 189 815 | | |
| 40 | 204 962 | −570 | 717 | 205 110 | 205 202±3 | f | 205 205 | | |
| 41 | 220 572 | −659 | 618 | 220 531 | 220 624±4 | g | 220 627 | | |
| 42 | 236 225 | −757 | 527 | 235 994 | 236 085±4 | h | 236 091 | | |
| 43 | 251 932 | −864 | 442 | 251 509 | | | 251 606 | | |
| 44 | 267 700 | −980 | 362 | 267 082 | 267 175±7 | i | 267 180 | 267 189 | p |
| 45 | 283 539 | −1105 | 288 | 282 721 | 282 834±8 | i | 282 819 | 282 824 | p |
| 46 | 299 455 | −1240 | 218 | 298 432 | 298 520±4 | j | 298 531 | 298 528 | p |
| 47 | 315 456 | −1386 | 151 | 314 221 | 314 330±5 | j | 314 320 | 314 311 | p |
| 48 | 331 546 | −1542 | 88 | 330 091 | 330 196±5 | j | 330 191 | 330 177 | p |
| 49 | 347 733 | −1710 | 28 | 346 051 | 346 156±6 | j | 346 151 | 346 131 | p |
| 50 | 364 020 | −1888 | −29 | 362 102 | 362 195±7 | j | 362 202 | 362 178 | p |
| 51 | 380 413 | −2079 | −84 | 378 251 | 378 367±7 | j | 378 351 | 378 325 | p |
| 52 | 396 915 | −2281 | −136 | 394 498 | | | 394 598 | 394 572 | p |
| 53 | 413 542 | −2496 | −185 | 410 860 | 410 949±8 | j | 410 960 | 410 932 | p |
| 54 | 430 283 | −2724 | −233 | 427 326 | 427 425±9 | j | 427 426 | 427 402 | p |
| 55 | 447 156 | −2965 | −279 | 443 913 | 444 022±10 | j | 444 013 | 443 989 | p |
| 56 | 464 158 | −3220 | −322 | 460 616 | | | 460 716 | 460 696 | p |
| 57 | 481 298 | −3489 | −365 | 477 444 | 477 550±70 | k | 477 544 | 477 530 | p |
| 58 | 498 579 | −3773 | −405 | 494 401 | | | 494 501 | 494 494 | p |
| 59 | 516 007 | −4073 | −444 | 511 491 | | | 511 591 | 511 598 | p |
| 60 | 533 587 | −4387 | −482 | 528 718 | 528 790±10 | j | 528 818 | 528 835 | p |
| 61 | 551 319 | −4719 | −518 | 546 082 | | | 546 182 | 546 221 | p |
| 62 | 569 207 | −5067 | −553 | 563 587 | 563 540±30 | l | 563 687 | 563 749 | p |
| 63 | 587 273 | −5432 | −588 | 581 253 | 581 460±100 | k | 581 353 | 581 433 | p |
| 64 | 605 502 | −5815 | −621 | 599 066 | 599 230±110 | k | 599 166 | 599 265 | p |
| 65 | 623 919 | −6216 | −654 | 617 049 | | | 617 149 | 617 273 | p |
| 66 | 642 526 | −6636 | −685 | 635 205 | 635 268±20 | j | 635 305 | 635 441 | p |
| 67 | 661 276 | −7074 | −716 | 653 485 | | | 653 585 | 653 783 | p |
| 68 | 680 293 | −7533 | −747 | 672 013 | | | 672 113 | 672 305 | p |
| 69 | 699 453 | −8012 | −777 | 690 664 | | | 690 764 | 691 009 | p |
| 70 | 718 824 | −8511 | −807 | 709 507 | 709 490±100 | m | 709 607 | 709 895 | p |
| 71 | 738 423 | −9031 | −836 | 728 557 | | | 728 657 | 728 975 | p |
| 72 | 758 219 | −9572 | −865 | 747 782 | | | 747 882 | 748 245 | p |
| 73 | 778 258 | −10 136 | −894 | 767 228 | 768 050±600 | m | 767 328 | 767 731 | p |
| 74 | 798 488 | −10 722 | −923 | 786 843 | 787 464±93 | n | 786 943 | 787 414 | p |
| 75 | 819 002 | −11 331 | −952 | 806 719 | | | 806 819 | 807 311 | p |
| 76 | 839 729 | −11 964 | −981 | 826 784 | | | 826 884 | 827 417 | p |
| 77 | 860 700 | −12 620 | −1010 | 847 070 | | | 847 170 | 847 759 | p |
| 78 | 881 929 | −13 301 | −1039 | 867 589 | | | 867 689 | 868 319 | p |
| 79 | 903 412 | −14 007 | −1068 | 888 337 | 889 007±120 | o | 888 437 | 889 110 | p |
| 80 | 925 130 | −14 739 | −1098 | 909 293 | | | 909 393 | 910 125 | p |
| 81 | 947 154 | −15 497 | −1127 | 930 531 | | | 930 631 | 931 376 | p |
| 82 | 969 429 | −16 281 | −1157 | 951 991 | 952 925±140 | o | 952 091 | 952 871 | p |
| 83 | 991 969 | −17 091 | −1187 | 973 690 | 975 134±140 | o | 973 790 | 974 640 | p |
| 84 | 1 014 824 | −17 930 | −1218 | 995 676 | | | 995 776 | 996 681 | p |
| 85 | 1 037 891 | −18 795 | −1249 | 1 017 847 | | | 1 017 947 | 1 018 984 | p |
| 86 | 1 061 190 | −19 687 | −1280 | 1 040 223 | | | 1 040 323 | 1 041 265 | p |
| 87 | 1 084 894 | −20 610 | −1311 | 1 062 973 | | | 1 063 073 | 1 064 045 | p |
| 88 | 1 108 840 | −21 561 | −1343 | 1 085 936 | | | 1 086 036 | 1 087 027 | p |
| 89 | 1 133 129 | −22 541 | −1375 | 1 109 213 | | | 1 109 313 | 1 110 322 | p |

TABLE VI. (*Continued*).

| Z | DF no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 90 | 1 157 188 | −23 544 | −1407 | 1 132 236 | | | 1 132 336 | 1 133 723 | p |
| 91 | 1 182 006 | −24 584 | −1440 | 1 155 982 | | | 1 156 082 | 1 157 582 | p |
| 92 | 1 206 879 | −25 650 | −1484 | 1 179 745 | 1 180 700±3000 | m | 1 179 845 | 1 181 377 | p |

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[d]N. Acquista and J. Reader, J. Opt. Soc. Am. **71**, 569 (1981).
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[j]J. Sugar *et al.*, Ref. 49.
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[l]M. Finkenthal, H. W. Moos, A. Bar-Shalom, N. Spector, A. Zigler, and E. Yarkoni, Phys. Rev. A **38**, 288 (1988).
[m]D. R. Kania *et al.*, Ref. 48.
[n]J. F. Seely, C. M. Brown, and W. E. Behring, Ref. 46.
[o]J. F. Seely, *et al.*, Ref. 44.
[p]J. F. Seely, C. M. Brown, and U. Feldman, Ref. 47.

TABLE VII. Energy for the $4s$-$4p_{3/2}$ transitions of Cu-like ions (in $cm^{-1}$).

| Z | DF no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 81 761 | −99 | 2419 | 84 081 | 84 103 | a | 84 103 | | |
| 33 | 99 237 | −133 | 2108 | 101 212 | 101 245 | a | 101 250 | | |
| 34 | 116 717 | −172 | 1870 | 118 415 | 118 462 | a | 118 463 | | |
| 35 | 134 325 | −216 | 1693 | 135 802 | 135 854 | a | 135 851 | | |
| 36 | 152 151 | −265 | 1538 | 153 424 | 153 476±2 | b | 153 474 | | |
| 37 | 170 268 | −321 | 1411 | 171 359 | 171 410±2 | c | 171 409 | | |
| 38 | 188 742 | −382 | 1302 | 189 661 | 189 714±2 | d | 189 712 | | |
| 39 | 207 627 | −450 | 1207 | 208 384 | 208 433±3 | e | 208 436 | | |
| 40 | 226 979 | −524 | 1124 | 227 578 | 227 627±3 | f | 227 630 | | |
| 41 | 246 848 | −606 | 1051 | 247 294 | 247 344±4 | g | 247 346 | | |
| 42 | 267 288 | −695 | 986 | 267 579 | 267 632±4 | h | 267 632 | | |
| 43 | 288 349 | −791 | 929 | 288 486 | | | 288 540 | | |
| 44 | 310 081 | −896 | 877 | 310 062 | 310 140±10 | i | 310 116 | 310 110 | p |
| 45 | 332 539 | −1010 | 831 | 332 361 | 332 372±11 | i | 332 415 | 332 411 | p |
| 46 | 355 776 | −1132 | 790 | 355 434 | 355 473±6 | j | 355 489 | 355 486 | p |
| 47 | 379 847 | −1264 | 754 | 379 337 | 379 386±7 | j | 379 393 | 379 390 | p |
| 48 | 404 808 | −1405 | 721 | 404 124 | 404 166±8 | j | 404 180 | 404 178 | p |
| 49 | 430 719 | −1556 | 693 | 429 856 | 429 884±9 | j | 429 913 | 429 912 | p |
| 50 | 457 640 | −1718 | 668 | 456 591 | 456 640±10 | j | 456 648 | 456 646 | p |
| 51 | 485 633 | −1889 | 647 | 484 391 | 484 522±12 | j | 484 448 | 484 449 | p |
| 52 | 514 762 | −2072 | 629 | 513 319 | | | 513 377 | 513 381 | p |
| 53 | 545 104 | −2266 | 614 | 543 452 | 543 508±15 | j | 543 510 | 543 520 | p |
| 54 | 576 714 | −2472 | 603 | 574 845 | 574 917±17 | j | 574 904 | 574 917 | p |
| 55 | 609 679 | −2689 | 594 | 607 584 | 607 652±18 | j | 607 643 | 607 659 | p |
| 56 | 644 064 | −2920 | 588 | 641 733 | 641 972±62 | k | 641 793 | 641 816 | p |

tions. The $E_{\rm rcor}$ for $U^{63+}$ we used were corrected for this difference.

## III. QUANTUM ELECTRODYNAMIC CORRECTIONS

As was mentioned earlier, screening of the self-energy is a source of major uncertainty in estimating QED corrections. There are three approximations commonly used in DF codes—to be referred to as the $\langle r \rangle$ method, the $\rho$ method, and the Welton method, for brevity.

### A. The $\langle r \rangle$ method

In this method, the expectation value of $r$ of a DF orbital is matched with that of a hydrogenic, point-nucleus ion with the same quantum numbers and an effective $Z_{\rm eff}$ whose $\langle r \rangle$ value is the same as the DF value. Then, Mohr's self-energy[9-11] is interpolated for this $Z_{\rm eff}$ to provide a "screened" self-energy for the DF orbital. This approximation fitted well the screened self-energy of the 1$s$ orbitals of neutral heavy elements calculated by

TABLE VII. (*Continued*).

| $Z$ | DF no QED | QED Welton | Relativistic correlation | Theory total | Experiment | Expt. Ref. | Present predictions | Other predictions | Predictions Ref. |
|---|---|---|---|---|---|---|---|---|---|
| 57 | 679 954 | −3163 | 586 | 677 377 | 677 780±100 | l | 677 438 | 677 465 | p |
| 58 | 717 427 | −3419 | 585 | 714 593 | | | 714 654 | 714 694 | p |
| 59 | 756 570 | −3689 | 588 | 753 468 | | | 753 530 | 753 585 | p |
| 60 | 797 469 | −3974 | 593 | 794 088 | 794 155±30 | j | 794 150 | 794 212 | p |
| 61 | 840 212 | −4274 | 601 | 836 539 | | | 836 601 | 836 687 | p |
| 62 | 884 893 | −4589 | 611 | 880 915 | 880 987±78 | m | 880 978 | 881 088 | p |
| 63 | 931 628 | −4921 | 624 | 927 331 | 927 470±300 | l | 927 394 | 927 523 | p |
| 64 | 980 499 | −5268 | 639 | 975 869 | 976 000±140 | m | 975 933 | 976 086 | p |
| 65 | 1 031 632 | −5633 | 656 | 1 026 655 | | | 1 026 719 | 1 026 905 | p |
| 66 | 1 085 137 | −6015 | 676 | 1 079 797 | 1 079 900±60 | j | 1 079 862 | 1 080 054 | p |
| 67 | 1 141 073 | −6414 | 697 | 1 135 355 | | | 1 135 421 | 1 135 680 | p |
| 68 | 1 199 686 | −6834 | 722 | 1 193 574 | 1 193 100±210 | k | 1 193 640 | 1193 887 | p |
| 69 | 1 260 965 | −7271 | 748 | 1 254 442 | | | 1 254 508 | 1 254 815 | p |
| 70 | 1 325 107 | −7729 | 776 | 1 318 155 | 1 318 500±300 | n | 1 318 222 | 1 318 583 | p |
| 71 | 1 392 259 | −8206 | 807 | 1 384 859 | | | 1 384 927 | 1 385 329 | p |
| 72 | 1 462 523 | −8705 | 840 | 1 454 658 | | | 1 454 726 | 1 455 180 | p |
| 73 | 1 536 090 | −9225 | 875 | 1 527 740 | 1 528 400±400 | n | 1 527 809 | 1 528 304 | p |
| 74 | 1 613 053 | −9767 | 912 | 1 604 199 | 1 605 000±390 | o | 1 604 268 | 1 604 853 | p |
| 75 | 1 693 665 | −10 333 | 951 | 1 684 284 | 1 685 600±430 | o | 1 684 354 | 1 684 948 | p |
| 76 | 1 778 012 | −10 921 | 993 | 1 768 084 | | | 1 768 154 | 1 768 847 | p |
| 77 | 1 866 294 | −11 533 | 1037 | 1 855 797 | | | 1 855 867 | 1 856 631 | p |
| 78 | 1 958 702 | −12 171 | 1082 | 1 947 613 | | | 1 947 684 | 1 948 482 | p |
| 79 | 2 055 416 | −12 834 | 1130 | 2 043 712 | 2 043 800±630 | p | 2 043 784 | 2 044 697 | p |
| 80 | 2 156 606 | −13 524 | 1181 | 2 144 264 | | | 2 144 336 | 2 145 278 | p |
| 81 | 2 262 554 | −14 241 | 1233 | 2 249 547 | | | 2 249 619 | 2 250 630 | p |
| 82 | 2 373 407 | −14 986 | 1288 | 2 359 709 | 2 360 400±840 | p | 2 359 782 | 2 360 829 | p |
| 83 | 2 489 404 | −15 760 | 1346 | 2 474 990 | 2 475 600±920 | q | 2 475 063 | 2 476 290 | p |
| 84 | 2 610 829 | −16 563 | 1405 | 2 595 671 | | | 2 595 745 | 2 597 065 | p |
| 85 | 2 737 812 | −17 396 | 1468 | 2 721 884 | | | 2 721 958 | 2 723 460 | p |
| 86 | 2 870 631 | −18 259 | 1532 | 2 853 904 | | | 2 853 979 | 2 855 430 | p |
| 87 | 3 009 740 | −19 155 | 1600 | 2 992 185 | | | 2 992 260 | 2 993 833 | p |
| 88 | 3 155 245 | −20 084 | 1670 | 3 136 831 | | | 3 136 907 | 3 138 535 | p |
| 89 | 3 307 549 | −21 047 | 1743 | 3 288 245 | | | 3 288 322 | 3 290 123 | p |
| 90 | 3 466 325 | −22 036 | 1819 | 3 446 108 | 3 449 500±1800 | q | 3 446 185 | 3 448 514 | p |
| 91 | 3 633 004 | −23 068 | 1897 | 3 611 833 | | | 3 611 911 | 3 614 414 | p |
| 92 | 3 807 141 | −24 133 | 1975 | 3 784 983 | 3 787 000±2000 | n | 3 785 061 | 3 787 735 | p |

[a]Table VI, footnote a.
[b]Table VI, footnote b.
[c]Table VI, footnote c.
[d]Table VI, footnote d.
[e]Table VI, footnote e.
[f]Table VI, footnote f.
[g]Table VI, footnote g.
[h]Table VI, footnote h.
[i]Table VI, footnote i.
[j]J. Sugar *et al.*, Ref. 49.
[k]J. Reader and G. Luther, Ref. 43.
[l]J. F. Seely *et al.*, Ref. 16.
[m]G. A. Doschek *et al.*, Ref. 45.
[n]D. R. Kania *et al.*, Ref. 48.
[o]J. F. Seely, C. M. Brown, and W. E. Behring, Ref. 46.
[p]J. F. Seely, C. M. Brown, and U. Feldman, Ref. 47.
[q]J. F. Seely *et al.*, Ref. 44.

Desiderio and Johnson[25] and Cheng and Johnson.[26] These two calculations and a recent theoretical work by Indelicato and Mohr,[27] which introduces screening as a perturbation to the nuclear Coulomb field, remain the only treatment of the self-energy screening based on a QED procedure while using approximate wave functions for a many-electron atom. As is shown later, the $\langle r \rangle$ method, which is the default in the DF codes by Grant *et al.*,[1,2] still leaves out a significant number of $Z$-dependent terms.

### B. The $\rho$ method

In this approximation, the square of a DF orbital $\psi_{\mathrm{DF}}$ is integrated from the origin to a short distance $r_0$, usually a fraction of the Compton wavelength $\lambda_0$ ($\sim$ Bohr radius/137), and the integral is compared to a similar integral calculated with a point-nucleus, hydrogenic wave function $\psi_{\mathrm{hyd}}$ with the same quantum numbers:

$$\rho=\int_0^{r_0}|\psi_{\mathrm{DF}}|^2 d\tau \Big/ \int_0^{r_0}|\psi_{\mathrm{hyd}}|^2 d\tau \; . \tag{9}$$

This ratio $\rho$ ($\leq 1$) is then used to scale Mohr's hydrogenic self-energy.[9–11] We chose $r_0=0.3\lambda_0$ because this value reproduced known inner-shell x-ray wavelengths well, although *transition energies* are rather insensitive to the choice of $r_0$.

### C. The Welton method

Welton[28] proposed to treat the self-energy as fluctuations in the classical trajectory of a bound electron due to the nuclear field. This method uses an effective potential to correct the lowest-order contribution (in $Z\alpha$, where $\alpha$ is the fine-structure constant) to the one-electron self-energy from two-electron interaction by adjusting the potential for the changes in the electronic charge density at the nucleus. This potential can be derived, for example, from Welton's semiclassical arguments.[28] It has been shown by Dupont-Roc, Fabre, and Cohen-Tannoudji[29] that for self-energy, the effective Hamiltonian based on the Welton model leads to the proper nonrelativistic limit.

For an $ns$ orbital, this method leads to a screening correction

$$\delta\varepsilon_{ns}=\frac{\langle ns|\nabla^2 U_N|ns\rangle_{\mathrm{DF}}}{\langle ns|\nabla^2 U_N|ns\rangle_{\mathrm{hyd}}}\varepsilon_{ns} \; , \tag{10}$$

where the subscript hyd stands for a hydrogenic wave function, $U_N$ is the nuclear potential, and $\varepsilon_{ns}$ is Mohr's point-nucleus, hydrogenic self-energy[9–11] corrected for finite nuclear-size effects.[18] For orbitals with $l \geq 1$, the above correction, which is proportional to the square of the wave function at the origin, vanishes, and the $g-2$ correction provides the leading screening correction

$$\delta\varepsilon_{nl}=\frac{\langle nl|\beta\boldsymbol{\alpha}\cdot\mathbf{E}|nl\rangle_{\mathrm{DF}}}{\langle nl|\beta\boldsymbol{\alpha}\cdot\mathbf{E}|nl\rangle_{\mathrm{hyd}}}\varepsilon_{nl} \quad \text{for } l \geq 1 \; , \tag{11}$$

where $\mathbf{E}$ is the nuclear electric field. This approximation was checked against experiments and was found to provide reasonable estimates.[4,5,30,31]

The $\rho$ and Welton methods produce very similar numerical results on *transition energies* for low-$Z$ ions, but they begin to depart from each other at $Z\sim 80$ and above. Of the three approximations presented above, the $\langle r \rangle$ method was found to lead to transition energies with the poorest agreement with known experimental data, particularly for high-$Z$ ions, in many comparisons we have made. The predictions by Seely *et al.*[14–17] are based on QED corrections using the $\langle r \rangle$ approximation. In addition to the hydrogenic self-energies for $n=1$ and 2 by Mohr,[9–11] preliminary values for $n=3$–5 and $|\kappa|=1$ and 2, where $\kappa$ is the Dirac quantum number, have been reported recently.[32] We used these new hydrogenic self-energies for $n=3$ and 4 instead of scaling $n=2$ values by $n^{-3}$, as is commonly done. The hydrogenic self-energy for $\kappa=-3$ ($=d_{5/2}$) is not available. We used the $3d_{5/2}$ result for $Z=0$ by Klarsfeld and Maquet[33] after scaling it by $(Z\alpha)^4$.

For the vacuum polarization, we also included corrections[34–36] of the order of $\alpha$ and $(Z\alpha)^2$ compared to the Uehling potential, but contributions from these terms are smaller than the uncertainties in the screening of the self-energy. The sum of the "screened" self-energy based on the $\rho$ or Welton method and the above-mentioned vacuum polarization corrections is listed in Tables II–VII.

## IV. COMPARISON WITH EXPERIMENTAL DATA

A large collection of experimental data is available for the resonance transitions reported in this article, mostly for ions with low to moderate $Z$. Since most experimental values are for transitions $ns$-$np_{1/2}$ and $ns$-$np_{3/2}$, we concentrate on comparing theory and experiment for these transitions.

Both theoretical results and experimental data are listed in Tables II–VII. In these tables, the first column lists the atomic number, the column marked "DF no QED" lists theoretical transition energies obtained from single-configuration *DF* wave functions (solutions of $H_0$) and the energy-dependent Breit operator, Eq. (7), without the Coulomb repulsion (which is included in $H_0$). The column marked "QED" lists QED corrections with the self-energy screened by either the $\rho$ or Welton method as noted. The relativistic correlation $E_{\mathrm{rcor}}$ defined by Eq. (1) is listed in the column marked "Relativistic correlation" while the sum of the second, third, and fourth columns is listed in the column marked "Theory total."

Experimental values and their sources are listed in the columns marked "Experiment" and "Expt. Ref." respectively. Our predicted values, which are based on our "Theory total" minus the difference between the theory and experiment after adjusting the difference to have "smoothly varying" first and second derivatives, are listed in the column marked "Present predictions" Standard fitting methods such as the least-square fitting or a simple polynomial do not work well in this case because we are interested in extrapolating the fitted results to higher $Z$, for which either experimental data are inaccurate or unavailable. Standard methods tend to introduce higher-order derivatives that eventually render extrapolations useless for $Z$ too far from the last data point used. The last two columns list predictions by others and their sources. The difference between our theoretical transition energies, "Theory total," and experimental values are plotted in Figs. 4–9.

### A. Li isoelectronic sequence

It is difficult to decide any preference among the three "screening" schemes based on the comparison with the experimental data for $Z \leq 42$ (see Figs. 4 and 5). The experimental data—which are included in Tables II and III—seem to have more scatter for heavier ions ($Z > 20$) than lighter ones, particularly for the $2p_{3/2}$ transition for $Z > 30$. The close agreement between the values based on the $\rho$ and Welton methods shown in Figs. 4 and 5 also holds for Na- and Cu-like ions. The wavelengths for the $2p_{1/2}$ and $2p_{3/2}$ transitions of $Xe^{51+}$ were measured by Martin *et al.* using the beam-foil method[37] (Tables II and III). Their transition energies are too large to be compatible with the trend seen in the experimental data for $Z \leq 42$, though the large uncertainty in their $2p_{3/2}$ result encompasses our theoretical and predicted values.

Recently Schweppe *et al.*[38] reported an experimental value for the $2p_{1/2}$ transition in $U^{89+}$. Our result with the $\rho$ method, 280.68 eV, comes closest to the experimental value, 280.59±0.10 eV (see Fig. 6). There are, however, several higher-order corrections that are missing in our theory, such as the nuclear polarization[39] and the exchange of two virtual photons between bound electrons, which are expected to be of the order of a few tenths of an electron volt. A simple change in the rms radius of the uranium nucleus—from 5.751 fermi used in Ref. 18 to our value of 5.863 fermi—reduced the transition energies of $U^{89+}$ by about 1 eV. Recently, Blundell, Johnson, and Sapirstein[40] recalculated the $2p_{1/2}$ transition energy using the MBPT and a nonspherical nuclear charge distribution; their value is 281.023 eV, which includes an empirical estimate of the "screened" QED correction of −41.225 eV to be compared with our value of −41.574 eV. This QED correction was also estimated by Indelicato and Desclaux[5] using the Welton method with extensive MCDF wave functions and a nonspherical nuclear charge distribution; their "screened" QED correction is −41.100 eV and the $2p_{1/2}$ transition energy is 281.6±0.9 eV. Although none of these estimates can be justified from a rigorous QED procedure, it is clear that the uncertainty in QED corrections in this case could be as

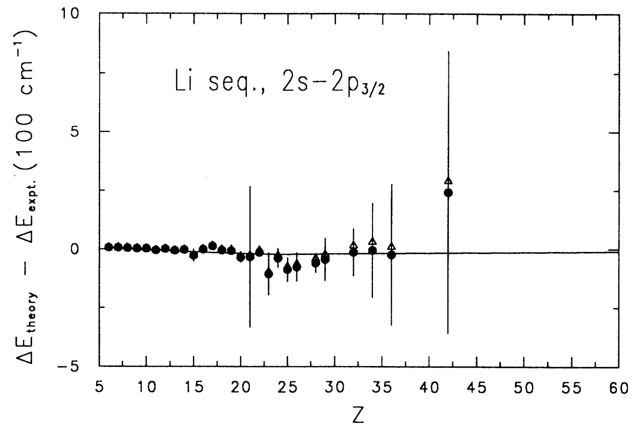


FIG. 5. Difference between theory and experiment for the $2s \rightarrow 2p_{3/2}$ transition energies $\Delta E$ of Li-like ions. The solid curve is the smoothed difference that was used to obtain our predicted values in Table III. See Fig. 4 caption for other explanations.

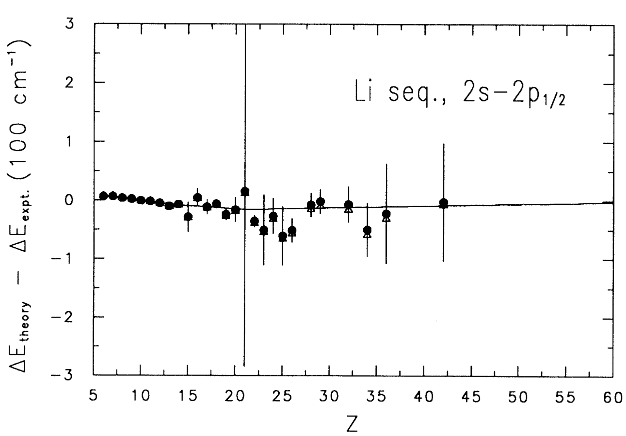


FIG. 4. Difference between theory and experiment for the $2s \rightarrow 2p_{1/2}$ transition energies $\Delta E$ of Li-like ions. Filled circles used theoretical values based on the $\rho$ method for QED screening, while the triangles used theoretical values based on the Welton method. The solid curve is the smoothed difference that was used to obtain our predicted values in Table II. Error bars attached to the circles represent experimental uncertainties only. The same error bars also apply to the triangles. Experimental uncertainties for the ions with no visible error bars are smaller than the size of the circles.

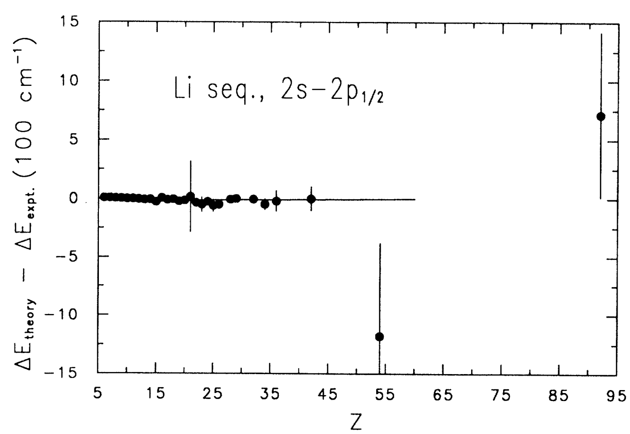


FIG. 6. Difference between theory and experiment for the $2s \rightarrow 2p_{1/2}$ transition energies $\Delta E$ of Li-like ions. Filled circles used theoretical values based on the $\rho$ method for QED screening. Experimental data for $Xe^{51+}$ and $U^{89+}$ were measured using the beam-foil method (Refs. 37 and 38). See Fig. 4 caption for other explanations.

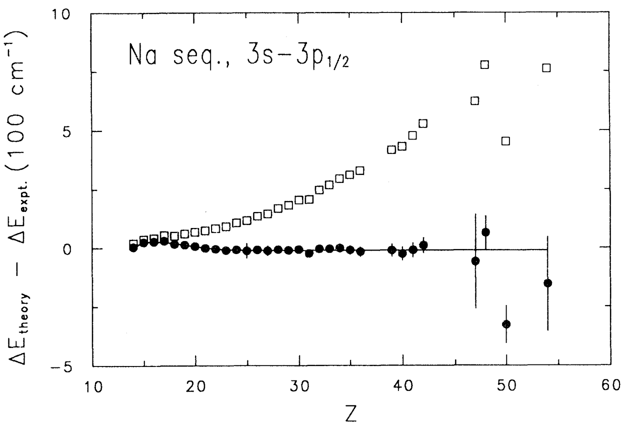


FIG. 7. Differece between theory and experiment for the $3s \rightarrow 3p_{1/2}$ transition energies $\Delta E$ of Na-like ions. Filled circles used theoretical values based on the Welton method for QED screening, while the square used theoretical values based on the $\langle r \rangle$ method. The solid curve is the smoothed difference that was used to obtain our predicted values in Table IV. See Fig. 4 caption for other explanations.

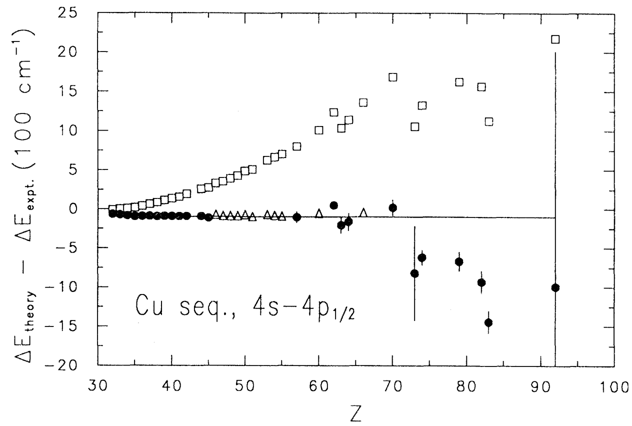


FIG. 9. Difference between theory and experiment for the $4s \rightarrow 4p_{1/2}$ transition energies $\Delta E$ of Cu-like ions. Filled circles used theoretical values based on the Welton method for QED screening, while the squares used theoretical values based on the $\langle r \rangle$ method. The solid curve is the smoothed difference that was used to obtain our predicted values in Table VI. Triangles represent the difference between theoretical values based on the Welton method and experimental data from the Texas experimental tokamak (TEXT) (Ref. 49). Experimental data for $Z \geq 70$ used spectra from laser-generated plasmas.

much as $\pm 0.5$ eV, or about $\pm 4000$ cm$^{-1}$.

As is shown in Fig. 6, the $2p_{1/2}$ transition energy of $Xe^{51+}$ by Martin *et al.*[37] is larger than our theoretical value, while that of $U^{89+}$ by Schweppe *et al.*[38] is smaller than ours. The trend apparent in the data for $Z \leq 42$ in Fig. 6 seems to be more compatible with the $U^{89+}$ result than the $Xe^{51+}$ value.

Since there are no experimental data for $54 < Z < 92$, it is difficult for us to reliably extend the trend observed at lower $Z$ in the difference between theory and experiment to $Z \sim 50$ and above. Experimental data to fill this gap are sorely needed, not only to establish the systematics of missing terms in the theory, but also because more rigorous theoretical results are likely to be first obtained for ions with a few bound electrons. Experimental data with a relative accuracy of one part in $10^4$ or better would be most useful.

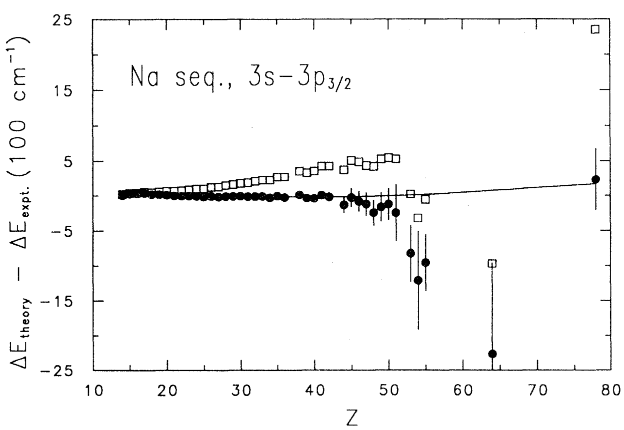


FIG. 8. Difference between theory and experiment for the $3s \rightarrow 3p_{3/2}$ transition energies $\Delta E$ of Na-like ions. The solid curve is the smoothed difference that was used to obtain our predicted values in Table V. The data for $Pt^{67+}$ was measured in an EBIT (Ref. 42), while other experimental data above $Z = 50$ used spectra from laser-generated plasmas. See the captions for Figs. 4 and 7 for other explanations.

The difference between our theoretical transition energies ("Theory total") and our predicted values for some ions are plotted as solid curves in Figs. 4 and 5 and are listed in Tables II and III. We note that the relatively large uncertainty of $\pm 300$ cm$^{-1}$ in the expermental $2s$-$2p$ transition energies listed[41] for $Sc^{18+}$ is too pessimistic–the actual uncertainty is more likely to be $\pm 40$ cm$^{-1}$. The transition energies predicted by Seely[14] have rapid changes in $Z$ dependence between $Z = 40$ and 50, a trend not supported by the comparison of our results with experiment, shown in Figs. 4 and 5.

### B. Na isoelectric sequence

The theoretical results and experimental data are presented in Tables IV and V. For Na-like ions with $Z \leq 40$, theoretical transition energies based on the $\rho$ and Welton methods agree with experiment within 100 cm$^{-1}$ for both the $3p_{1/2}$ and $3p_{3/2}$ transitions. However, transition energies based on the $\langle r \rangle$ method not only differ from the experiment by several hundred cm$^{-1}$ but also the difference steadily increases with $Z$, although the percentage difference does not increase as much (Figs. 7 and 8). The rapidly growing gaps between the theory based on the Welton method and experiment for $50 \geq Z \geq 70$ in Figs. 7 and 8 are likely to be experimental artifacts because we do not expect terms missing in our theory to have such a sudden strong $Z$ dependence there.

Cowan *et al.* recently measured[42] the wavelength for the $3p_{3/2}$ transition of $Pt^{67+}$ using an electron beam ion trap (EBIT). Their value is in close agreement with our values based on either the $\rho$ or Welton method but not with the value from the $\langle r \rangle$ method. This agreement is consistent with the trend seen in Fig. 8 for $Z<45$, suggesting that the experimental transition energies for ions between $Z=52$ and 64 are probably too large. We note that the experimental transition energies obtained from spectra of laser-generated plasmas tend to be too large (i.e., blue-shifted) compared to the trend observed for ions with lower $Z$. We will return to this point again for Cu-like ions.

The difference between our theoretical transition energies and our predicted values are plotted as solid curves in Figs. 7 and 8 and are compared to those predicted by Seely *et al.*[17] in Tables IV and V. The energies for the $3p_{1/2}$ transition predicted by Seely *et al.* are smaller than our theory for $Z>80$, while those for the $3p_{3/2}$ transition continue to be larger than our theory. There is no apparent theoretical reason to expect these opposite trends.

### C. Cu isoelectronic sequence

This is a sequence for which experimental values are available all the way to $U^{63+}$. Our theoretical values are presented in Tables VI and VII. Unlike the QED corrections based on the Welton or $\rho$ method, the difference between our theory with the $\langle r \rangle$ method and experiment rises rapidly to 2000 $cm^{-1}$ or more for $Z>70$, as is shown in Figs. 9 and 10. Also, the scatter and trend seen in the experimental data for $Z>70$ indicate that such data have larger uncertainties in magnitude—though relative accuracy deteriorates slowly—for both the $4p_{1/2}$ and $4p_{3/2}$ transitions. Experimental values for $55<Z<92$ obtained from spectra of laser-generated plasmas[43–48] exhibit a tendency for the difference between theory and experiment for the $4p_{3/2}$ transition (Fig. 10) to be increasingly negative (i.e., experimental energies are too high) from $Z\sim55$. More recent experimental values[49] for ions with $46<Z<70$ generated in the Texas experimental tokamak (TEXT) are in excellent agreement

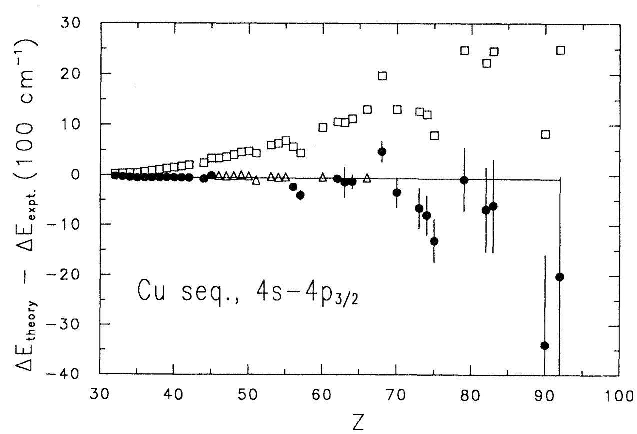


FIG. 10. Difference between theory and experiment for the $4s\rightarrow4p_{3/2}$ transition energies $\Delta E$ of Cu-like ions. The solid curve is the smoothed difference that was used to obtain our predicted values in Table VII. See Fig. 9 caption for other explanations.

with our values based on the Welton and $\rho$ methods, clearly establishing a trend with almost no $Z$ dependence (see triangles in Figs. 9 and 10). It is likely that the existing experimental energies from spectra of laser-generated plasmas in general are too high, as is the case for the Na-like ions. The data from laser-generated plasmas seem to have systematic problems that make the measured transition energies too high.

Our predicted transition energies are plotted as solid curves in Figs. 9 and 10 and are compared to those predicted by Seely, Brown, and Feldman[47] in Tables VI and VII. We emphasize, however, that the correct $Z$ dependence of the solid curves in Figs. 9 and 10 for $Z>80$ is unlikely to be as simple as we have assumed, since we expect higher-order relativistic corrections omitted in our theory to grow rapidly beyond $Z\sim80$. The energies predicted by Seely *et al.* for both the $4p_{1/2}$ and $4p_{3/2}$ transitions continue to be larger than our theoretical values, reaching differences of 1500–2700 $cm^{-1}$, or 0.1–0.02 Å in wavelength for $U^{+63}$. Some of these differences can be attributed to the use of different nuclear parameters in the DF codes[1,2] used by Seely *et al.*[14–17] and us,[3,4] but most of the difference is due to the different $Z$ dependence of the QED corrections in the DF codes.

## V. CONCLUSION

We have shown that the theoretical transition energies based on the $\rho$ and Welton methods to "screen" the self-energy agree well with experimental data for ions with net charges of about 40 or less, while the theoretical values based on the $\langle r \rangle$ method tend to depart from experiment almost linearly with $Z$. Moreover, we find the experimental transition energies from spectra of laser-generated plasmas have a tendency to be too high at $Z>70$. One possibility is that the red wing of a line profile is severely attenuated by self-absorption and other plasma effects, thus shifting the apparent peak toward the blue wing. To establish a clear $Z$ dependence in the difference between theory and experiment and verify the data collected by using laser-generated plasmas, more experimental data are needed for ions with $Z>70$, obtained from sources other than laser-generated plasmas. Heavy Cu-like ions can be produced by existing ion traps or large tokamaks, and wavelength measurements with such sources with relative uncertainties less than one part in $10^4$ are highly desirable. In addition, accurate experimental values for high-$Z$ ($50<Z<92$) Li-like ions are indispensable for testing future theories for the "screening" of the self-energy and other higher-order relativistic effects based on a rigorous QED formalism. Meanwhile, we offer our predicted transition energies in Tables II–VII to serve as "road signs" for experimentalists.

After our manuscript was submitted, Knize[50] published data on selected Li-like ions with $24\leq Z\leq34$, which were reinterpretations of the experiments reported by Hinnov, Denne, and co-workers.[51] Some of the reinterpreted data agree better with our predicted values and some agree worse than that reported earlier, indicating no clear preference for either set of transition energies.

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*Permanent address: Korea Atomic Energy Research Institute, Taejon 302-353, Korea.

†Present address: Laboratoire de Physique Atomique et Nucléaire, Université P&M Curie, 75252 Paris CEDEX 05, France.



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