BREIT AND QED EFFECTS IN SPECTRA OF THE $4s^2\,{}^1S_0$–$4s4p\,{}^3P_1,{}^1P_1$ TRANSITIONS IN THE Zn SEQUENCE

L. H. Hao*, J. J. Liu

School of Electronic Communication Engineering, Hainan Tropical Ocean University, Sanya, Hainan, 572022, China; e-mail: lhhao_1020@163.com

The $4s^2$–$4s4p$ E_1 transitions for Zn-like ions from Z in the range 30–92 are calculated using the multi-configuration Dirac–Hartree–Fock (MCDHF) method. The results obtained are in good agreement with other theoretical and experimental data and demonstrate the applicability of this method to high-precision atomic structure calculations of both few-electron systems and large atomic systems, such as Zn-like ions, along the entire isoelectronic sequence. We also report herein the calculations of many-electron quantum electrodynamic (QED) and Breit effects for the $^3P_0$, $^3P_1$, $^3P_2$, and $^1P_1$ states for all Zn-like ions in the range $30 \le Z \le 100$.

Keywords: *core-valence correlation, valence-valence correlation, energy levels, transition.*

ЭФФЕКТЫ БРЕЙТА И КВАНТОВОЙ ЭЛЕКТРОДИНАМИЧЕСКОЙ КОРРЕКЦИИ В ПЕРЕХОДАХ $4s^2\,{}^1S_0$–$4s4p\,{}^3P_1,{}^1P_1$ Zn-ПОДОБНЫХ ИОНОВ

L. H. Hao*, J. J. Liu

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Школа инженерных коммуникаций, Хайнанский университет тропического океана, Санья, провинция Хайнань, 572022, Китай; e-mail: lhhao_1020@163.com

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Методом Дирака–Хартри–Фока рассчитаны переходы $4s^2$–$4s4p$ E_1 для Zn-подобных ионов при Z = 30–92. Полученные результаты хорошо согласуются с известными данными и демонстрируют полезность предлагаемого метода для высокоточных расчетов атомной структуры не только малоэлектронных систем, но и больших атомных систем, таких как вся изоэлектронная последовательность Zn-подобных ионов. Приведены расчеты многоэлектронных квантовых электродинамических эффектов и эффектов Брейта для состояний $^3P_0$, $^3P_1$, $^3P_2$ и $^1P_1$ для всех Zn-подобных ионов в диапазоне $30 \le Z \le 100$.

***Ключевые слова*:** *корреляция ядро–валентность, корреляция валентность–валентность, энергия уровня, переход.*

Introduction. For high-precision atomic structure calculations, two aspects of multicharged ions have always been the focus of theoretical investigations. The first is the relativistic electron–electron correlation energy, whereas the other is the quantum electrodynamic (QED) correction. Theoretical studies of two-valence electron ions along the zinc isoelectronic sequence have been published by multiple authors. Fine-structure energy levels, wavelengths, and transition rates for Z from 48 to 54 [1], 55 to 69 [2], and 70 to 92 [3] were presented using the multi-configuration Dirac–Hartree–Fock (MCDHF) method. Transition rates, oscillator strengths, and line strengths were calculated for electric-dipole (E_1) transitions between the even-parity

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$4s^2$, $4p^2$, $4s4d$, $4d^2$, $4p4f$, and $4f^2$ states and the odd-parity $4s4p$, $4s4f$, $4p4d$, and $4d4f$ states in Zn-like ions with the nuclear charges Z ranging from 32 to 100 using the relativistic many-body perturbation theory (RMBPT) by Safronova and Safronova [4]. The $4s4p$ excitation energies and $4s^2$–$4s4p$ E_1 transitions of Zn-like ions from $Z = 30$ to 92 were shown using the relativistic configuration interaction (RCI) by Chen and Cheng [5]. Many-electron quantum electrodynamic (QED) effects for the $4s^2\,{}^1S_0$–$4s4p\,{}^1P_1$ transition in high-Z Zn-like ions with Z = 70, 74, 76, 79, 82, 83, 90, and 92 were reported using the relativistic many-body perturbation theory (RMBPT) by Blundell [6]. The spin-forbidden transition $4s^2\,{}^1S_0$–$4s4p\,{}^3P_1$ and the hyperfine-induced (HPF) transition $4s^2\,{}^1S_0$–$4s4p\,{}^3P_0$ for ions between $Z = 30$ (Zn) and $Z = 47$ (Ag) were reported using the multiconfiguration Dirac–Fock (MCDF) method by Liu et al. [7]. High-accuracy calculations of term energies and wavelengths of resonance lines in Zn-like ions from $Z = 30$ to 92 were performed using the relativistic multi-reference Møller-Plesset (MR-MP) perturbation theory by Vilkas and Ishikawa [8]. Energy levels and radiative transition probabilities were presented for the $n = 4$, $\Delta n = 0$ transitions of the ions Rb VIII to Xe XXV along the zinc isoelectronic sequence using the relativistic Hartree–Fock method by Biémont et al. [9]. Excitation energies and oscillator strengths from the ${}^1S_0$ ground state to the first ${}^3P_1$ and ${}^1P_1$ excited states of Zn-like ions were calculated using the multiconfiguration relativistic random-phase approximation (MCRRPA), including excitation channels from the core electrons, by Chou et al. [10]. Isoelectronic studies of the $4s4p\,{}^3P_J$ energy levels in the Zn sequence from Z = 30 to 56 were shown using the semiempirical parametrization by Curtis [11].

A large number of experimental studies of the energies of $n = 4$ states have been made. For example, the extreme ultraviolet resonance lines of Zn-like ions of Yb, W, Au, Pb, Th, U [12], and Ba [13] were observed using an electron-beam ion trap and a flat-field spectrometer. Accurate wavelengths for resonance lines of the Cu I and Zn I isoelectronic sequences for Pd ($Z = 46$) to Dy ($Z = 66$) were identified using the TEXT tokamak at the Fusion Research Center in Austin, Texas by Sugar et al. [14]. Spectra of the Zn-like ions Rb VIII, Sr IX, Y X, Zr XI, Nb XII, and Mo XIII were excited with sparks and laser-produced plasmas and observed with normal- and grazing-incidence vacuum spectrographs by Litzén and Reader [15]. Spectroscopic measurements of highly-charged Zn-like Sm and Er [16], and Ga [17] were performed at the National Institute of Standards and Technology (NIST) using an electron-beam ion trap (EBIT). The extreme ultraviolet radiation emitted from highly-charged Rb-like Dy^{29+} to Ni-like Dy^{38+} ions was measured at the National Institute of Standards and Technology using an electron-beam ion trap (EBIT) by Kilbane et al. [18]. Zn-like ions of elements from Yb ($Z = 70$) to U ($Z = 92$) in an electron-beam ion trap were observed by Träbert et al. [19]. The extreme ultraviolet spectra of highly-charged Ha, Ta, Au [20], and Pt [21] were produced with an electron-beam ion trap (EBIT) at the National Institute of Standards and Technology, and their proper identification is important for plasma diagnostics in astrophysics as well as in fusion energy research.

Much work has been done for providing more accurate theoretical results comparable to experimental results, but for Z in the range from 30 to 100, the electron–electron correlation and QED problems still need further investigation. Precise measurements of transition energies in mid- to high-Z many-electron ions are particularly challenging to theorists attempting to develop such relativistic approaches. For the excitation energies of the $4s4p\,{}^3P_1$ and ${}^1P_1$ states from the $4s^2\,{}^1S_0$ ground state of Zn-like ions of experimental error can require inclusion not only of the more traditional effects of relativistic many-electron systems, such as the use of the Coulomb and Breit interactions within a Dirac formalism for the electron, but also field-theoretic effects such as the QED Corrections, which are dominated by radiative corrections from electron self-energies and vacuum polarizations. Accurate relativistic atomic structure [22] calculations are thus crucial to the testing of strong-field QED effects where screening and corrections can be important.

In this paper, in addition to the well-known problems arising from the necessity of considering some of the core electrons within the atom and the effects of electron correlation, relativity has to be taken into account for accurate calculations. The calculation methods used are based on the MCDHF approach, as represented by GRASPVU (a general-purpose relativistic atomic structure package developed at Vanderbilt University). It is a modification and extension of the GRASP92 codes of Parpia et al. [23]. Additionally, we include both Coulomb and Breit contributions in the Breit-Dirac-Fock potential and then treat the residual Breit and Coulomb interactions perturbatively. QED corrections are made by a combination of phenomenological and *ab initio* methods. In the following section, we give a brief description of this method. Our MCDHF calculations of Zn-like ions will then be presented and compared with other theories and with the experiment.

Theory. The calculations have been performed using the fully relativistic multiconfiguration Dirac–Hartree–Fock (MCDHF) approach with the MCDFGME program [22] of Desclaux and Indelicato. The theoretical basis of our present computational approach has been widely discussed elsewhere [24–26], so we do not repeat it. We made two calculations, one with the valance-valence (VV) correlation and one including

the core-valance (CV) correlation. Zn-like configurations consist of core and valence electrons. The core is defined as a Ni-like ground state configuration containing the closed 1*s*, 2*s*, 2*p*, 3*s*, 3*p*, and 3*d* subshells, and the valence electrons come from the 4*s* and 4*p* subshells. Our calculations start from the reference configurations $4s^2$ for the ground state and the 4*s*4*p* for the excited states. For simplicity, the Ni-like core is not listed here. In our basic CI expansions, we include single and double excitations from these reference configurations. We considered the active space consisting of all the orbitals in the set with the principal quantum number $n \le 6$, and only $l \le 4$ were included with $n = 7$. CV contributions from the inner core electrons are small and calculated separately, as corrections with smaller basis sets of $n \le 5$ and $l \le 3$ for the 2*s*, 2*p*, 3*s* core and 4*s*, 4*p* valence electrons. The remaining CV excitations from the 1s subshell and core-core (CC) excitations are found to contribute less than 0.01 eV to the excitation energies and are neglected here. We start by optimizing all the orbitals on the full active space of CV correlation CSFs (including all *l* values): $3d^{10}\{4\}^2$.

When deriving the specific form of MCDHF equations to solve, we start by applying the variational principal to a functional of energies. It is common to use the extended optimal level (EOL) technique, where a linear combination of the most important energy levels is used. In the next step we generated all CSFs of the form $3d^9\{3,4\}^1\{4,5\}^1\{3,4,5\}^1$ with the constraint of only orbitals with $l \le 3$.

Finally, we include more VV by adding to the restricted active spaces all CSFs of the form $3d^{10}\{4,5\}^1\{4,5,6\}^1$ and $3d^{10}\{4,5\}^1\{4,5,6,7s,7p,7d,7f\}^1$ with $l \ne 3$, and optimize the orbitals 5*f*, 6*s*, 6*p*, 6*d*, 6*f*, 6*g*, 7*s*, 7*p*, 7*d*, and 7*f*.

In the subsequent relativistic configuration interaction (CI) calculations, the transverse photon or Breit interaction

$$H_{\text{Breit}} = -\sum_{i<j}^{N}\left[\frac{\alpha_i\alpha_j}{2r_{ij}} + \frac{(\alpha_i r_{ij})(\alpha_j r_{ij})}{2r_{ij}^3}\right] \quad (1)$$

may be included in the Hamiltonian [27]. The contributions from QED (self-energy and vacuum polarization) corrections have also been taken into account in our calculations. The formulas for self-energy and vacuum polarization can be found elsewhere [27]. The transverse photon or Breit interaction as well as vacuum polarization, self-energy, and finite nuclear mass corrections may be added to the Dirac–Coulomb Hamiltonian (for a different approach in which the Breit interaction and QED effects are treated self-consistently, we refer to the MCDFGME code by Desclaux and Indelicato [23]). In this implementation of the RCI program, an iterative Davidson method was used together with a spare matrix representation allowing for large expansions.

Results and discussions. In Table 1, we compare our results for transition wavelengths λ of Zn-like ions with nuclear charges *Z* ranging from 30 to 92. Also, some available theoretical and experimental results are tabulated for comparison. Our MCDHF values are compared with the theoretical values from [2, 4, 8] and the experimental results from [12, 28–30]. We see that in two transitions the CV+VV correlation results are very close to the experimental results in the difference range from 0 to 0.345%. Also, our calculations results are also generally in good agreement with the MBPT results from [2, 4, 8] and data including the CV correlation by MCDHF calculations for mid- to high-*Z* ions (Z = 54–92), the difference being about 0.006–1.076% for most cases. In general, our results agree better with the experiment than the RMBPT results of [4, 8] in this part of the isoelectronic sequence, except the results for the $^1P_1$ state with $Z = 82$ and 90. This may be because we have included a limited number of configurations in our calculation. In our previous work and paper [5], we find that the $n \ge 5$ layer electrons have a great influence on the E_1 transitions. In the work presented here, we have increased the number of configurations included to $n = 7$ or the size of the orbital set in a systematic manner until good convergence was obtained.

The dramatic improvement in the MCDHF results at high *Z* comes from two changes: better QED (SE and VP) calculations and Breit corrections. In Table 2, we compare QED energies calculated here with the results from [2, 5, 6, 31]. Our QED energies are slightly closer to Blundell's revised results [31], with differences ranging from 0.001 to 0.016 eV. In view of the difficulty of these QED calculations, the agreement among theories is quite reasonable. We know that the QED calculation and Breit corrections contributions should be taken into account.

The details of QED calculation and Breit corrections calculations can be found in Fig. 1. As an illustration of contributions to the total energy, we show in Fig. 1 the breakdowns of Breit and QED (SE and VP) excitation energies for 34 Zn-like ions for the $^3P_0$, $^3P_1$, $^3P_2$, and $^1P_1$ states. Figure 1 shows that Breit and QED corrections increase rapidly with *Z* and become more important at high *Z*. We see that for the light ions ($Z \le 40$) these corrections are very small at the existing level of accuracy of treating electron correlations. However, for mid- to high-*Z* ions these corrections become essential and somewhat improve the final accu-

TABLE 1. Computed and Measured Wavelengths (Å) for the $4s^2\ ^1S_0$–$4s4p\ ^{3,1}P_1$ Transitions in Zn-Like Ions

Z	$4s^2\ ^1S_0$–$4s4p\ ^3P_1$			$4s^2\ ^1S_0$–$4s4p\ ^1P_1$		
	MCDHF (CV+VV)	Theory	Experiment	MCDHF (CV+VV)	Theory	Experiment
30	3092.326			2145.571		
32	1601.501		1600.09 [28]	1088.348		1088.45 [28]
34	1094.212		1094.7 [28]	759.313		759.1 [28]
36	831.986		832.268 [28]	585.525		585.357 [28]
38	670.362		671.017 [28]	475.528		475.336 [28]
40	560.337			398.488		
42	480.491		480.820 [28]	341.005		340.909 [28]
44	419.601			296.162		
46	371.825			260.005		
48	333.286			230.088		
50	301.520			204.831		
52	274.919			183.188		
54	252.316		252.473 [28]	164.415	164.520 [8]	164.412 [28]
56	232.870	233.126 [2]		147.980	148.090 [8]	147.47 [29]
58	215.990	216.189 [2]		133.475		
60	201.170	201.337 [2]		120.594	120.665 [8]	120.58 [29]
62	188.065	188.204 [2]		109.111	109.131 [8]	109.11 [29]
64	176.411	176.505 [2]		98.848	98.818 [8]	98.87 [29]
66	165.911	166.008 [2]		89.612	89.586 [8]	89.65 [29]
68	156.441	156.535 [2]		81.298	81.293 [8]	81.33 [29]
70	147.848	147.949 [4]	148.170 [30]	73.806	73.824 [8]	73.8070(66) [12]
72	140.018	140.303 [4]	140.048 [30]	67.032	66.750 [4]	67.015 [30]
74	132.821	132.928 [4]		60.929	60.963 [8]	60.9300(54) [12]
76	126.218	126.314 [4]		55.394	55.422 [8]	55.384 [30]
78	120.112	120.212 [4]		50.379	50.360 [4]	
80	114.459	114.563 [4]		45.843	45.819 [4]	
82	109.182	109.309 [4]		41.723	41.720 [8]	41.7185(45) [12]
84	104.281	104.417 [4]		37.989	37.966 [4]	
86	99.718	99.866 [4]		34.596	34.577 [4]	
88	95.432	95.596 [4]		31.518	31.498 [4]	
90	91.458	91.602 [4]		28.725	28.7234 [8]	28.7227(67) [12]
92	87.705	87.860 [4]		26.187	26.1838 [8]	26.1868(36) [12]

TABLE 2. QED Corrections (eV) to the $^1P_1$ Excitation Energies of Zn-Like Ions

Z	This work	[31]	[5]	[6]	[2]
52	–0.263	–0.279	–0.255		–0.252
54	–0.315	–0.328	–0.305		–0.304
60	–0.515	–0.516	–0.491		
64	–0.680	–0.678	–0.651		
66	–0.771	–0.772	–0.744		
68	–0.882	–0.875	–0.846		
70	–0.991	–0.988	–0.958	–0.939	
74	–1.252	–1.249	–1.213	–1.192	
76	–1.405	–1.397	–1.358	–1.334	
82	–1.932	–1.922	–1.872	–1.839	
90	–2.860	–2.852	–2.774	–2.729	
92	–3.140	–3.132	–3.045	–2.994	

racy. As seen in Fig. 1, with the increasing of the nuclear charge number, the vacuum polarization energy increases whereas the self-energy increases in the negative direction, and the self-energy occupies a large space in QED corrections. So the trend of the QED excited energy level is gradually increasing in the negative direction as functions of Z. We note that QED excitation energies are also determined mainly by cancellations between the $4p$ and $4s$ electrons. But as contributions from $4p_{1/2}$ and $4p_{3/2}$ are both small compared to those from $4s$, QED corrections are dominated by the latter and thus similar in size among all thirty-four $4s4p$ states along the entire isoelectronic sequence. We show in Fig. 1 that the Breit increase rapidly with Z and become more important at high Z. It is interesting to note that the contribution from the Breit is more than from the VP in Fig. 1a,b and the contribution from the VP is more than from the Breit in Fig. 1c,d. This is apparently due to the fact that in the high-Z jj-coupling limit, the $^3P_0$ and $^3P_1$ states become a $4s4p_{1/2}$ doublet while the $^3P_2$ and $^1P_1$ states become a $4s4p_{3/2}$ doublet. Contributions to the excitation energies thus come mainly from energy differences between the $4p_{1/2}$ electron from the two lower excited states or the $4p_{3/2}$ electron from the two upper excited states with the $4s$ electron from the ground state, hence the similarities in the contributions between the $^3P_0$ and $^3P_1$ states and between the $^3P_2$ and $^1P_1$ states.

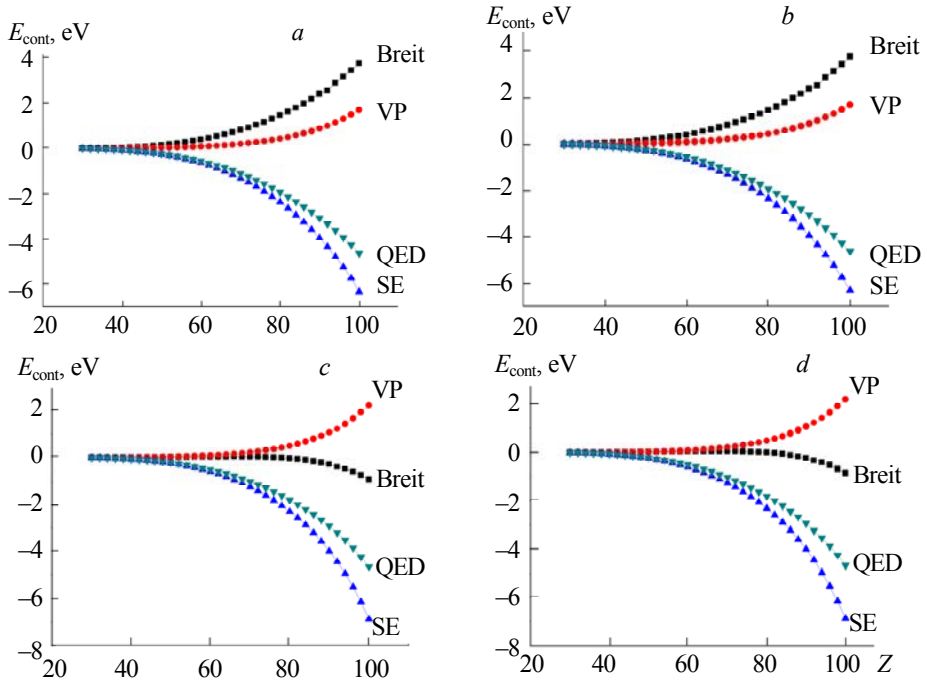

Fig. 1. Contributions from the Breit interaction, self-energy (SE), vacuum polarization (VP), and quantum electrodynamic (QED) to the excitation energies (eV) of the $4s4p\ ^3P_0$ states in Zn-like ions as functions of Z.

In Tables 3 and 4, the radiative lifetimes of the $^1P_1$ and $^3P_1$ states are compared with other theories [2, 5, 7, 10, 32] and with the experiment [33–37]. Since theoretical energies may not be very accurate, theoretical transition rates are often adjusted by replacing theoretical with empirical transition energies. For low- to mid-Z ions, the $4s^2\ ^1S_0$–$4s4p\ ^3P_1$ spin-forbidden transition is allowed through singlet–triplet mixings and its transition matrix element is proportional to the small $^1P_1$ mixing coefficient, which in turn scales approximately like the inverse of the $^{1,3}P_1$ level splitting. As a result, the radiative lifetimes are often adjusted for the transition energy $\Delta E = E(^{1,3}P_1) - E(^1S_0)$ using the equation

$$\tau_{adjusted} = \tau_{original}(\Delta E_{theor}/\Delta E_{expt})^3 \qquad (2)$$

while those for the $^3P_1$ states of low- to mid-Z ions may be further adjusted for the singlet-triplet interval energy $\delta E = E(^1P_1) - E(^3P_1)$ with the equation [32]

$$\tau_{adjusted} = \tau_{original}(\Delta E_{theor}/\Delta E_{expt})^3(\delta E_{expt}/\delta E_{theor})^2. \qquad (3)$$

In Tables 3 and 4, the theoretical results from RCI [5] and MCDF [7] have already been adjusted with empirical transition energies in those works, and the RCI $^3P_1$ lifetimes have further been adjusted with the singlet-triplet splittings.

TABLE 3. Lifetimes (ns) for the $4s^2\ ^1S_0$–$4s4p\ ^3P_1$ Transition in Zn-Like Ions

Z	MCDHF	MCDF [7]	RCI [5]	MCRRPA [10]	CIV3 [32]	Experiment	Z	MCDHF
30	22371.365	25490	22375	32971			62	0.139
32	1009.189	975.6	1011	1089			64	0.117
34	166.882	165.6	167.5				66	0.102
36	47.396	47.30	47.45	49.81	46.19	47(10) [33]	68	0.087
38	17.857	17.85	17.85		16.82		70	0.075
40	8.062	8.05	8.03				72	0.068
42	4.118	4.12	4.11	4.22	3.99	3.73(0.20) [34]	74	0.059
44	2.315						76	0.051
46	1.408						78	0.046
48	0.918		0.914	0.926			80	0.042
50	0.625						82	0.037
52	0.448						84	0.035
54	0.334		0.334	0.335			86	0.034
56	0.252						88	0.032
58	0.201						90	0.029
60	0.162						92	0.025

TABLE 4. Lifetimes (ns) for the $4s^2\ ^1S_0$–$4s4p\ ^1P_1$ Transition in Zn-Like Ions

Z	MCDHF	MCDF [7]	RCI [5]	MCRRPA [10]	Experiment
30	1.355	1.316	1.361		1.45(0.15) [35]
32	0.317	0.315	0.318	0.293	0.29(0.03) [36]
34	0.160	0.159	0.161		0.20(0.02) [37]
36	0.0998	0.0991	0.100	0.0953	0.101(0.010) [33]
38	0.0689	0.0685	0.0691		
40	0.0505	0.0503	0.0507		
42	0.0386	0.0384	0.0388	0.0374	
44	0.0303				
46	0.0241				
48	0.0194	0.0193 [2]	0.0197	0.0191	
50	0.0159	0.0159 [2]	0.0161		
52	0.0131	0.0130 [2]			
54	0.0109	0.0107 [2]	0.0110	0.0107	
56	0.00899		0.00908	0.00885	
58	0.00749				
60	0.00618				
62	0.00508		0.00513		
64	0.00421				
66	0.00345				
68	0.00279				
70	0.00229				
72	0.00190				
74	0.00149		0.00157		
76	0.00122				
78	0.00098				
80	0.00083				
82	0.00064				
84	0.00052				
86	0.00041				
88	0.00033				
90	0.00027				
92	0.00022				

For the lifetimes of the $^1P_1$ state, the agreement among the theories and the experiment is within 10%, except for Se V (as large as 20%). For the lifetimes of the $^3P_1$ states, the agreement is also within 10%. This shows the sensitivity of the intercombination transition on electron correlations, as these spin-forbidden $^3P_1$ transition rates depend critically on the mixing with the $^1P_1$ state for low-Z ions. As can be seen from Tables 3 and 4, our calculated lifetimes lie between the other two theoretical predictions [5, 7] and are slightly closer to Chen and Cheng's revised results [5], with differences ranging from 0 to 5.10%. Indeed, if no energy adjustment is made, the $^3P_1$ lifetimes from the MCRRPA [10] would be larger than the MCDHF lifetimes by 2.1 for zinc and 13% for Kr VII. In addition, the theory provides us with computed transition rates $A_{1,3} = A(4s^2\,{}^1S_0–4s4p\,{}^{1,3}P_1)$, while the measurable and, for diagnostics, interesting properties are the lifetime $\tau_{\text{original}(1,3)} = 1/A_{1,3}$. In Tables 3 and 4, we predict new data for several lifetimes where no other theoretical and/or experimental results are available. About these results, we do not make any empirical energy adjustment. We hope that these results will be useful in analyzing older experiments and planning new ones.

Conclusion. We have shown that the present MCDHF theory yields very accurate relativistic correlation wavelengths and lifetimes even for large atomic systems such as 30-electron Zn-like ions with the nuclear charge Z ranging from 30 to 92. When combined with our QED and Breit corrections, theoretical transition wavelengths agree well with the experiment for all 4*s*4*p* excited states along the entire isoelectronic sequence. We demonstrate that MCDHF results can provide stringent tests of the strong-field QED theory and unveil the importance of subtle relativistic effects such as Breit corrections when compared with high-precision spectral measurements of high-Z ions. For many-open-shell complex systems, more compact and efficient basis sets may be needed for high-precision atomic structure calculations. The results from the present calculations provide benchmark values for future theoretical and experimental studies of the zinc isoelectronic sequence.

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