PHYSICAL REVIEW A VOLUME 50, NUMBER 5 NOVEMBER 1994

Energies and fine structures of $1s^2\,2snp$ (n=2,3) $^1P^o$ and $^3P^o_{2,1,0}$ states of Be-like ions

X.-W. Zhu and Kwong T. Chung
Department of Physics, North Carolina State University, Raleigh, North Carolina 27695-8202

(Received 8 April 1994)

The energies and wave functions of the Be-like $1s^22snp$ (n=2,3) $^1P^o$ and $^3P^o_{2,1,0}$ states are calculated with a full-core plus correlation method for ions from B II to Ne VII, Mg IX, and Si XI. The relativistic corrections and fine structures are calculated with the first-order perturbation theory. Higher-order effects are estimated. The calculated excitation energies (relative to the $1s^22s^2$ ground state) are compared with the experiment. Intermediate coupling between the $^3P^o_1$ and $^1P^o_1$ states is also considered. Most of the predicted $^3P^o_J$ energies agree with the experiment to within a few cm^{-1}. The fine-structure splittings of the $1s^22s2p\,^3P^o_{2,1,0}$ states calculated in this work all agree with the best experimental data in the literature. Our results show that for systems of $Z \geq 9$, it is critically important to consider intermediate coupling. For Si XI, it shifts the $2s2p\,^{3,1}P^o_1$ levels by 86 cm^{-1} and the $2s3p\,^{3,1}P^o_1$ energies by 193 cm^{-1}. The predicted $2s2p\,^1P^o$ energies are slightly higher than the experimental data; the discrepancy increases from 14 cm^{-1} for Z=5 to 93 cm^{-1} for Z=14.

PACS number(s): 31.20.Di, 31.20.Tz, 31.30.Jv, 31.50.+w

I. INTRODUCTION

The accurate oscillator strengths and lifetimes of the Be-like ions are of experimental interest. Their importance in astrophysics has also been emphasized in the literature [1, 2]. To obtain a reliable oscillator strength and lifetime, accurate energies and wave functions of the excited state of Be-like ions are needed. A considerable amount of theoretical work has been done on the $1s^22snp$ excited states of the Be-like isoelectronic sequence [3–10]. An interesting feature of the Be-like $2s3p$ states is discussed by Kim, Martin, and Weiss [7]. In normal cases, a $2s3p\,^3P^o$ will give a lower energy than the $2s3p\,^1P^o$ due to the exchange interaction. However, this ordering is inverted for $Z \geq 6$ in Be-like systems and this inversion is reversed again at about Z=22.

Edlén [11, 12] has made a detailed study of the $1s^22l2l'$ excited states of Be-like ions by combining the multiconfiguration Dirac-Fock (MCDF) calculation [3] with experimental observation. His analysis leads to rather accurate results for the excitation energies and fine structures. The transition energies between different excited states are also given in other works [13–16]. Most of these works are interested in the calculation of atomic oscillator strengths. Although a nonrelativistic approach is adopted by some workers, relatively few accurate nonrelativistic energies are published in the literature. One of the most elaborate computation on the $1s^22s2p\,^1P^o$ nonrelativistic energies is given by Sims and Whitten [13]. Their upper bounds for C III and O V are higher than the upper bounds calculated in this work by approximately 0.15 eV.

There is much experimental interests in the study of Be-like $2s3p\,^3P^o$ systems, for example, the differential lifetime measurements of the $2s3s\,^3S_1$-$2s3p\,^3P^o_J$ and $2p^2\,^3P_J$-$2s3p\,^3P^o_{J'}$ transitions [17]. If one tries to measure the lifetime of the upper level, one needs to know the transition probabilities to all lower levels. Furthermore, one needs to find transitions which permits the resolution of the decays from the three fine-structure components of the $1s^22s3p\,^3P^o_{2,1,0}$. This task is complicated by not knowing the exact fine structure and the position of the $1s^22s3p\,^3P^o_1$ level as well as its relative position to the $1s^22s3p\,^1P^o_1$ level. The needed spectroscopic information on term values of the levels involved is not available for many of the ions of interest such as Mg and Si. Accurate theoretical energies can be very useful in these experimental studies. For larger Z, the results from different authors in the literature disagree with each other. Especially for $1s^22s3p\,^1P^o$ and $^3P^o_{2,1,0}$ states. Some of the experimental data are quite approximate and others are lacking.

Recently, we have calculated the energies and fine structures of the $2snl$ ($n \leq 3$) excited states of the Beryllium atom [18] using a full-core plus correlation method (FCPC). Most of the predicted energies agree with the experiment to about 1 cm^{-1}. The predicted fine-structure splittings for $2s2p\,^3P^o_J$ and $2s3p\,^3P^o_J$ agree well with those in the experiment [19]. One would like to find out whether the FCPC method is also effective for Be-like excited systems as Z becomes larger. For beryllium, the relativistic perturbation is small. By carrying out a calculation along the isoelectronic sequence, we can study how the relativistic effects increase with Z. In this work, we use FCPC for the Be-like $2snp$ (n = 2, 3) $^1P^o_1$ and $^3P^o_{2,1,0}$ states for ions with Z=5–14. We will compare our results with the available experimental and theoretical data in the literature whenever possible.

II. THEORY

The Hamiltonian and perturbation operators used in this work are the same as these of Chung, Zhu, and Wang [20]. They are not repeated here. Multiconfiguration interaction wave function and LS-coupling scheme are adopted. A restricted variational method [21] is used to saturate the functional space of the wave function as in Ref. [18]. In this method, one first obtains a "basic wave function," Ψ_b, and an energy upper bound E_b using the conventional variation method. We have

$$\Psi_b(1,2,3,4) = \Psi_0(1,2,3,4) + \Psi_1(1,2,3,4), \tag{1}$$

where

$$\Psi_0(1,2,3,4) = A\Phi_{1s1s}(1,2)\Phi_{2snp}(3,4) \tag{2}$$

and

$$\Psi_1(1,2,3,4) = A\sum_i C_i\Phi_{n(i)l(i)}(1,2,3,4). \tag{3}$$

$l(i)$ represents a particular angular component, and $n(i)$ represents the various terms of the wave function associated with this $l(i)$. A is the antisymmetrization operator and C_i are the linear parameters. $\Phi_{1s1s}(1,2)$ is a predetermined $1s1s$-core wave function. It is the same as in Ref. [20]. $\Phi_{2snp}(3,4)$ represents the wave function of the outer electrons. Only two $[l_1,l_2]$ angular components, [0,1] and [1,2], are included in $\Phi_{2snp}(3,4)$. Most of the other correlation effects are included in Ψ_1, which accounts for the intershell as well as the intrashell correlations. In this work, $\Psi_1(1,2,3,4)$ contains about 910–1162 terms of basis functions and $\Phi_{2snp}(3,4)$ contains 49 terms. The angular and spin components of the wave function in Ψ_1 are similar to those of Ref. [18]. The radial basis functions in each angular component contain a set of nonlinear parameters which are determined in the energy optimization process.

To carry out the restricted variation calculation, the basic wave function Ψ_b is used as a single term in an improved wave function that is given by

$$\Phi(1,2,3,4) = D_0\Psi_b(1,2,3,4) + \Psi_2(1,2,3,4), \tag{4}$$

where

$$\Psi_2(1,2,3,4) = A\sum_{i=1}^{I} D_i\Phi_{n(i)l(i)}(1,2,3,4). \tag{5}$$

By solving the secular equation constructed from Eq. (4), one can compute the energy improvements over the basic energy E_b. For details of this method, we refer the reader to Ref. [18, 21].

The relativistic and mass polarization operators are from Pauli-Breit approximation which are the same as

TABLE I. Nonrelativistic energy of the $1s^22snp$ ($n = 2,3$) $^{3,1}P^o$ states of Be-like system (ΔE_{rv} is the extrapolated energy from the restricted variational calculation).

Z	State	Upper bound E (a.u.)	Core Corr. (μ a.u.)	$\Delta E_{higher\,l}$ (μ a.u.)	ΔE_{rv} (μ a.u.)	Total E_{nonrel} (a.u.)
5	$2s2p\,^1P^o$	-24.014 074 6	-247.6	-136.52	-168.30	-24.014 626 9
	$2s2p\,^3P^o$	-24.178 490 6	-247.6	-26.90	-123.49	-24.178 888 6
	$2s3p\,^1P^o$	-23.692 068 6	-247.6	-23.70	-102.75	-23.692 442 7
	$2s3p\,^3P^o$	-23.692 570 7	-247.6	-20.34	-124.08	-23.692 962 7
6	$2s2p\,^1P^o$	-36.068 386 8	-259.8	-194.82	-214.44	-36.069 055 8
	$2s2p\,^3P^o$	-36.296 097 9	-259.8	-36.51	-145.74	-36.296 539 9
	$2s3p\,^1P^o$	-35.355 197 8	-259.8	-29.14	-123.80	-35.355 610 5
	$2s3p\,^3P^o$	-35.351 581 6	-259.8	-23.19	-135.76	-35.352 000 4
7	$2s2p\,^1P^o$	-50.627 766 6	-268.8	-233.07	-246.33	-50.628 514 8
	$2s2p\,^3P^o$	-50.916 576 0	-268.8	-43.23	-210.74	-50.917 098 7
	$2s3p\,^1P^o$	-49.380 442 8	-268.8	-34.00	-135.22	-49.380 880 8
	$2s3p\,^3P^o$	-49.373 613 6	-268.8	-25.52	-161.52	-49.374 069 5
8	$2s2p\,^1P^o$	-67.689 687 2	-275.7	-263.29	-287.95	-67.690 514 1
	$2s2p\,^3P^o$	-68.038 666 6	-275.7	-48.17	-232.98	-68.039 223 5
	$2s3p\,^1P^o$	-65.767 317 5	-275.7	-38.56	-149.93	-65.767 781 7
	$2s3p\,^3P^o$	-65.757 823 0	-275.7	-28.02	-185.84	-65.758 312 6
9	$2s2p\,^1P^0$	-87.253 106 8	-281.3	-289.06	-327.04	-87.254 004 2
	$2s2p\,^3P^0$	-87.661 736 9	-281.3	-52.49	-251.35	-87.662 322 0
	$2s3p\,^1P^0$	-84.515 610 7	-281.3	-42.71	-160.23	-84.516 094 9
	$2s3p\,^3P^0$	-84.503 815 4	-281.3	-30.89	-181.97	-84.504 309 5
10	$2s2p\,^1P^o$	-109.317 546 3	-285.8	-308.51	-294.32	-109.318 434 9
	$2s2p\,^3P^o$	-109.785 445 1	-285.8	-55.83	-269.19	-109.786 056 0
	$2s3p\,^1P^o$	-105.625 211 9	-285.8	-46.03	-167.81	-105.625 711 5
	$2s3p\,^3P^o$	-105.611 323 3	-285.8	-33.54	-194.52	-105.611 837 1
12	$2s2p\,^1P^o$	-160.948 035 0	-292.7	-335.00	-296.70	-160.948 959 5
	$2s2p\,^3P^o$	-161.534 073 0	-292.7	-60.57	-286.94	-161.534 713 2
	$2s3p\,^1P^o$	-154.928 083 6	-292.7	-51.33	-191.18	-154.928 618 9
	$2s3p\,^3P^o$	-154.910 478 8	-292.7	-36.02	-207.19	-154.911 014 8
14	$2s2p\,^1P^o$	-222.579 848 5	-297.9	-355.91	-309.26	-222.580 811 6
	$2s2p\,^3P^o$	-223.283 673 5	-297.9	-64.24	-306.87	-223.284 342 6
	$2s3p\,^1P^o$	-213.675 693 3	-297.9	-55.31	-190.84	-213.676 237 4
	$2s3p\,^3P^o$	-213.654 724 0	-297.9	-38.12	-207.56	-213.655 267 7

those in Chung and Zhu [18]. The relativistic perturbation operators include: P^4, the Darwin term, the electron-electron contact term, the orbit-orbit interaction, the spin-orbit, spin-other-orbit, and spin-spin interactions. The explicit expressions of the operators are given in Refs. [20] and [18]. The mass polarization correction to the nonrelativistic energy is calculated by including the mass polarization operator in the Hamiltonian and rediagonalized the secular equation. The wave function with this mass polarization is used to calculate the relativistic corrections using first-order perturbation theory. The results obtained are not very different from the ones using the conventional first-order perturbation theory. The isotopes used in the present work are ^{11}B, ^{12}C, ^{14}N, ^{16}O, ^{19}F, ^{20}Ne, ^{24}Mg, and ^{28}Si. The masses are taken from Wapstra and Audi [22].

The contribution from QED effect is estimated using the same approach as in Ref. [20] for the $2s$ electron and in Ref. [18] for the p electrons. Since the relativistic corrections are only computed in the context of first-order theory with the Pauli-Breit operators, the possible higher-order contribution needs to be considered. The higher-order relativistic effect and nuclear size effect are estimated by using a method described in Chung *et al.*, [20]. The effective nuclear charges used for $1s^22s3p$ are determined by considering that the $2s$ electron is in the field of $1s1s$ core and the $3p$ electron is in the field of $1s1s2s$. But for $1s^22s2p$, we assume that the $2s$ is the outer electron. The main reason is that, for a hydrogen-like system, the radius of a $2p$ orbital is smaller than that of the $2s$ orbital (see, e.g., Bethe and Salpeter [23]). A more ideal solution is if one can determine the $1s1s2s$ and $1s1s2p$ fractional parentage percentages in the $1s1s2s2p$ states. However, we do not have a good method to determine these percentages for our wave function. Hence, our calculated QED and higher-order relativistic corrections are subject to this uncertainty.

For the fine structure, the perturbation operators are the same as Ref. [18]. We use first-order perturbation theory to calculate the $2snp\,{}^3P^o_J$ splittings. The QED and higher-order relativistic effects are estimated using the same method as before. For $J = 2$–0 splittings, this gives a rather accurate result. However, the $J = 2$–1 splittings will not be accurate if we do not consider the shift due to the coupling of the ${}^1P^o_1$ and ${}^3P^o_1$ states. This shift is given by

$$\Delta E = \frac{|\langle\Psi({}^1P^o_1)|H_{so} + H_{soo}|\Psi({}^3P^o_1)\rangle|^2}{E({}^1P^o_1) - E({}^3P^o_1)}, \qquad (6)$$

where H_{so} and H_{soo} are the spin-orbit and spin-other-orbit perturbation operators, respectively. This energy shift is positive for the higher state and negative for the lower state. In computing this shift, the relativistic corrections are included in E $({}^1P^o_1)$ and E $({}^3P^o_1)$.

III. RESULTS AND DISCUSSION

As in Ref. [18], we first calculate the nonrelativistic energy upper bound for the excited states with the basic wave function, Ψ_b. These upper bounds give substantial improvement over those in the literature. For example, for $2s2p\,{}^3P^o$, the multiconfiguration results in Hibbert [14] are -24.1274 a.u. for Z=5, and -109.7288 a.u. for Z=10. Our upper bounds are $-24.178\,491$ and $-109.786\,056$ a.u., respectively. Similar improvements are also obtained for other states. Sims and Whitten [13] calculated the $2s2p\,{}^1P^o$ states of C III and O V. Their results, $-36.062\,83$ and $-67.684\,33$ a.u. are higher than the upper bounds in this work, $-36.068\,387$ and $-67.689\,687$ a.u. by about 0.15 eV.

In the next step, we make significant improvements over these upper bounds with the restricted variation calculation. For example, for $1s^22s2p\,{}^1P^o$, the contributions from the restricted variation calculation ranges from -168.30 μa.u. to -309.26 μa.u. from B II to Si XI. Similar improvements are also obtained for other states.

As in Ref. [18], the orbital angular momenta of the electrons in our wave function only range from $l = 0$ to 6. The energy contributions from the $l \geq 7$ terms may also be appreciable. They need to be extrapolated. We use the same procedure as in Ref. [18] to extrapolate the higher l contributions. In addition to the restricted variation and higher l contribution, we also need to include the core correction for the FCPC results. These core corrections are discussed in Ref. [20]. By combining the extrapolated results and the corrections, we obtain the nonrelativistic energy. These results are given in Table I.

In Table VI[1] we give the mass polarization (ΔE_{MP}) and relativistic corrections of the $2s2p$ systems. For $2s2p\,{}^3P^o_J$ only center of gravity energy is given in this table. By subtracting these from the $1s1s$ core results, they give the corresponding $2s2p$ double-electron ionization contributions. The results for the $1s1s$ cores are the same as those of Ref. [20]. In addition to the relativistic perturbations considered in this reference, we have also included the effect from the intermediate coupling between the ${}^3P^o$ and ${}^1P^o$ states. Adding the estimated corrections from QED, higher-order relativistic and nuclear size effects, we obtain the total two-electron ($2s2p$) IP. The IP of the $2p$ electron is obtained by subtracting the predicted $2s$ IP [20] from the $2s2p$ IP. The excitation energy of the $2s2p$ state is obtained by subtracting the $2s2p$ IP from the IP of $2s2s$ [20]. The corresponding results for the $2s3p$ states are presented in Table VII[1].

In Chung and Zhu [18], the contribution of the relativistic effects of the nl electron in a Be $2snl$ atom to the "binding" or "antibinding" of this electron is tabulated

---

[1] **See AIP document no. PAPS PLRAAN-50-3818-8 for eight pages of ionization potential and excitation energy of Be-like $2s2p\,{}^{3,1}P$ and $2s3p\,{}^{3,1}P$ states Tables VI and VII. Order by PAPS number and journal reference from American Institute of Physics, Physics Auxiliary Publication Service, 500 Sunnyside Blvd., Woodbury, NY 11797. The prepaid price is \$1.50 each microfiche (60 pages), or \$5.00 for photocopies of up to 30 pages, and \$0.15 for each additional page over 30 pages. Airmail additional. Make checks payable to the American Institute of Physics.**

TABLE II. Relativistic perturbation contributions to the binding of np electron in Be-like system (in cm^{-1}). The entries in this table is equal to $\Delta E_{rel}(1s^22snp) - \Delta E_{rel}(1s^22s)$, where ΔE_{rel} is the sum of the expectation values of relativistic perturbation operators. $\Delta E_{rel}(1s^22s)$ are from Refs. [24, 25].

Z	$2s2p\,^1P^o$	$2s2p\,^3P^o$	$2s3p\,^1P^o$	$2s3p\,^3P^o$
5	17.5	11.4	7.4	1.3
6	28.9	9.5	12.8	0.8
7	17.5	-16.1	11.5	-7.1
8	-21.7	-81.8	0.1	-39.6
9	-104.1	-215.0	-25.7	-79.5
10	-277.5	-438.4	-77.7	-155.5
12	-1 006.1	-1 308.4	-301.4	-478.5
14	-2 521.0	-3 030.0	-764.6	-1 152.9

and discussed. The conclusion is that for the beryllium atom, the relativistic effects of the np ($n = 2, 3$) electrons are small by themselves, but their presence contributes to the shielding of the $2s$ electron from the nucleus. This shielding reduces the relativistic correction of the $2s$ electron. Thus, the overall relativistic correction of the np orbital reduces its binding energy. In this work, we can also study this effect along the isoelectronic sequence. We subtracted the relativistic correction of the $1s^22s$ state [24, 25] from that of the $1s^22snp$ as in Ref. [18]. The results are shown in Table II. For small Z ions such as B II and C III, the shielding of $2s$ electron is more significant than the np relativistic contribution. The net result is antibinding. As Z gets larger, the relativistic correction of the np electron becomes more significant which lowers the overall energy. The effect becomes binding. The transition from antibinding to binding occurs at Z=7 for the triplets and at Z=8 for the singlets. The results in Table II seem to suggest that the shielding of the singlets are more significant than the triplets.

In Table III, we give a comparison of the $1s^22snp\,^1P^o$ excitation energies calculated in this work with those of the experiment and other theoretical results. As in Chung and Zhu [18], we are still facing a challenge that our predicted energies are a few cm^{-1} too high even for low Z systems. This discrepancy increases somewhat as Z increases. It is interesting to note that, the predicted Si XI $2s2p\,^1P^o$ excitation energy agree with the experiment almost exactly before the intermediate coupling is considered. However, the inclusion of this coupling raises the $2s2p\,^1P_1^o$ excitation energy by 86.4 cm^{-1} to 329 772 cm^{-1}. This is 82 cm^{-1} higher than the datum quoted in Bashkin and Stoner [26] and Kelly [27], and it is 93 cm^{-1} higher than that of Martin and Zalubas [31].

The effect from intermediate coupling is even stronger between the $2s3p\,^{3,1}P_1^o$ states. The main reason is that $E(2s3p\,^3P_1^o)$ lies much closer to $E(2s3p\,^1P_1^o)$ in comparison with the 2s2p states. For example, for Z=10, 12, and 14, the factor $|\langle 2s2p\,^1P_1^o|H_{so} + H_{soo}|2s2p\,^3P_1^o\rangle|^2$, is about sixteen times that of the 2s3p states, but the energy factor is more than 33 times larger. Consequently, the shift of the $2s3p\,^{3,1}P_1^o$ energy due to the intermediate coupling is more than twice as that of the corresponding $2s2p\,^{3,1}P_1^o$ states.

The fine-structure splittings of the $2snp$ ($n = 2, 3$) $^3P_{2,1,0}$ states are tabulated in Table IV for 2s2p

TABLE III. Comparison of excitation energy of Be-like $1s^22snp\,^1P^o$ (n=2,3, in cm^{-1}).

Z	This work	Expt.	ΔE[a]	Other theory	Edlén[b]	This work	Expt.	ΔE	Other author
		$2s2p\,^1P^o$					$2s3p\,^1P^o$		
5	73 410.7	73 396.60[c,d]	14.1		73 396.6	144 112.1	144 103.17[c,d]	8.9	
6	102 370.2	102 352.04[c,d]	18.2		102 351	258 939.9	258 931.29[c,d]	8.6	258 942[e]
7	130 710.2	130 693.9[c,d]	16.3		130 694	404 534.1	404 522.4[c,d]	11.7	404 557[e]
8	158 817.4	158 797.7[c,d]	19.7		158 797	580 841.0	580 824.9[c,d]	16.1	580 897[e]
9	186 879.0	186 841[c,d]	38		186 845	787 870.1	787 833[c,d]	37	
		186 844[f]	35				787 844[f]	26	
10	214 987	214 952[d]	35		214 954	1 025 655	$1\,025.69\times10^3$[c,d]		
12	271 750	271 687[c,d,g]	63	271 650[h]	271 697	1 593 744	$1\,593.6\times10^3$[c,g]		1 593 279[h]
							1 593 908[d]	-164	1 593 662[e]
14	329 772	329 690[c,d]	82	329 712[h]	329 678	2 285 653	$2\,285.04\times10^3$[d]		2 285 057[h]
		329 679[i]	93				2 285 040[c,i]	613	2 285 432[e]

[a] ΔE= This work - experiment.
[b] Edlén [11, 12].
[c] Bashkin and Stoner [26].
[d] Kelly [27].
[e] Kim, Martin, and Weiss [7].
[f] Engström [29].
[g] Martin and Zalubas [30].
[h] Ando, Safronova, and Tolstikhina [5].
[i] Martin and Zalubas [31].

TABLE IV. Fine-structure resolved excitation energy and splitting for the $1s^22s2p\,^3P_J^o$ states of Be-like system [in cm^{-1}, E_J is the excitation energies from first-order perturbation theory. ΔE_J (H.R.) is the higher order relativistic contribution].

	J value			Splitting	
	2	1	0	2–1	2–0
		$Z=5$			
E_J	37 361.5	37 345.4	37 339.4		
ΔE_J (H.R.)	0.003	-0.003	-0.007		
ΔE_J (QED)	0.025	-0.025	-0.050		
Theor. (this work)	37 361.5	37 345.4	37 339.3	16.1	22.2
Expt.^{a,b}	37 358.3	37 342.4	37 336.7	15.9	21.6
Theor.-Expt.	3.2	3.0	2.6	0.2	0.6
Edlén^{c}	37 358.3	37 342.4	37 336.7	15.9	21.6
LCV^{d}				17.70	24.42
		$Z=6$			
E_J	52 452.76	52 396.74	52 373.33		
ΔE_J (H.R.)	0.019	-0.019	-0.037		
ΔE_J (QED)	0.077	-0.077	-0.154		
Theor. (this work)	52 452.86	52 396.64	52 373.14	56.22	79.72
Expt.^{a,b}	52 447.11	52 390.75	52 367.06	56.36	80.05
Theor.-Expt.	5.75	5.89	6.08	-0.14	-0.33
Edlén^{c}	52 447	52 391	52 367	56	80
LCV^{d}				61.19	86.76
FHS^{e}		52 369			78.9
		$Z=7$			
E_J	67 413.3	67 270.2	67 207.6		
ΔE_J (H.R.)	.070	-0.070	-0.140		
ΔE_J (QED)	0.186	-0.186	-0.372		
Theor. (this work)	67 413.6	67 269.9	67 207.1	143.7	206.5
Expt.^{a,b}	67 416.3	67 272.3	67 209.2	144.0	207.1
Theor.-Expt.	-2.7	-2.4	-2.1	-0.3	-0.6
Edlén^{c}	67 417	67 272	67 210	145	207
LCV^{d}				153.38	220.49
		$Z=8$			
E_J	82 379.6	82 075.5	81 938.9		
ΔE_J (H.R.)	.207	-0.207	-0.413		
ΔE_J (QED)	0.382	-0.382	-0.763		
Theor. (this work)	82 380.2	82 074.9	81 937.7	305.3	442.5
Expt.^{a,b}	82 382.0	82 075.3	81 939.2	306.7	442.8
Theor.-Expt.	-1.8	-0.4	-1.5	-1.4	-0.3
Edlén^{c}	82 386	82 079	81 942	307	444
LCV^{d}				322.63	467.57
		$Z=9$			
E_J	97 440.1	96 868.7	96 607.5		
Inter. coupling		-2.0			
ΔE_J (H.R.)	0.517	-0.517	-1.034		
ΔE_J (QED)	0.700	-0.700	-1.399		
Theor. (this work)	97 441.3	96 865.5	96 605.1	575.8	836.2
Expt.^{a}	97 441	96 867	96 605	574	836
Theor.-Expt.	0	-1	0	2	0
Edlén^{c}	97 452	96 876	96 615	576	837
Other Expt.	97 437^{b}	96 867^{b}	96 601^{b}	570	836
	97 427^{f}	96 850^{f}	96 590^{f}	577	837
		$Z=10$			
E_J	112 687	111 703	111 248		
Inter. coupling		-5.0			
ΔE_J (H.R.)	1.144	-1.144	-2.288		
ΔE_J (QED)	1.181	-1.181	-2.363		
Theor. (this work)	112 689	111 696	111 243	993	1 446
Expt.^{b}	112 700	111 706	111 251	994	1 449
Theor.-Expt.	-11	-10	-8	-1	-3
Edlén^{c}	112 700	111 708	111 254	992	1 446

TABLE IV. *(Continued).*

		J value		Splitting	
Other Expt.[a]	112 704	111 710	111 255	994	1 449
LCV[d]				1 097.3	1 607.5
		Z=12			
E_J	144 085	141 661	140 520		
Inter. coupling		-24.0			
ΔE_J (H.R.)	4.321	-4.321	-8.642		
ΔE_J (QED)	2.829	-2.829	-5.658		
Theor. (this work)	144 092	141 630	140 506	2 462	3 586
Expt.[g]	144 091	141 631	140 504	2 460	3 587
Theor.-Expt.	1	-1	2	2	-1
Edleń[c]	144 096	141 636	140 508	2 460	3 588
Other Expt.	144 162[a]	141 700[a]	140 575[a]	2 462	3 587
	144 162[b]	141 980[b]	140 528[b]	2 182	3 634
AST[i]	144 306	141 775	140 625	2 531	3 681
		Z=14			
E_J	177 303	172 255	169 852		
Inter. coupling		-86.1			
ΔE_J (H.R.)	12.817	-12.817	-25.633		
ΔE_J (QED)	5.757	-5.757	-11.513		
Theor. (this work)	177 322	172 150	169 815	5 172	7 507
Expt.[h]	177 318	172 144	169 802	5 174	7 516
Theor.-Expt.	4	6	13	-2	-9
Edleń[c]	177 309	172 141	169 800	5 168	7 509
Other Expt.[a,b]	176 810	171 560	169 140	5 250	7 670
AST[i]	177 617	172 346	169 973	5 271	7 644

[a] Kelly [27].

[b] Bashkin and Stoner [26].

[c] Edlén [11, 12].

[d] Laughlin, Constantinides, and Victor [6].

[e] Fleming, Hibbert, and Stafford [8].

[f] Engström [29].

[g] Martin and Zalubas [30].

[h] Martin and Zalubas [31].

[i] Ando, Safronova, and Tolstikhina [5].

and Table V for $2s3p$. The experiment data for the $1s^22s2p\,^3P_{2,1,0}$ splittings are comparatively more complete [26–31]. Edlén [11, 12] has also recommended the energy values of the J levels on the basis of his analysis. Laughlin, Constantinides, and Victor [6] predicted the splittings using a model potential. Ando, Safronova, and Tolstikhina [5] also calculated the spittings for $Z > 10$ systems using MCDF and MZ. MZ is a $1/Z$ expansion method. In Table IV, we compare our prediction with the experiment. The effect of the intermediate coupling is quite apparent. For example, before intermediate coupling, our Mg IX $J=2$–1 splitting, 2438 cm^{-1}, is different from the 2460 cm^{-1} of Martin and Zalubas [30] and 2462 cm^{-1} of Kelly [27]. The coupling lowers the $2s2p^3P_1^o$ by 23.97 cm^{-1} and changes the $J=2$–1 splitting to 2462 cm^{-1} which agrees with the experiment almost exactly. Similar improvements are also obtained for Ne VII and Si XI. The predicted $2s2p\,^3P_J^o$ excitation energies agree with the experimental data very closely for all Z considered. This is unexpected, considering the possible uncertainty in our QED and higher order relativistic corrections. Nevertheless, this agreement seems to suggest that the method we used is suitable for $2s2p\,^3P_J^o$ states. In comparison with other theoretical prediction, we note that our fine-structure splitting results differ from those of Laughlin *et al.* [6] by about 5–8 %. percent. Considering the simplicity of the model potential, this agreement is quite good. The MCDF and MZ results in Ando *et al.* [5] are somewhat different and they consider the MZ results to be more reliable. Some of their MZ results are also given in Table IV. Their fine-structure splittings for Mg IX and Si XI differ from ours by less than three percent. Recently, the excitation energy of the C III $1s^22s2p\,^3P_1^o$ is predicted to be 52 369 cm^{-1} by Fleming *et al.* [8] and 52 343 cm^{-1} by Fischer [9]. They agree well with our result, 52 396 cm^{-1}, and the experimental result of 52 390 cm^{-1}.

The excitation energies and fine-structure splittings for the $2s3p\,^3P_J^o$ states are given in Table V. For higher Z, the experimental data for these states are less complete. For Z=5 – 9, our results for E_J agree with the data quoted in Bashkin and Stoner [26] and Kelly [27] quite well. The discrepancies range from 0.3 to 5 cm^{-1}. The agreement on fine-structure splitting is excellent in all cases. For Z=10, the data quoted in Bashkin and Stoner [26] and Kelly [27] are quite different. Our results agree much better with those of Bashkin and Stoner. For Mg IX, the E_J quoted in Bashkin and Stoner is very ap-

TABLE V. Fine-structure resolved excitation energy and splitting for the $1s^22s3p\,^3P^o_J$ states of Be-like system [in cm^{-1}, E_J is the excitation energies from first order perturbation theory. ΔE_J(H.R.) is the higher-order relativistic contribution].

	J value			Splitting	
	2	1	0	2–1	2–0
		$Z=5$			
E_J	143 994.19	143 990.85	143 989.60		
Inter. coupling		-0.06			
ΔE_J (QED)	0.002	-0.002	-0.004		
Theor. (this work)	143 994.19	143 990.79	143 989.59	3.40	4.60
Expt.[a]	143 993.89	143 990.45	143 989.15	3.44	4.74
Theor.-Expt.	0.30	0.34	0.44	-0.04	-0.14
		$Z=6$			
E_J	259 726.50	259 713.38	259 707.92		
Inter. coupling		0.11			
ΔE_J (H.R.)	0.001	-0.001	-0.003		
ΔE_J (QED)	0.009	-0.009	-0.018		
Theor. (this work)	259 726.51	259 713.48	259 707.90	13.03	18.61
Expt.[a,b]	259 724.30	259 711.22	259 705.55	13.08	18.75
Theor.-Expt.	2.21	2.26	2.35	-0.05	-0.14
KMW[c]		259 736			
		$Z=7$			
E_J	406 027.0	405 991.4	405 975.8		
Inter. coupling		0.4			
ΔE_J (H.R.)	0.007	-0.007	-0.014		
ΔE_J (QED)	0.027	-0.027	-0.054		
Theor. (this work)	406 027.0	405 991.8	405 975.7	35.2	51.3
Expt.[a,b]	406 022.8	405 987.5	405 971.6	35.3	51.2
Theor.-Expt.	4.2	4.3	4.1	-0.1	0.1
KMW[c]		406 024			
		$Z=8$			
E_J	582 915.9	582 837.7	582 802.5		
Inter. coupling		1.4			
ΔE_J (H.R.)	0.026	-0.026	-0.052		
ΔE_J (QED)	0.063	-0.063	-0.126		
Theor. (this work)	582 916.0	582 839.0	582 802.3	77.0	113.7
Expt.[b]	582 917.0	582 839.8	582 803.1	77.2	113.9
Theor.-Expt.	-1.0	-0.8	-0.8	-0.2	-0.2
KMW[c]		582 908			
		$Z=9$			
E_J	790 477.5	790 327.2	790 258.5		
Inter. coupling		3.9			
ΔE_J (H.R.)	0.074	-0.074	-0.149		
ΔE_J (QED)	0.126	-0.126	-0.252		
Theor. (this work)	790 477.7	790 330.9	790 258.1	146.8	219.6
Expt.[a]	790 474	790 326	790 253	148	221
Theor.-Expt.	4	5	5	-1	-1
Other Expt.[d]	790 460	790 312	790 240	148	220
		$Z=10$			
E_J	1 028 758.0	1 028 495.3	1 028 373.7		
Inter. coupling		10.1			
ΔE_J (H.R.)	0.182	-0.182	-0.364		
ΔE_J (QED)	0.227	-0.227	-0.455		
Theor.(this work)	1 028 758.4	1 028 505.0	1 028 372.9	253.4	385.5
Expt.[a]	1 028 754.7	1 028 499.3	1 028 366.5	255.4	388.2
Theor.-Expt.	3.7	5.7	6.4	-2.0	-2.7
Other Expt.[b]	1 028 775	1 028 519	1 028 386	236	369
		$Z=12$			
E_J	1 597 804.8	1 597 144.0	1596 832.9		
Inter. coupling		50.2			
ΔE_J (H.R.)	0.666	-0.666	-1.332		
ΔE_J (QED)	0.534	-0.534	-1.069		

TABLE V. *(Continued)*.

		J value		Splitting	
Theor. (this work)	1 597 806	1 597 193	1 596 830	613	976
Expt.[a]	$1\,598.4\times10^3$	$1\,597.7\times10^3$	$1\,597.4\times10^3$	0.7×10^3	1.0×10^3
AST[e]	1 597 926	1 597 287	1 596 917	639	1009
		$Z=14$			
E_J	2 290 743.6	2 289 349.4	2 288 686.0		
Inter. coupling		193.1			
ΔE_J (H.R.)	2.562	-2.562	-5.123		
ΔE_J (QED)	1.292	-1.292	-2.583		
Theor. (this work)	2 290 747	2 289 539	2 288 678	1 208	2 069
AST[e]	2 290 887	2 289 640	2 288 771	1 247	2 116

[a] Bashkin and Stoner [26].

[b] Kelly [27].

[c] Kim, Martin, and Weiss [7].

[d] Engström [29].

[e] Ando, Safronova, and Tolstikhina [5].

proximate, our prediction does not agree with these data. On the other hand, our prediction is close to the prediction of Ando *et al.* [5] with the largest discrepancy being 120 cm^{-1}. The predicted fine-structure splittings only differ by about 3%.

For Si XI $2s3p\,^3P^o_J$, no experimental data is available. Our E_J differs from that of Ando *et al.* [5] by less than 140 cm^{-1}. Again, our fine-structure splittings are smaller than theirs by about three percent.

IV. CONCLUSION

The purpose of this work is to carry out a FCPC calculation for the $2snp\,^{1,3}P^o_J$ states to test the accuracy of the method along the isoelectronic sequence and to provide some reliable theoretical Mg IX and Si XI $2s3p\,^{1,3}P^o_J$ data for experimental workers. From the agreement between our $E(2s2p\,^3P^o_J)$ and experiment and that of $E(2s3p\,^3P^o_J)$ for $Z \leq 10$, the predicted Mg IX and Si XI $E(2s3p\,^3P^o_J)$ are probably quite accurate. They should be useful for experiments on these systems.

In obtaining an accurate nonrelativistic energy, it is necessary to consider the higher l contributions. The restricted variation method also provides an effective procedure to saturate the functional space. The results in Table I shows how important they contribute to the final energy.

There has been much interest in the coupling of $^1P^o_1$ and $^3P^o_1$ in the literature [7, 32–38]. Our results show that this coupling is strong and it is critically important for the fine-structure splitting for $Z \geq 9$, especially for $2s3p\,^{1,3}P^o_J$. In general, the inclusion of this coupling leads to results which are in close agreement with experiment. The predicted fine structures in this work are probably quite reliable.

As in Chung and Zhu [18], the predicted $2snp\,^1P^o_1$ energies do not agree with experiment closely. The fact that this discrepancy increases with Z seems to suggest that the main problem is not insufficient correlation in the nonrelativistic wave function. Most of the discrepancy may still come from errors in QED. However, we do not have a better method to handle this problem at this time.

ACKNOWLEDGMENTS

This work is supported by the National Science Foundation Grant No. PHY 93-14907.

---

[1] D. E. Blackwell, Quart. J. R. Astron. Soc. **16**, 361 (1975).
[2] A. K. Dupree, P. V. Foukal, and C. Jordan, Astrophys. J. **209**, 621 (1976).
[3] K. T. Cheng, Y.-K. Kim, and J. P. Desclaux, At. Data Nucl. Data Tables **24**, 111 (1979).
[4] E. Markiewicz, P. R. Mczachran, and M. Cohen, Phys. Scr. **23**, 828 (1981).
[5] K. Ando, U. I. Safronova, and I. Y. Tolstikhina, Phys. Scr. **46**, 107 (1992).
[6] C. Laughlin, E. R. Constantinides, and G. A. Victor, J. Phys. B **11**, 2243 (1978)
[7] Y.-K. Kim, W. C. Martin, and A. W. Weiss, J. Opt. Soc. Am. B **5**, 2215 (1988).
[8] J. Fleming, A. Hibbert, and R. P. Stafford, Phys. Sci. **49**, 316 (1994).
[9] C. F. Fischer, Phys. Sci. **49**, 323 (1994).
[10] V. H. S. Kwong, Z. Fang, T. T. Gibbons, W. H. Parkinson, and L. P. Smith, Astrophys. J. **411**, 431 (1993).
[11] B. Edlén, Phys. Scr. **20**, 129 (1979).
[12] B. Edlén, Phys. Scr. **28**, 51 (1983).
[13] J. S. Sims and R. C. Whitten, Phys. Rev. A **8**, 2220 (1973).
[14] A. Hibbert, J. Phys. B **9**, 2805 (1976).
[15] C. M. Moser, R. K. Nesbet, and M. N. Gupta, Phys. Rev. A **13**, 17 (1976).
[16] A. Hibbert, J. Phys. B **7**, 1417 (1974).

[17] E. Träbert (private communication).

[18] K. T. Chung and X.-W. Zhu, Phys. Rev. A **48**, 1944 (1993).

[19] L. Johansson, Ark. Fys. **23**, 119 (1962).

[20] K. T. Chung, X.-W. Zhu, and Z.-W. Wang, Phys. Rev. A **47**, 1740 (1993).

[21] K. T. Chung and X.-W. Zhu, Phys. Scr. **48**, 292 (1993).

[22] A. H. Wapstra and G. Audi, Nucl. Phys. A **432**, 1 (1985).

[23] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two- Electron Atoms* (Springer-Verlag, Berlin, 1957), p. 17.

[24] K. T. Chung, Phys. Rev. A **44**, 5421 (1991).

[25] K. T. Chung, Phys. Rev. A **45**, 7766 (1992).

[26] S. Bashkin and J. O. Stoner, Jr., *Atomic Energy Level & Grotrian Diagrams* II (Elsevier, New York, 1975).

[27] R. L. Kelly, J. Phys. Chem. Ref. Data. **16**, 1 (1987), Suppl. 1.

[28] A. Ölme, Phys. Scr. **1**, 256 (1970).

[29] L. Engström, Phys. Scr. **31**, 379 (1985).

[30] W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data **9**, 46 (1980).

[31] W. C. Martin and R. Zalubas, J. Phys. Chem. Ref. Data **12**, 323 (1983).

[32] D. G. Ellis, Phys. Rev. A **28**, 1223 (1983).

[33] V. A. Boiko, S. A. Pikuz, U. I. Safronova, and A. Y. Faenov, J. Phys. B **10**, 1253 (1977).

[34] D. H. Sampson, R. E. H. Clark, and S. J. Goett, Phys. Rev. A **24**, 2979 (1981); D. H. Sampson, S. J. Goett, and R. E. H. Clark, At. Data Nucl. Data Tables **30**, 125 (1984).

[35] A. K. Bhatia and H. E. Mason, Astron. Astrophys. **103**, 324 (1981)

[36] H Odabasi, J. Opt. Soc. Am. **59**, 583 (1969).

[37] R. Glass, J. Phys. B **12**, 1633 (1979).

[38] A. Hibbert, J. Phys. B **12**, L661 (1979).