$1s2s2p^2\,{}^5P$-$1s2p^3\,{}^5S^\circ$ transition and fine structure of Be-like systems

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Using an *LSJ*-coupling scheme and a configuration-interaction wave function, the relativistic energies, transition wavelengths of the $1s2s2p^2\,{}^5P$ and $1s2p^3\,{}^5S^\circ$, are studied. The relativistic correction, Breit-Pauli operator, and mass polarization correction are calculated for ions from Be I to Ne VII. Very good agreement with experiment is obtained in many cases. For example, the calculated transition wavelengths for Be I, N VI, O V, and Ne VII are 1910.15, 825.45, 694.75, and 526.57 Å. It is to be compared with the corresponding experimental data of 1909.5±0.6, 825.55±0.1, 694.75±0.1, and 526.65±0.1 Å. The calculated fine-structure values agree reasonably well with other theoretical results and with experiments. Some interesting comparisons between the existing theoretical data will also be discussed.

I. INTRODUCTION

In the past ten years, encouraging progress has been made on the energy spectra of Li-like quartets. This progress is made possible by the close interaction between experiment and theory.[1–10] These quartet states are core excited but they do not couple to the continuum through the Coulomb potential. Hence optical emission is the main stabilization mechanism for the higher-excited quartets. Experimentally, a high-resolution beam-foil technique has been carried out which determines the observed wavelength to well within 0.1 Å in the ultraviolet region. Theoretically, large *LS*-coupling wave functions are used with relativistic corrections to calculate the energy accurate to a few meV. With the help of theoretical data, the emission spectral lines in the experiment are unambiguously identified. Therefore the spectra of Li-like quartets are considered to be well established for some low-Z systems.

For four-electron systems, the corresponding core-excited states would be the quintets. There are considerably fewer theoretical data available. In 1980, Bunge[11] identified the 3489-Å line in the Li spectra to be the transition between Li^- $1s2s2p^2\,{}^5P$ and $1s2p^3\,{}^5S^\circ$. This has stimulated considerable interest in searching for similar transitions in the isoelectronic sequence. This is done for Be I,[12] B II,[13,14] F VI,[15] Ne VII,[16] C III, N IV, and O V.[17,18] Theoretically, the transition energies are calculated with various versions of the multiconfiguration Dirac-Fock methods,[19,20,16,17] multiconfiguration Hartree-Fock method,[13,21] and others.[22,23] In this work, an attempt is made to calculate the transition wavelengths and fine structures with multiconfiguration-interaction wave functions. The relativistic correction, mass polarization, and Breit-Pauli operators are included using first-order perturbation theory. The procedure is similar to the earlier work on Li-like $1s2s2p\,{}^4P^\circ$-$1s2p2p\,{}^4P$ transitions.[24] In Sec. II the perturbation operators and the basis set of wave functions will be presented. Sections III and IV give the computation procedure, results, and discussions. Section V is a brief summary and conclusion.

II. THEORY

The Hamiltonian for the berylliumlike system in atomic units is given by

$$H=H_0+H_1+H_2+H_3+H_4+H_5+H_{\rm so}+H_{\rm soo}+H_{\rm ss}\ , \tag{1}$$

where

$$H_0=\sum_{i=1}^{4}\left[-\frac{1}{2}\nabla_i^2-\frac{Z}{r_i}\right]+\sum_{\substack{i,j=1\\ i<j}}^{4}\frac{1}{r_{ij}}\ , \tag{2}$$

$$H_1=-\frac{1}{8c^2}\sum_{i=1}^{4}\mathbf{P}_i^4 \tag{3}$$

is the mass correction,

$$H_2=\frac{Z\pi}{2c^2}\sum_{i=1}^{4}\delta(\mathbf{r}_i) \tag{4}$$

is the Darwin term,

$$H_3=-\frac{1}{M}\sum_{\substack{i,j=1\\ i<j}}^{4}\nabla_i\cdot\nabla_j \tag{5}$$

is the mass polarization,

$$H_4=-\frac{1}{2c^2}\sum_{\substack{i,j=1\\ i<j}}^{4}\frac{1}{r_{ij}}\left[\mathbf{P}_i\cdot\mathbf{P}_j+\frac{\mathbf{r}_{ij}(\mathbf{r}_{ij}\cdot\mathbf{P}_i)\cdot\mathbf{P}_j}{r_{ij}^2}\right] \tag{6}$$

is the retardation potential, and

$$H_5=-\frac{\pi}{c^2}\sum_{\substack{i,j=1\\ i<j}}^{4}(1+\tfrac{8}{3}\mathbf{s}_i\cdot\mathbf{s}_j)\delta(\mathbf{r}_{ij}) \tag{7}$$

is the electron Fermi contact term, where M is the nuclear mass in a.u. and $c=137.036$. The spin-orbit, spin-spin and spin-other orbit operators are given by

$$H_{\rm so}=\frac{Z}{2c^2}\sum_{i=1}^{4}\frac{\boldsymbol{l}_i\cdot\mathbf{s}_i}{r_i^3}\ , \tag{8}$$

$$H_{ss}=\sum_{\substack{i,j=1\\ i<j}}^{4}\frac{1}{c^2 r_{ij}^3}\left[\mathbf{s}_i\cdot\mathbf{s}_j-\frac{3(\mathbf{s}_i\cdot\mathbf{r}_{ij})(\mathbf{s}_j\cdot\mathbf{r}_{ij})}{r_{ij}^2}\right], \tag{9}$$

$$H_{soo}=-\frac{1}{2c^2}\sum_{\substack{i,j=1\\ i\neq j}}^{4}\left[\frac{1}{r_{ij}^3}(\mathbf{r}_i-\mathbf{r}_j)\times\mathbf{P}_i\right]\cdot(\mathbf{s}_i+2\mathbf{s}_j), \tag{10}$$

where $\mathbf{l}_i$ and $\mathbf{s}_i$ are the orbital and spin angular momentum of the ith electron. The wave function is a linear combination of basis functions which are the eigenfunctions of L^2, S^2, L_z, and S_z. L and S are the total orbital and spin angular momentum of the atomic system. Hence

$$\Psi_{LSMS_z}=A\sum_{\substack{l(i)\\ n(i)}}C_{n(i)}^{l(i)}\varphi_{n(i)}(R)Y_{l(i)}^{LM}(\hat{R})\chi_{SS_z}, \tag{11}$$

where A is the antisymmetrization operator and $C_{n(i)}^{l(i)}$ are the linear parameters. R represents, collectively, the radial parts of $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$, $\mathbf{r}_4$, and $\hat{R}$ represents their angular part. $\varphi_{n(i)}$ represents the set of all possible radial functions and $Y_{l(i)}^{LM}$ represents the set of all possible orbital angular functions. In actual calculation, truncation is necessary. The radial function is given by the product of the Slater-type orbitals:

$$\varphi_{n(i)}(R)=\prod_{j=1}^{4}r_j^{n_j}\exp(-\alpha_j r_j) \tag{12}$$

and the angular function is given by

$$\begin{aligned}Y_{l(i)}^{LM}(\hat{R})=\sum_{m_j}&\langle l_1 m_1 l_2 m_2|l_{12}m_{12}\rangle\\ &\times\langle l_{12}m_{12}l_3 m_3|l_{123}m_{123}\rangle\\ &\times\langle l_{123}m_{123}l_4 m_4|LM\rangle\prod_{j=1}^{4}Y_{l_j m_j}(\Omega_j).\end{aligned} \tag{13}$$

The spin function χ_{SS_z} is a quintet which is the eigenfunction of the total spin angular momentum with the eigenvalue of $S=2$. Each choice of $l(i)$ represents a particular partial wave for which a set of nonlinear parameters α is chosen through energy optimization. The linear parameters C are then determined by solving the secular equation from

$$\delta\langle H_0\rangle=\delta\frac{\langle\Psi|H_0|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{14}$$

This secular equation also determines the nonrelativistic zeroth-order energy E_0. The relativistic and mass-polarization corrections are obtained by using the first-order perturbation theory. That is,

$$\Delta E_{rel}=\langle\Psi|H_1+H_2|\Psi\rangle, \tag{15}$$

$$\Delta E_{msp}=\langle\Psi|H_3|\Psi\rangle, \tag{16}$$

and

$$\Delta E_{ret}=\langle\Psi|H_4|\Psi\rangle. \tag{17}$$

Since the spins of the individual electron are all parallel in a quintet, the spin function χ_{SS_z} is symmetric with respect to the exchange of any pair of spin coordinates. To have an antisymmetric total wave function, the spatial part of the wave function must be antisymmetric with respect to interchange of electron coordinates. Hence the wave function vanishes when $\mathbf{r}_i=\mathbf{r}_j$ and the expectation value for $\delta(\mathbf{r}_{ij})$ vanishes for any pair of i,j. As a consequence, the operator H_5 does not contribute to the energy of a four-electron quintet system. We now have the "center of gravity" energy E_{cg}

$$E_{cg}=E_0+\Delta E_{rel}+\Delta E_{msp}+\Delta E_{ret}. \tag{18}$$

The fine-structure energy levels are obtained by constructing the wave function with the LSJ scheme

$$\Psi_{LSJJ_z}=\sum_{M,S_z}\langle LSMS_z|JJ_z\rangle\Psi_{LSMS_z} \tag{19}$$

and

$$(\Delta E_{fs})_J=\langle\Psi_{LSJJ_z}|H_{so}+H_{soo}+H_{ss}|\Psi_{LSJJ_z}\rangle. \tag{20}$$

III. COMPUTATION

We started the calculation with the B II system by selecting a number of orbital angular partial waves. To achieve high accuracy, one usually needs to include a larger number of linear parameters in the wave function with each linear parameter corresponding to a set of $n(i)$. However, there is advantage to keeping the size of the wave function small for many reasons. Hence a term-selection process is installed to test the contribution of each term and to select a much smaller wave function without compromising the energy appreciably. For example, for the B II ^5P state, a 134-term wave function is selected from a 239-term wave function. Fourteen partial waves are adopted for this state. Some other partial waves are also tried, but their contributions to the energy are too small. The convergence pattern for this state is shown in Table I. In this table, ΔE gives the contribution to the binding energy when the corresponding partial wave is added. For example, the energy for the wave function with the first two partial wave (51 terms total) is $-17.208\,241$ a.u. The nonlinear parameters in each partial wave are individually optimized. A few of the α_1 are fixed to be 5.0 since they are very close to the optimized value and further optimization will not change the energy at the eighth digit. Each term in N corresponds to a set of $n(i)$, the powers of r in the Slater orbital. It is too complicated to give the 134 sets of $n(i)$ in this table. It will be supplied to the interested reader on request.

For the $^5S^\circ$ state calculation, it converges comparatively faster. An 89-term wave function is selected from a 139-term wave function. Eleven partial waves are used for this state. Once the partial waves and terms for B II ^5P and $^5S^\circ$ states are selected, the same partial waves and terms are also used for all other Z ions. For Be I, C III, N IV, and O V, the nonlinear parameters are reoptimized for each ion. This is actually quite laborious.

TABLE I. Convergence of nonrelativistic energy and wave function of $1s2s2p^2\,^5P$ B II (in a.u.). N is the number of linear parameters (the corresponding power of r will be supplied on request) and α_i are the nonlinear parameters. ΔE is the binding energy contributed by adding the corresponding partial wave.

	$[(l_1,l_2)l_{12},l_3]l_{123},l_4$	N	α_1	α_2	α_3	α_4	$-\Delta E$
1	[(0,0)0,1]1,1	37	4.90	2.0947	2.268	1.869	17.202 659 5
2	[(0,0)0,2]2,2	14	5.00	1.764	2.376	2.61	0.005 581 7
3	[(0,1)1,2]1,1	24	5.00	2.88	2.588	1.875	0.006 229 5
4	[(0,1)1,2]1,1	5	1.75	5.28	3.3644	1.50	0.001 337 6
5	[(0,0)0,1]1,1	10	2.5	2.035	4.52	1.869	0.001 300 1
6	[(0,2)2,3]1,1	8	5.0	2.8	2.8468	1.875	0.000 738 8
7	[(1,1)0,1]1,1	6	4.90	3.78	1.43	2.04	0.000 624 6
8	[(0,0)0,3]3,3	7	5.0	1.323	3.24	3.132	0.000 429 1
9	[(2,2)0,1]1,1	3	4.9	5.67	1.43	2.04	0.000 081 6
10	[(0,0)0,4]4,4	3	5.0	1.029	2.808	3.654	0.000 061 5
11	[(0,3)3,4]1,1	5	5.0	4.2	2.8468	1.6875	0.000 099 3
12	[(0,2)2,3]2,1	3	5.0	2.52	2.562	2.5	0.000 053 5
13	[(0,1)1,2]2,1	5	5.0	2.4	4.374	1.8	0.000 031 2
14	[(0,2)2,3]1,1	4	1.75	2.52	2.562	5.0	0.000 012 9
Total		134					17.219 243 9

For large-Z systems, we expect the nonlinear parameters to vary linearly with Z. Therefore, the results for F VI and Ne VII are obtained by simply scaling the nonlinear parameters from the wave functions of O V.

IV. RESULTS AND DISCUSSION

Although there have been many theoretical works on transition wavelengths in the literature,[14–17,19–23] very few energies have been given for either the ^5P or $^5S^\circ$ state. The only available data are given by Mannervik *et al.*[13] for B II and Agentoft *et al.*[12] for Be I where a multiconfiguration Hartree-Fock method is used. For B II, they obtain $-17.213\,540$ and $-16.866\,147$ a.u. for the ^5P and $^5S^\circ$ states, respectively. Compared with the nonrelativistic energies $-17.219\,244$ and $-16.875\,801$ a.u. obtained in this work, our results are lowered by 155 meV for ^5P and 263 meV for $^5S^\circ$. Since our results are upper bounds to the true nonrelativistic eigenvalues, the lower value should be considered as more accurate. In a very recent work by Brage and Froese-Fischer,[21] they have improved their agreement with experiment significantly. The energies of these states are not given in this reference, but based on the nonrelativistic-energy data Brage communicated to me, their results are higher by about 0.0006 a.u. for the ^5P states and about 0.001 a.u. for the $^5S^\circ$ states.[21]

The relativistic and mass polarization corrections to the energy are calculated by Eqs. (15)–(17). The relativistically corrected energies together with the nonrelativistic energies are given in Table II. Our method is somewhat different from that of Refs. 13 and 21 where perturbation operators are included in the matrix diagonalization and thus the energies are corrected to much higher order. The reason that we use strictly first-order perturbation theory is because the H_1, H_2, H_4, H_5, H_{so}, H_{soo}, and H_{ss} in Eq. (1) are only correct to first order by themselves. For the ions of interest in this work, the two methods will give essentially the same result for all perturbations except for H_1+H_2. In the case of H_1+H_2, the difference in the perturbation energy increases with Z. For O V, this perturbation energy differs by 0.000 969 a.u. for $^5S^0$ and 0.000 901 a.u. for ^5P when the two methods are compared. Also included in Table II are the transition wavelengths from previous theory and experiment.

The best theoretical data on these transition wavelengths are by Brage and Froese-Fischer.[21] Our result compares well with their result. However, in making this comparison, two more important differences should be noted. First, the retardation effect (orbit-orbit interaction) is not included in Ref. 21. We find this effect rather important. The contributions to the transition-wavelength range from -0.21 Å for Be I to -0.55 Å for F VI and -0.61 Å for Ne VII. Second, in both Refs. 13 and 21, the contact term from the spin-spin interaction is included. This corresponds to the $\mathbf{s}_i\cdot\mathbf{s}_j$ term in Eq. (7). From our discussion in Sec. III, it should not make a contribution to the quintet energy. As a check, we calculated the energy contribution of H_5 to both ^5P and $^5S^\circ$ and found none.

Comparing our wavelengths with that of the experiment, the results for O V and Ne VII lie within the experimental uncertainty. The results for Be I and N IV lie at the edge of the experimental uncertainty. Our B II result agrees with the result of Martinson *et al.*[14] but lies outside the uncertainty quoted more recently by Mannervik *et al.*[13] For C III and F VI, our results lie outside of the experimental uncertainty. In making these comparisons, one should keep in mind that the Lamb shift is neglected in the present work. Hata and Grant[19] have noted strong configuration mixing beyond the LS coupling states in

TABLE II. Energies and transition wavelengths of the $1s2s2p^2\,{}^5P$ and $1s2p^3\,{}^5S^\circ$ (E in a.u.).

	Z						
	4	5	6	7	8	9	10
$^5S^\circ$							
Nonrelativistic	−10.184 155 1	−16.875 801 1	−25.322 816 0	−35.522 557 5	−47.473 945 1	−61.176 333 6	−76.629 413 2
Relativistic	−10.185 941 0	−16.880 273 2	−25.332 337 6	−35.540 562 6	−47.505 367 7	−61.227 552 0	−76.708 731 5
^5P							
Nonrelativistic	−10.422 509 5	−17.219 243 9	−25.769 826 4	−36.072 119 5	−48.125 508 9	−61.929 427 0	−77.483 822 5
Relativistic	−10.424 488 4	−17.224 255 0	−25.780 569 0	−36.092 567 2	−48.161 216 9	−61.987 681 4	−77.574 036 3
1 a.u.→Å	455.661	455.657	455.656	455.653	455.649	455.646	455.646
			Center-of-gravity transition wavelength (in Å)				
Ref. 19			1003.7	816.4	688.1		
Ref. 20			1008.1	820.0	690.9	596.6	524.5
Ref. 21	1907.8	1323.1	1015.8	825.1	694.7	599.6	526.9
This work	1910.15	1324.65	1016.56	825.45	694.75	599.43	526.57
Experiment	1909.46±0.6[a]	1323.92±0.07[b] 1324.5±0.5[f]	1016.06±0.05[c]	825.55±0.1[c]	694.75±0.1[c]	599.67±0.1[d]	526.65±0.1[e]

[a]Converted from air wavelength in Ref. 12.
[b]Reference 13.
[c]Reference 17.
[d]Reference 15.
[e]Reference 16.
[f]Reference 14.

their work. Our result seems to support the finding of Brage and Froese-Fischer[21] that this mixing is not important to the transition-wavelength calculation.

There is another point worthwhile mentioning. As remarked earlier, the nonlinear parameters in the F VI and Ne VII are scaled from O V in this work. Since we get perfect agreement with experiment for O V, we expect that our results may gradually get worse as Z deviates from 8. From this standpoint, the comparison of our results with F VI and Ne VII experiments is somewhat unexpected.

It is interesting to compare the perturbation corrections of $1s2s2p^2\,{}^5P$ with that of Li-like $1s2s2p\,{}^4P^\circ$ and similarly for $1s2p^3\,{}^5S^\circ$ with $1s2p2p\,{}^4P$.[24] In each case, an additional $2p$ electron is added. This comparison is given in Table III. Intuitively, one would expect the $\langle H_1+H_2\rangle$ correction to become larger with the extra $2p$ electron. This is not the case for $Z=4$ and $Z=5$ ^5P states and the $Z=4$ $^5S^\circ$ state. It may be caused by two factors: The repulsion of the electrons reduces the contribution from each $2p$ electron and the penetration of the $2p$ electron shields the $2s$ electron more from the nucleus.

TABLE III. Comparison of perturbation corrections for $1s2s2p^2\,{}^5P$ and $1s2p^3\,{}^5S^\circ$ with $1s2s2p\,{}^4P^\circ$ and $1s2p2p\,{}^4P$ systems (in a.u., see Ref. 24, [−2] implies $\times 10^{-2}$ to the quoted number in the table).

Z	4	5	6	7	8	9	10
$1s2p^3\,{}^5S^\circ$							
$\Delta E_{\rm rel}[-2]$	−0.180 30	−0.457 52	−0.979 39	−1.858 53	−3.246 71	−5.293 05	−8.187 26
$\Delta E_{\rm mps}[-4]$	−0.615	−1.108	−1.792	−2.387	−2.993	−3.417	−4.226
$\Delta E_{\rm ret}[-4]$	0.786	2.140	4.515	8.189	13.438	20.538	29.769
$1s2s2p^2\,{}^5P$							
$\Delta E_{\rm rel}[-2]$	−0.198 46	−0.507 40	−1.091 75	−2.082 74	−3.639 57	−5.938 51	−9.190 00
$\Delta E_{\rm mps}[-4]$	−0.475	−0.813	−1.279	−1.675	−2.078	−2.355	−2.892
$\Delta E_{\rm ret}[-4]$	0.531	1.441	3.028	5.472	8.955	13.661	19.755
$1s2s2p\,{}^4P^\circ$							
$\Delta E_{\rm rel}[-2]$	−0.2009	−0.5086	−1.0821	−2.0439	−3.537 11	−5.7353	
$\Delta E_{\rm mps}[-4]$	−0.32	−0.51	−0.76	−0.97	−1.17	−1.31	
$\Delta E_{\rm ret}[-4]$	0.35	0.85	1.69	2.96	4.73	7.10	
$1s2p2p\,{}^4P$							
$\Delta E_{\rm rel}[-2]$	−0.1806	−0.4540	−0.9619	−1.8131	−3.1365	−5.0803	
$\Delta E_{\rm mps}[-4]$	−0.61	−0.98	−1.48	−1.89	−2.31	−2.58	
$\Delta E_{\rm ret}[-4]$	0.69	1.71	3.41	5.96	9.54	14.33	

TABLE IV. Spin-orbit, spin-spin, and spin-other-orbit energies for the $1s2s2p^2\,{}^5P_3$ states of Be-like systems (in a.u., [−3] implies $\times 10^{-3}$ to the quoted number in the table).

Z	4	5	6	7	8	9	10
$\langle H_{so}\rangle$[−3]	0.043 85	0.072 16	0.357 12	0.743 46	1.378 59	2.350 18	3.759 70
$\langle H_{ss}\rangle$[−4]	−0.0363	−0.0943	−0.1927	−0.3418	−0.5520	−0.8336	−1.1972
$\langle H_{soo}\rangle$[−3]	−0.041 54	−0.1101	−0.226 71	−0.405 41	−0.658 32	−1.000 84	−1.441 64

For larger Z, these effects become relatively less important as can be seen from this table. The retardation effect mostly comes from the interaction of the $2p$-$1s$ electrons. It is interesting to note that the ratio of ΔE_{ret} for ${}^5S^\circ$ to ${}^5P$ is about 1.5 and that of ${}^4P$ to ${}^4P^\circ$ is about 2.0 which are the ratios of the number of $2p$ electrons. In comparing $1s2p2p\,{}^4P$ with $1s2s2p2p\,{}^5P$, one notices that the presence of the extra $2s$ electron reduces ΔE_{ret} slightly and this reduction increases uniformly from $Z=4$ to $Z=9$. The ratio of ΔE_{ret} for ${}^5S^\circ$ to ${}^4P$ increases from 1.139 for $Z=4$ to 1.433 for $Z=9$, showing the effect of Coulomb repulsion which becomes relatively less important as nuclear charge increases. The mass-polarization corrections behave much the same way as that of the retardation perturbation.

For the fine structure, the $\langle H_{so}\rangle$, $\langle H_{soo}\rangle$, and $\langle H_{ss}\rangle$ are calculated for the ${}^5P_3$ states. These results are given in Table IV. The results for $J=1$ and $J=2$ are obtained using the Wigner-Eckert theorem. From these energies, the transition wavelengths and fine-structure splittings are evaluated. These results are given in Table V. For the most part, the fine structures of this calculation lie between that of MCDF-OL (Ref. 17) and Hata and Grant.[19] The comparison with experiments is reasonable but not exceptional. Adding QED contributions improves the agreement only very slightly.[19] The experimental ν_{32} of C III and ν_{21} of F VI in this table are computed from the quoted wavelengths. In the case of F VI, ν_{21} is given to be 453 cm^{-1} in Ref. 15. However, this contradicts the quoted fine-structure wavelengths and these wavelengths do give the correct λ_{cg} in this reference.

In comparing the calculated fine structures with experiments, we noted that the N IV results give the best agreement, whereas the C III results differ slightly. For O V, the experimental result for ν_{32} is 188±2 cm^{-1}. However, for this system, the error bars differ by 0.05 Å in the quoted two wavelengths. Assuming that the fine-structure uncertainty comes only from this difference (most favorable case) the uncertainty in ν_{32} would be ±10 cm^{-1}. Hence the 182.6 cm^{-1} obtained in this work would be within the experimental uncertainty. Our ν_{21} for O V, 243 cm^{-1}, is clearly too small compared with the 252±4 cm^{-1}. In the case of F VI, our 424 cm^{-1} compares well with the revised ν_{21} of 419±20 cm^{-1} (from 453

TABLE V. Fine structures for the $1s2s2p^2\,{}^5P_J$ states of Be-like systems (experimental data are taken from Ref. 17 for $Z=6,7,8$, Ref. 15 for $Z=9$, and Ref. 16 for $Z=10$).

		Transition wavelength λ_J (Å)			Fine-structure splitting (cm^{-1})				
Z	J	This work	Expt.	$\Delta\lambda$		This work	Expt.	Ref. 19	Ref. 16
	1	1910.02			ν_{21}	6.09		6.65	
4	2	1910.24			ν_{32}	−2.83		−0.52	
	3	1910.14							
	1	1324.74			ν_{21}	6.16		22.98	
5	2	1324.85			ν_{32}	−21.81		6.13	
	3	1324.47							
	1	1015.96	1015.43±0.05	0.53	ν_{21}	58.23	63.5(1.5)	59.63	57
6	2	1016.57	1016.09±0.05	0.48	ν_{32}	23.89	21.3[a]	30.21	21
	3	1016.81	1016.31±0.05	0.50					
	1	824.51	824.60±0.05	−0.09	ν_{21}	126.70	127(1)	129.19	125
7	2	825.37	825.47±0.05	−0.10	ν_{32}	77.52	79.5(.8)	86.72	73
	3	825.90	826.01±0.05	−0.11					
	1	693.40	693.36±0.05	0.04	ν_{21}	242.88	252(4)	247.34	242
8	2	694.57	694.57±0.05	0.00	ν_{32}	182.60	188(2)	194.95	176
	3	695.45	695.48±0.10	−0.03					
	1	597.61	597.80±0.10	−0.19	ν_{21}	424.21	419(20)[b]	433.19	426
9	2	599.13	599.30±0.08	−0.17	ν_{32}	361.87	396(20)	378.50	354
	3	600.43	600.73±0.08	−0.30					
	1	524.21	524.20±0.20	0.01	ν_{21}	692.67	711(22)	709.46	700
10	2	526.12	526.16±0.10	−0.04	ν_{32}	644.87	680(7)	665.17	633
	3	537.91	528.05±0.10	−0.14					

[a]Calculated from wavelength.

[b]Calculated from wavelength, quoted to be 453 cm^{-1} in Ref. 15. See discussion in text.

cm^{-1}). But our ν_{32}, 362 cm^{-1}, is too small compared with the 396±20 cm^{-1} from the experiment. For Ne VII the calculated ν_{21}, 693 cm^{-1}, lies on the edge of experimental uncertainty, 711±22 cm^{-1}. But the calculated ν_{32}, 645 cm^{-1}, is substantially smaller than the 680±7 cm^{-1} from the experiment.

The B II result in this work differs drastically with that of Hata and Grant.[19] Unfortunately, no experimental data are available to make a more critical assessment in this case. It should be noted that the "spin-orbit operator" defined as Eq. (8) does not contain the Coulomb field from the other electrons. Therefore the spin-orbit result given in Table IV is not equivalent to the MCDF results of Ref. 19 even though the total fine-structure results agree reasonably well for $Z > 5$ systems.

V. CONCLUSION

In this work, the energies, transition wavelengths, and fine structures for the $1s2s2p\,^2\,^5P$ and $1s2p^3\,^5S^\circ$ are studied for $Z=4-10$. The wavelength results agree well with experiments. This in itself does not guarantee that our individual states are calculated to high accuracy since the wavelength comes from the difference of two energies. However, compared with the accurate multiconfiguration Hartree-Fock calculation of Mannervik *et al.*,[13] our B II nonrelativistic results are better by 263 and 155 meV. This is probably a good indication that our results are quite accurate. The fine structure compares reasonably with experiment, but in some cases our data lie outside of the uncertainty quoted in the experiment.

Although the Li-like quartet optical spectra have been well studied in the literature, the Be-like quintet data are still very limited. I hope the accuracy provided in this investigation can be extended to higher excited quintet states so as to help experimental identification of the Be-like spectra in the near future.

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