Relativistic energy, fine structure, and hyperfine structure of the high-lying core-excited states $^5P(n)$ $(n=1-7)$ and $^5S^o(m)$ $(m=1-5)$ for Be-like boron and carbon

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(Received 5 November 2003; published 21 April 2004)

The variational method with multiconfiguration interaction wave function is used to obtain the energies of high-lying core-excited states $^5P(n)$ $(n=1-7)$ and $^5S^o(m)$ $(m=1-5)$ in Be-like boron and carbon, including the mass polarization and relativistic corrections. Restricted variational method is carried out to extrapolate a better energy. The oscillator strengths, transition rates, and wavelengths are also calculated. The results are compared with other theoretical and experimental data in the literature. The fine structure and hyperfine structure of core-excited states for this system are also investigated.

DOI: 10.1103/PhysRevA.69.042513 PACS number(s): 32.10.Fn, 32.70.Cs, 31.30.Jv

I. INTRODUCTION

In the past few decades, the core-excited states of beryllium-like ions have attracted considerable attention to both theoretical [1–12] and experimental [13–18]. The high-lying core-excited quintet state of beryllium-like ions is a complex four-electron atomic system with high orbital, spin, and angular momentum quantum numbers, which can be stable against Coulomb autoionization because of well-known angular-momentum and parity-selection rules. The progress in beam-foil and beam-gas electron spectroscopy offers the possibility to study excitation mechanisms for this system by creating such quintet states with very large cross sections. The studies of the core-excited states of beryllium-like ions play an important role in developing the excited-state theory of multielectron atoms and better understanding the complicated correlation effects between electrons.

Bruch *et al.* [1] were the first to discuss the possibility of observing optical transitions between quintet states of Be, who suggested that transitions among the quintet states of Be could be responsible for some of the unidentified lines in the Be beam-foil spectrum. Later, Bruch, Schneider, and collaborators [13–15] extended their electron-spectroscopic studies to Be-like boron and carbon. In the calculation of energies and transition rates for some high-lying states of high multiplicities in light atoms and ions, Beck and Nicolaides [2] found the wavelength of the $1s2s2p^2\ ^5P$-$1s2p^3\ ^5S^o$ transition in B^+ should lie close to 131.0 nm by using the first-order theory of oscillator strengths. Their results were consistent with beam-foil data (132.45 ± 0.05 nm, lifetime 0.75 ± 0.08 ns) reported in 1970 by Martinson *et al.* [16] and 0.65 ± 0.04 ns subsequently obtained by Kernahan *et al.* [17]. Schneider *et al.* [3] presented a Grotrian diagram for the quintet states in C^{2+} obtained from calculated energies. Later, the $1s2s2p^2\ ^5P$-$1s2p^3\ ^5S^o$ transition in B^+ was improved in beam-foil spectroscopy and multiconfiguration Hartree-Fock (MCHF) calculations by Mannervik *et al.* [5]. Their experimental wavelength and lifetime [5] 132.392 ± 0.007 nm and 0.65 ± 0.01 ns are more than five times more accurate than previous experimental results. The theoretical results 131.16 nm and 0.601 ns of Mannervik *et al.* [5] are in good agreement with previous theoretical predictions of Beck and Nicolaides [2], but not very close to the experimental values of themselves. Subsequently, Brage and Fischer [4] extended the MCHF calculation allowing for more correlation and including relativistic effects, thus obtaining a value of 132.31 nm for the transition wavelength in very good agreement with the experimental results. So far, to our knowledge, quite few calculations of the high-*n* core-excited states for Be-like system have been reported due to the restriction of resolution from experiments and the numerical unsteadiness in theoretical calculations, and the identification of the transition line among the high-*n* core-excited quintet states of Be-like ions is very difficult.

In the past two decades, some theoretical methods [6–10] have been used to explore fine structure and hyperfine structure of core-excited states for Be-like isoelectronic sequence. Cheng *et al.* [6] reported the fine and hyperfine structure of the doubly excited states of the $^7Li^-$ spectrum using multiconfiguration Dirac-Fock method. Yang and Chung [7] first reported the results of fine structure and hyperfine structure of the lowest core-excited states of Be-like isoelectronic sequence. To our knowledge, few calculations of fine structure and hyperfine structure have been investigated for the corresponding core-excited states of Be-like system.

In this paper, variational method with multiconfiguration interaction wave function is carried out on the high-lying core-excited states $^5P(n)$ $(n=1-7)$ and $^5S^o(m)$ $(m=1-5)$ for the Be-like boron and carbon. The relativistic energies, the fine structure, the hyperfine parameters, and the coupling constants are reported and discussed. The oscillator strengths, transition rates, and wavelengths are also given to compare with experiments. It is our hope to provide more reliable theoretical data to stimulate further experimental measurements.

II. THEORY

The nonrelativistic Hamiltonian for the Be-like ions is given in atomic units by

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TABLE I. Relativistic energies (a.u.) of the core-excited states $^5P(n)$ $(n=1-7)$ and $^5S^o(m)$ $(m=1-5)$ for Be-like boron and carbon. N_l is the number of the angular-spin components in the wave function.

Resonances	N_l	E_b	ΔE_{RV}	E_{nonrel} This work	E_{nonrel} Others		E_{rel}	E_{total} This work	E_{total} Others
					B^+				
$1s2s2p^2\ ^5P(1)$	44	−17.2200671	−0.0000829	−17.2201500	−17.213540[a]	−17.2201314[b]	−0.0050160	−17.2251660	−17.218608[a]
$1s2s2p3p\ ^5P(2)$	43	−16.5548652	−0.0000812	−16.5549464			−0.0050479	−16.5599943	
$1s2s2p4p\ ^5P(3)$	39	−16.4171265	−0.0000846	−16.4172111			−0.0050492	−16.4222603	
$1s2s2p5p\ ^5P(4)$	43	−16.3594842	−0.0000738	−16.3595580			−0.0050470	−16.3646050	
$1s2p2p5s\ ^5P(5)$	40	−16.3448892	−0.0000842	−16.3449734			−0.0046936	−16.3496670	
$1s2s2p6p\ ^5P(6)$	40	−16.3294026	−0.0000740	−16.3294766			−0.0050490	−16.3345257	
$1s2s2p7p\ ^5P(7)$	41	−16.3119175	−0.0000850	−16.3120025			−0.0050394	−16.3170419	
$1s2p^3\ ^5S^o(1)$	30	−16.8764307	−0.0000578	−16.8764885	−16.866147[a]	−16.8764239[b]	−0.0044869	−16.8809754	−16.870761[a]
$1s2p^23p\ ^5S^o(2)$	35	−16.2747458	−0.0000571	−16.2748029			−0.0044720	−16.2792749	
$1s2p^24p\ ^5S^o(3)$	33	−16.1453463	−0.0000575	−16.1454038			−0.0044801	−16.1498839	
$1s2p^25p\ ^5S^o(4)$	29	−16.0900374	−0.0000756	−16.0901130			−0.0044698	−16.0945828	
$1s2p^26p\ ^5S^o(5)$	29	−16.0611478	−0.0000829	−16.0612307			−0.0044648	−16.0656955	
					C^{2+}				
$1s2s2p^2\ ^5P(1)$	44	−25.7706181	−0.0000851	−25.7707032		−25.7706177[b]	−0.0107440	−25.7814472	
$1s2s2p3p\ ^5P(2)$	49	−24.5764092	−0.0000835	−24.5764927			−0.0107209	−24.5872136	
$1s2p2p3s\ ^5P(3)$	45	−24.3245807	−0.0000884	−24.3246691			−0.0097160	−24.3343850	
$1s2s2p4p\ ^5P(4)$	45	−24.2919942	−0.0000832	−24.2920774			−0.0107170	−24.3027945	
$1s2s2p5p\ ^5P(5)$	39	−24.1704162	−0.0000863	−24.1705025			−0.0106778	−24.1811803	
$1s2p^3\ ^5S^o(1)$	29	−25.3234479	−0.0000575	−25.3235054		−25.3234390[b]	−0.0095387	−25.3330442	
$1s2p^23p\ ^5S^o(2)$	32	−24.2161488	−0.0000570	−24.2162058			−0.0094612	−24.2256670	
$1s2p^24p\ ^5S^o(3)$	30	−23.9465602	−0.0000658	−23.9466260			−0.0094468	−23.9560728	
$1s2p^25p\ ^5S^o(4)$	32	−23.8283594	−0.0000542	−23.8284136			−0.0094472	−23.8378608	
$1s2p^26p\ ^5S^o(5)$	31	−23.7659362	−0.0000726	−23.7660088			−0.0094423	−23.7754511	

[a]Reference [5].
[b]Reference [7].

$$\hat{H}_0 = \sum_{i=1}^{4}\left[-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right] + \sum_{\substack{i,j=1\\ i<j}}^{4}\frac{1}{r_{ij}}. \tag{1}$$

The basic wave function ψ_b can be written as

$$\psi_b(1,2,3,4) = A\sum_i C_i \phi_{n(i),l(i)}(R) Y_{l(i)}^{LM}(\Omega)\chi_{SS_z}, \tag{2}$$

where A is the antisymmetrization operator and the radial basis function are Slater orbitals:

$$\phi_{n(i),l(i)}(R) = \prod_{j=1}^{4} r_j^{n_j}\exp(-\alpha_j r_j). \tag{3}$$

A different set of nonlinear parameters α_j is used for each angular-spin component. The linear parameters C_i and the nonlinear parameters α_j are determined in the energy optimization process.

The upper bounds E_b of the core-excited quintet states are calculated using the Rayleigh-Ritz variation method,

$$\delta E_b = \delta\langle H_0\rangle = \delta\frac{\langle\psi_b|H_0|\psi_b\rangle}{\langle\psi_b|\psi_b\rangle}. \tag{4}$$

In the variational calculation, the 2*s* electron of these quintet states could be stable against equivalent 1*s* electrons because of the Pauli exclusion principle.

Restricted variational method is used to further improve energy E_b. The basic wave function ψ_b is used as a single term in an improved wave function [19] that is given by

$$\Phi(1,2,3,4) = D_0\psi_b(1,2,3,4) + \psi_2(1,2,3,4), \tag{5}$$

where

$$\psi_2(1,2,3,4) = A\sum_{i=1}^{I} D_i\Phi_{n(i)l(i)}(1,2,3,4). \tag{6}$$

To saturate the functional space, ψ_2 takes the same form as $\psi_b(1,2,3,4)$, but the nonlinear parameters are much different from those of $\psi_b(1,2,3,4)$. Each of nonlinear parameters in the basis function of ψ_2 is optimized in the restricted variational calculation. The total nonrelativistic energy is obtained by adding improvement from restricted variation

TABLE II. Wavelengths λ (nm), oscillator strength (f_l, f_v, f_a), transition rates (s^{-1}), and lifetime τ (ns) of some core-excited quintet states for Be-like Boron and Carbon. The numbers in brackets indicates the powers of 10.

Transitions	Source	f_l	f_v	f_a	A_l	A_v	A_a	τ	λ
				B^+					
$1s2p^3\ ^5S^o(1)$	This work	0.1405	0.1405	0.1416	1.599[9]	1.598[9]	1.611[9]	0.625	132.386
$\rightarrow 1s2s2p^2\ ^5P(1)$									
	Others[a]	0.143	0.142					0.65±0.01	132.392±0.007[b]
	Others[c]	0.143	0.149					0.65±0.04	132.45±0.05[b]
$1s2s2p3p\ ^5P(2)$	This work	0.107[−4]	0.112[−4]	0.257[−4]	1.181[4]	1.241[4]	2.842[4]	84674.01	141.959
	Others[a]								141.3
$1s2s2p4p\ ^5P(3)$	This work	0.872[−4]	0.853[−4]	0.132[−4]	1.972[5]	1.928[5]	2.987[5]	5070.99	99.334
$1s2s2p5p\ ^5P(4)$	This work	0.0003	0.0003	0.0002	8.015[5]	8.106[5]	6.109[5]	1247.66	88.243
$1s2p2p5s\ ^5P(5)$	This work	0.1891	0.1870	0.1927	5.723[8]	5.659[8]	5.832[8]	1.747	85.762
	Others[a]								85.91, 85.77±0.02[b]
$1s2s2p6p\ ^5P(6)$	This work	0.0023	0.0023	0.0024	7.348[6]	7.345[6]	7.646[6]	136.09	83.386
$1s2s2p7p\ ^5P(7)$	This work	0.0008	0.0008	0.0007	2.726[6]	2.600[6]	2.255[6]	366.84	80.800
$1s2p^23p\ ^5S^o(2)$	This work	0.0738	0.0730	0.0888	5.582[8]	5.525[8]	6.719[8]	1.791	162.319
$\rightarrow 1s2s2p3p\ ^5P(2)$									
	Others[d]								162.4
$1s2p^24p\ ^5S^o(3)$	This work	0.0679	0.0679	0.0960	4.836[8]	4.833[8]	6.837[8]	2.068	167.291
$\rightarrow 1s2s2p4p\ ^5P(3)$									
$1s2p^25p\ ^5S^o(4)$	This work	0.0603	0.0609	0.0756	4.085[8]	4.545[8]	5.294[8]	2.448	168.749
$\rightarrow 1s2s2p5p\ ^5P(4)$									
$1s2p^26p\ ^5S^o(5)$	This work	0.0002	0.0002	0.0003	1.143[6]	1.451[6]	2.267[6]	874.89	160.460
$\rightarrow 1s2p2p5s\ ^5P(5)$									
				C^{2+}					
$1s2p^3\ ^5S^o(1)$	This work	0.1150	0.1150	0.1254	2.217[9]	2.216[9]	2.476[9]	0.451	101.618
$\rightarrow 1s2s2p^2\ ^5P(1)$									
	Others[e]							0.49±0.03	101.4±0.5
	Others[f]							0.49±0.03	101.606±0.005[b]
$1s2s2p3p\ ^5P(2)$	This work	0.0003	0.0003	0.0002	1.612[6]	1.545[6]	1.000[6]	620.35	61.094
	Others[e]								61.3
$1s2p2p3s\ ^5P(3)$	This work	0.1774	0.1770	0.1814	1.895[9]	1.891[9]	1.938[9]	0.528	45.627
	Others[e]								46.6
$1s2s2p4p\ ^5P(4)$	This work	0.0109	0.0109	0.0108	1.235[8]	1.239[8]	1.225[8]	8.097	44.228
$1s2s2p5p\ ^5P(5)$	This work	0.0488	0.0485	0.0480	6.953[8]	6.910[8]	6.837[8]	1.438	39.558
$1s2p^23p\ ^5S^o(2)$	This work	0.0610	0.0610	0.0830	7.637[8]	7.617[8]	1.039[9]	1.309	126.030
$\rightarrow 1s2s2p3p\ ^5P(2)$									
$1s2p^24p\ ^5S^o(3)$	This work	0.0030	0.0032	0.0012	4.141[7]	4.473[7]	1.621[7]	24.15	120.445
$\rightarrow 1s2p2p3s\ ^5P(3)$									
$1s2p^25p\ ^5S^o(4)$	This work	0.0004	0.0004	0.0003	8.061[6]	8.017[6]	7.633[6]	124.05	98.005
$\rightarrow 1s2s2p4p\ ^5P(4)$									
$1s2p^26p\ ^5S^o(5)$	This work	0.0004	0.0004	0.0002	6.390[6]	6.158[6]	2.919[6]	156.49	112.306
$\rightarrow 1s2s2p5p\ ^5P(5)$									

[a]Reference [5].
[b]Experimental.
[c]Reference [16].
[d]Reference [23].
[e]Reference [3].
[f]Reference [18].

TABLE III. Center-of-gravity total energies E_{CG} (in a.u.), fine-structure corrections ΔE_J (in a.u.), and fine-structure splittings $\nu_{J-J'}$ (in cm^{-1}) of the core-excited states $^5P(n)$ $(n=1-5)$ for Be-like boron and carbon.

		$^5P^e(1)$	$^5P^e(2)$	$^5P^e(3)$	$^5P^e(4)$	$^5P^e(5)$
			B^+			
E_{CG}		−17.2251660	−16.5599943	−16.4222603	−16.364605	−16.3495483
ΔE_J	$J=1$	−0.0000861	−0.0000683	−0.0000670	-0.0000814	−0.0001070
	$J=2$	0.0000151	0.0000046	0.0000030	0.0000172	0.0000098
	$J=3$	−0.0000261	−0.0000260	0.0000266	0.0000226	0.0000389
ν_{2-1}		22.20	15.99	15.36	21.63	25.62
Others		22.98[a]				
ν_{3-2}		2.42	4.71	5.18	1.20	6.38
Others		6.13[a]				
			C^{2+}			
E_{CG}		−25.7814472	−24.5872136	−24.3343850	−24.3027945	−24.1811803
ΔE_J	$J=1$	−0.0002647	−0.0001944	−0.0003109	−0.0001884	−0.0001914
	$J=2$	0.0000010	−0.0000116	−0.0000114	−0.0000129	0.0000057
	$J=3$	0.0001127	0.0000916	0.0001414	0.0000899	0.0000779
V_{2-1}		58.33	40.13	65.72	38.53	43.25
Others		59.63[a]				
		57[b]				
		63.5[c]				
v_{3-2}		24.51	22.64	33.52	22.56	15.85
Others		30.21[a]				
		21[b]				
		21.3[c]				

[a]Reference [9].
[b]Reference [10].
[c]Reference [18] (Expt.).

ΔE_{RV}. Then the nonrelativistic energy is given by $E_b + \Delta E_{RV}$.

In addition to the ΔE_{RV}, the total energy is further improved by including the mass polarization effect and relativistic corrections. The relativistic perturbation operators considered in this work are correction to the kinetic energy (P^4), Darwin term, electron-electron contact term, and orbit-orbit interaction. The mass polarization perturbation and the relativistic corrections are calculated using first-order perturbation theory. The perturbation operators are given by [20]

$$H' = H_k + H_D + H_{ee} + H_{mp} + H_{oo}, \tag{7}$$

where

$$\hat{H}_k = -\frac{1}{8C^2}\sum_{i=1}^{4} P_i^4 \quad \text{(correction to kinetic energy)}, \tag{8}$$

$$\hat{H}_D = \frac{Z\pi}{2C^2}\sum_{i=1}^{4} \delta(\boldsymbol{r}_i) \quad \text{(Darwin term)}, \tag{9}$$

$$\hat{H}_{ee} = -\frac{\pi}{C^2}\sum_{\substack{i,j=1 \\ i<j}}^{4}\left(1+\frac{8}{3}\boldsymbol{s}_i\cdot\boldsymbol{s}_j\right)\delta(\boldsymbol{r}_{ij}) \quad \text{(electron -electron interaction)}, \tag{10}$$

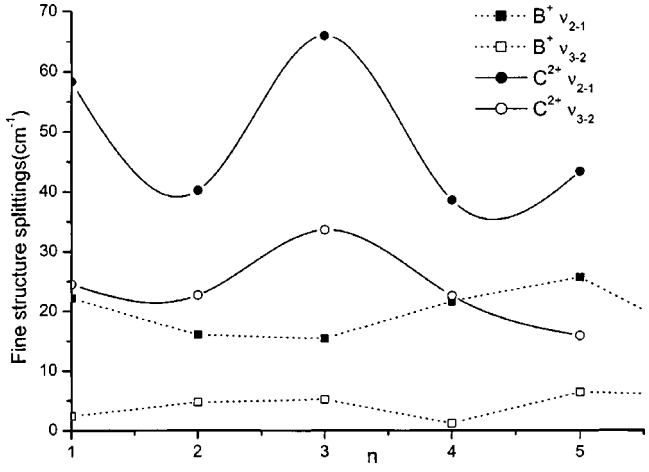

FIG. 1. Fine-structure splittings $\nu_{j-j'}$(in cm^{-1}) of core-excited states $^5P^e(n)$ $(n=1-5)$ for Be-like boron and carbon.

TABLE IV. Hyperfine parameters (in a.u.) of the core-excited states $^5P(n)$ $(n=1-3)$ and $^5S^o(m)$ $(m=1-3)$ for Be-like boron and carbon.

Resonances	a_c	a_{SD}	a_l	b_q
		B^+		
$1s2s2p^2\ ^5P^e(1)$	525.7025	0.43858	2.16935	0.87717
$1s2s2p3p\ ^5P^e(2)$	531.9075	0.30142	1.47869	0.60285
$1s2s2p4p\ ^5P^e(3)$	532.6763	0.28120	1.40294	0.56241
$1s2p^3\ ^5S^o(1)$	487.6366			
$1s2p^23p\ ^5S^o(2)$	489.4645			
$1s2p^24p\ ^5S^o(3)$	489.9915			
		C^{2+}		
$1s2s2p^2\ ^5P^e(1)$	916.1866	0.9023243	4.471033	1. 804649
$1s2s2p3p\ ^5P^e(2)$	925.2372	0.6058896	2.997254	1.211779
$1s2p2p3s\ ^5P^e(3)$	860.6288	1.0280430	5.073973	2.056086
$1s2p^3\ ^5S^o(1)$	843.2432			
$1s2p^23p\ ^5S^o(2)$	846.8645			
$1s2p^24p\ ^5S^o(3)$	847.4492			

$$\hat{H}_{oo} = -\frac{1}{2C^2}\sum_{\substack{i,j=1\\ i<j}}^{4}\frac{1}{\boldsymbol{r}_{ij}}\left[\boldsymbol{P}_i\cdot\boldsymbol{P}_j+\frac{\boldsymbol{r}_{ij}(\boldsymbol{r}_{ij}\cdot\boldsymbol{P}_i)\cdot\boldsymbol{P}_j}{\boldsymbol{r}_{ij}^2}\right] \quad \text{(orbit -orbit interaction)}, \tag{11}$$

$$\hat{H}_{mp} = -\frac{1}{M}\sum_{\substack{i,j=1\\ i<j}}^{4}\boldsymbol{\nabla}_i\cdot\boldsymbol{\nabla}_j \quad \text{(mass polarization term)}, \tag{12}$$

where M is the nuclear mass, the $\boldsymbol{s}_i$ and $\boldsymbol{P}_i$ are the spin and the linear momentum of the ith electron, respectively.

The relativistic and mass polarization corrections are given by

$$\Delta E_{rel} = \langle\psi_b|\hat{H}_k+\hat{H}_D+\hat{H}_{ee}+\hat{H}_{oo}+\hat{H}_{mp}|\psi_b\rangle. \tag{13}$$

The total energy becomes

$$E_{\text{total}} = E_b+\Delta E_{RV}+\Delta E_{rel}. \tag{14}$$

The fine-structure perturbation operators [8] are given by

$$H_{FS} = H_{SO}+H_{SOO}+H_{SS}, \tag{15}$$

where the spin-orbit, spin-other-orbit, and spin-spin operators are

$$H_{SO} = \frac{Z}{2c^2}\sum_{i=1}^{4}\frac{\boldsymbol{1}_i\cdot\boldsymbol{s}_i}{r_i^3}, \tag{16}$$

$$H_{SOO} = -\frac{1}{2c^2}\sum_{\substack{i,j=1\\ i\neq j}}^{4}\left[\frac{1}{r_{ij}^3}(\boldsymbol{r}_i-\boldsymbol{r}_j)\times\boldsymbol{P}_i\right]\cdot(\boldsymbol{s}_i+2\boldsymbol{s}_j), \tag{17}$$

$$H_{SS} = \frac{1}{c^2}\sum_{\substack{i,j=1\\ i<j}}^{4}\frac{1}{r_{ij}^3}\left[\boldsymbol{s}_i\cdot\boldsymbol{s}_j-\frac{3(\boldsymbol{s}_i\cdot\boldsymbol{r}_{ij})(\boldsymbol{s}_j\cdot\boldsymbol{r}_{ij})}{r_{ij}^2}\right]. \tag{18}$$

To calculate the fine-structure splitting, the *LSJ* coupling scheme is used:

$$\Psi_{LSJJ_Z} = \sum_{S_Z,L_Z}\langle LSL_ZS_Z|JJ_Z\rangle\psi_b(1,2,3,4). \tag{19}$$

The fine-structure energy levels are calculated by first-order perturbation theory:

$$(\Delta E_{FS})_J = \langle\Psi_{LSJJ_Z}|H_{SO}+H_{SOO}+H_{SS}|\Psi_{LSJJ_Z}\rangle. \tag{20}$$

For an N-electron system, the hyperfine interaction Hamiltonian can be represented as follows [21,22]:

$$H_{hfs} = \sum_{k=1}T^{(k)}\cdot M^{(k)}, \tag{21}$$

where $T^{(k)}$ and $M^{(k)}$ are spherical tensor operators of rank k in the electronic and nuclear space, respectively. The $k=1$ term represents the magnetic-dipole interaction between the magnetic field generated by the electrons and nuclear magnetic-dipole moments, the $k=2$ term the electric quadrupole interaction between the electric-field gradient from the electrons and the nonspherical charge distribution of the nucleus. The contributions from higher-order terms are much smaller and can often be neglected.

In the nonrelativistic framework, the electronic tensor operators, in atomic units, can be written as

$$T^{(1)} = \frac{\alpha^2}{2}\sum_{i=1}^{4}\left[2g_l r_i^{-3}l_i^{(1)}-\sqrt{10}g_s\{s_i^{(1)}C_i^{(2)}\}^{(1)}r_i^{-3}+\frac{8\pi}{3}g_s s_i^{(1)}\delta(\mathbf{r}_i)\right] \tag{22}$$

and

$$T^{(2)} = -\sum_{i=1}^{4}r_i^{-3}C_i^{(2)}, \tag{23}$$

where $g_l=(1-m_e/M)$ is the orbital electron g factor, and $g_s=2.002\ 319\ 3$ is the electron spin g factor. M is the nuclear mass. The tensor $\boldsymbol{C}_i^{(2)}$ is connected to the spherical harmonics $\boldsymbol{Y}_{lm}(\boldsymbol{i})$ by $C_m^{(l)}=\sqrt{4\pi/2l+1}\,\boldsymbol{Y}_{lm}$.

The hyperfine interaction couples the electronic angular momenta **J** and the nuclear angular momenta **I** to a total angular momentum $\mathbf{F}=\mathbf{I}+\mathbf{J}$. The uncoupling and coupling hyperfine constants are defined in atomic units as [21,22]

$$a_C = \langle\gamma LSLS|\sum_{i=1}^{N}8\pi\delta^3(\boldsymbol{r}_i)\boldsymbol{s}_0(i)|\gamma LSLS\rangle \quad \text{(Fermi contact)}, \tag{24}$$

TABLE V. Hyperfine coupling constants (in GHz) of the core-excited states $^5P(n)$ $(n=1-3)$ and $^5S^o(m)$ $(m=1-3)$ for Be-like boron and carbon. The numbers in brackets indicate the powers of 10.

	A_j			B_j		
Resonances	$J=3$	$J=2$	$J=1$	$J=3$	$J=2$	$J=1$
			B^+			
$1s2s2p^2\ ^5P^e(1)$	3.39871	4.17961	7.49181	−1.74611[−2]	1.74611[−2]	−1.74611[−3]
$1s2s2p3p\ ^5P^e(2)$	3.42243	4.23095	7.59463	−1.20004[−2]	1.20004[−2]	−1.20004[−3]
$ls2s2p4p\ ^5P^e(3)$	3.42550	4.23760	7.60695	−1.11954[−2]	1.11954[−2]	−1.11954[−3]
$1s2p^3\ ^5S^o(1)$		4.65964				
$1s2p^23p\ ^5S^o(2)$		4.67710				
$1s2p^24p\ ^5S^o(3)$		4.68214				
			C^{2+}			
$1s2s2p^2\ ^5P^e(1)$	−6.35909	−7.79724	−13.9653	−1.45272[−2]	1.45272[−2]	−1.45272[−3]
$1s2s2p3p\ ^5P^e(2)$	−6.38463	−7.87906	−14.1357	−9.75469[−3]	9.75469[−3]	−9.75469[−4]
$1s2p2p3s\ ^5P^e(3)$	−5.99503	−7.32134	−13.0999	−1.65513[−2]	1.65513[−2]	−1.65513[−3]
$1s2p^3\ ^5S^o(1)$		−8.62755				
$1s2p^23p\ ^5S^o(2)$		−8.66460				
$1s2p^24p\ ^5S^o(3)$		−8.67059				

$$a_{SD} = \langle \gamma LSLS | \sum_{i=1}^{N} 2\boldsymbol{C}_0^{(2)}(i)\boldsymbol{s}_0(i) r_i^{-3} | \gamma LSLS \rangle \quad \text{(spin dipolar)}, \tag{25}$$

$$a_l = \langle \gamma LSLS | \sum_{i=1}^{N} \boldsymbol{l}_0(i) r_i^{-3} | \gamma LSLS \rangle \quad \text{(orbital)}, \tag{26}$$

$$b_q = \langle \gamma LSLS | \sum_{i=1}^{N} 2\boldsymbol{C}_0^{(2)}(i) r_i^{-3} | \gamma LSLS \rangle \quad \text{(electric quadrupole)}, \tag{27}$$

and

$$A_J = \frac{\mu_I}{I} \frac{1}{[J(J+1)(2J+1)]^{1/2}} \langle \gamma J || T^{(1)} || \gamma J \rangle, \tag{28}$$

$$A_{J-1,J} = \frac{\mu_I}{I} \frac{1}{[J(2J-1)(2J+1)]^{1/2}} \langle \gamma J-1 || T^{(1)} || \gamma J \rangle, \tag{29}$$

$$B_J = 2Q \left[\frac{2J(2J-1)}{(2J+1)(2J+2)(2J+3)} \right]^{1/2} \langle \gamma J || T^{(2)} || \gamma J \rangle, \tag{30}$$

where μ_I is the nuclear magnetic moment. Q is the nuclear electric quadrupole moment.

III. RESULT AND DISCUSSION

The core-excited states of berylliumlike ions are a complex four-electron atomic system in which the correlation effects between electrons are very complicated. Many relevant angular and spin couplings are important for the energy. For each set of orbital angular momenta l_1, l_2, l_3, *and* l_4, there could be several ways to couple this set into the desired total orbital angular momentum. In this work, for the ^5P state, even parity, the important angular series $[l_1, l_2, l_3, l_4]$ are $[0,0,l,l]$, $[0,1\ l,(l+1)]$, $[1,1,l,l]$, $[0,2,(l+1),(l+1)]$, $[1,1,l,(l+2)]$, $[0,2,(l+1),(l+3)]$, etc. For the $^5S^o$ state, odd parity, the available angular series $[l_1, l_2, l_3, l_4]$ are $[0,1,l,l]$, $[1,1,l,(l+1)]$, $[0,2,(l+1),(l+2)]$, $[1,2,(l+1),(l+1)]$, $[1,2,(l+1),(l+3)]$, $[2,2,(l+1),(l+2)]$, etc. In both cases, the value of l is from 1 to 9, as the energy contribution from set with $l>9$ is small and negligible. In order to get the high quality wave function, the number of angular-spin components in the wave functions ranges from 29 to 49, and the number of linear parameters ranges from 662 to 1290. To improve the energy E_b obtained from ψ_b, the restricted variational method is used to compute energy contributions from each chosen angular-spin series. The relativistic corrections and the mass polarization are also included using first-order perturbation theory. The relativistic perturbation operators considered in this work are correction to the kinetic energy (P^4), Darwin term, electron-electron contact term, and orbit-orbit interaction. Table I presents the relativistic energies of the core-excited states $^5P(n)$ $(n=1-7)$ and $^5S^o(m)$ $(m=1-5)$ in B^+ and the core-excited states $^5P(n)$ $(n=1-5)$ and $^5S^o(m)$ $(m=1-5)$ in C^{2+}. For those high-n core-excited quintet states of this system, it is difficult to carry out high quality theoretical calculations due to the numerical unsteadiness. The variational wave functions are carefully chosen in this work to avoid the variational breakdown from the high-n states to the low-n states due to the very strong correlation effects between electrons. As Table I shows, for all cases, the relativistic energies in this work are lower and better than those of Mannervik (MCHF) [5], the improvement ranging from 0.007 a.u. to 0.01 a.u.

In Table I, the states for this system are numbered according to their position in the series; the lowest is denoted by

(1). Each core-excited quintet state is approximately identified by the following three factors: the energy, the relative contribution to normalization of the angular-spin components, and a check of the relativistic perturbation correction. In this case, we note that the relativistic effect of a $1s2p2pnl$ state is smaller than that of $1s2s2pnl'$ state. As Table I shows, for C^{2+}, the relativistic effect of $1s2p2p3s\ ^5P$ state −9716.0 μa.u. is apparently smaller than that of $1s2s2p3p\ ^5P$ state −10 720.9 μa.u. and $1s2s2p4p\ ^5P$ state −10 717.0 μa.u., so identifying $1s2p2p3s$ for $^5P(3)$ will be more reasonable than $1s2s2p4p$. It is consistent with the results in C^{2+} of Schneider *et al.* [3]. For the same reason, for B^+, the relativistic effect of $1s2p2p5s\ ^5P$ state −4693.6 μa.u. is apparently smaller than that of $1s2s2p5p\ ^5P$ state −5047.0 μa.u. and $1s2s2p6p\ ^5P$ state −5049.0 μa.u., so identifying $1s2p2p5s$ for $^5P(5)$ will be more reasonable than $1s2s2p6p$. It is different from the assignment in B^+ reported by Mannervik *et al.* [5].

The results of oscillator strengths and optical transition rates from the dipole length (f_l, A_l), dipole velocity (f_v, A_v), and dipole acceleration (f_a, A_a) formulas, lifetimes and the transition wavelengths have been given in Table II. In this work, the f_l, f_v, and f_a are in good agreement with each other. For example, the f_l, f_v, and f_a of $1s2s2p^2\ ^5P$ -$1s2p^3\ ^5S^o$ in B^+ are 0.1405, 0.1405, and 0.1416, respectively. The good agreement between the length, velocity, and acceleration results could be used as the indication of the accuracy of the wave function. For those high-n core-excited states, because these oscillator strengths are calculated with ψ_b only, and the open-channel part of the wave function is not included, the three results agree reasonably well. As Table II shows, the transition wavelengths in this work are in good agreement with the experimental value [16,5] and other theoretical data [3,23]. According to our theoretical energy levels in this work, the 85.77 nm line is suggested to assign to the $1s2p^3\ ^5S^o$-$1s2p2p5s\ ^5P(5)$ transition of B^+. The transitions $1s2p^3\ ^5S^o$-$1s2s2p3p\ ^5P(2)$, $1s2p^3\ ^5S^o$ -$1s2s2p4p\ ^5P(3)$, and $1s2p^3\ ^5S^o$-$1s2s2p5p\ ^5P(4)$ in B^+ could not be observed easily in experiment owing to the surprisingly large lifetimes and corresponding small oscillator strengths. To our knowledge, the identification of the transition line among high-n core-excited quintet states for B^+ is very difficult due to coinciding with the triplet transitions $1s^22s2p\ ^3P^o$-$1s^22p^2\ ^3P$ in B^+ and the restriction of resolution from experiments. Our results should be valuable in future experiments.

The relativistic energies given in Table I are the center-of-gravity energies. If including the effects of the spin-orbit, spin-other-orbit, and spin-spin interactions, we obtain the energies of the fine-structure resolved J levels. Table III gives the shifts of the various J levels from the center-of-gravity energy and the fine-structure splittings of the core-excited states $^5P(n)$ $(n=1-5)$ in Be-like boron and carbon. The fine-structure splittings in this work are in good agreement with other theoretical and experimental data [9,10,18]. Figure 1 gives the systematical change of the fine-structure splittings of the core-excited states $^5P(n)$ $(n=1-5)$ along with the n increasing for Be-like boron and carbon. In Fig. 1, we noted that the mutation of the fine-structure splittings at $1s2p2p5s\ ^5P(5)$ in B^+ and at $1s2p2p3s\ ^5P(3)$ in C^{2+} is reasonable according to the assignment of configuration structure for this high-n system as mentioned above.

Table IV gives the hyperfine structure of the core-excited states $^5P(n)$ $(n=1-3)$ and $^5S^o(m)$ $(m=1-3)$. We studied the hyperfine structure parameters: Fermi contact a_c, the spin dipolar a_{SD}, the orbital a_l, and the electric quadrupole b_q. The hyperfine coupling constants A_J and B_J are listed in Table V also. In this work, $Q=0.0847$ b, $\mu_I=1.800\ 645$ nm, $I=3$ for B^+ and $Q=0.034\ 26$ b, $\mu_I=-0.964\ 000$ nm, $I=3/2$ for C^{2+} are taken from Ref. [24].

IV. CONCLUSION

In this work, the relativistic energies, fine structure and hyperfine structure for the core-excited quintet states are studied for berylliumlike boron and carbon. The relativistic energies obtained in this work are much lower and better than those of the other theoretical data. The identifications of the energy levels for the high-n core-excited series are discussed. The 85.77 nm line in B^+ is suggested to assign to the $1s2p^3\ ^5S^o$-$1s2p2p5s\ ^5P(5)$ transition according to the accurate calculations of the energy levels and the wavelengths in this work. These available theoretical data should be useful for studying the observed spectra in future experiments.

ACKNOWLEDGMENTS

The authors are grateful to Dr. Kong T. Chung for his computer code. This work was supported by the National Natural Science Foundation of China under Grant No. 10374008, by the Ministry of Education P. R. China under Grant No. 20020007036, and by the Grant No. BIT-UBF-200307A05.

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