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K-shell photoionization of boron-like carbon ions: analysis of 1s−2p resonances*

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Close-coupling calculations based on an R-matrix formalism are performed for the 1s–2p resonance photoionizations from the low-lying states of boron-like carbon ions. The resonance energies, widths and oscillator strengths of 1s−2p core excitations are determined by analysing the calculated photoionization cross sections. Our calculations are in reasonable agreement with the experimental and theoretical results presented by other authors. The present numerical values may help to analyse the astrophysical and laboratory plasmas.

Keywords: photoionization, C II, resonance
PACC: 3280F, 3280D

1. Introduction

Transition energies, oscillator strengths and the autoionization widths associated with atomic or ionic inner-shell excitations are important to inner-shell absorption or emission spectroscopy. A great effort has been made to deal with these inner-shell processes by many authors. Recently, Zeng *et al*[1,2] have carried out close-coupling calculations for aluminium ions and obtained the cross sections of 1s-photoexcitations and 1s-photoionizations. They analysed the 1s–2p transitions and autoionizations of aluminium ions arising from aluminium plasmas. We find by using their results that a close-coupling method may provide us with reasonable agreement with experimental results of autoionization widths.

High-resolution spectroscopy in x-ray band is one of the most useful methods for detailed investigations of the dynamics and structure of x-ray sources. With the recent x-ray satellites, such as *Chandra* and *XMM-Newton*, the high-resolution spectroscopy of photoionized plasmas at x-ray energies is available; it is desirable to produce the corresponding theoretical atomic data as a counterpart of those spectra.[3]

Because of their astrophysical importance, carbon and its ions have been a subject of a number of theoretical and experimental studies. For B-like C II ion, as a part of the Opacity Project (OP),[4] Fernley *et al*[5] calculated energy levels and oscillator strengths of valence excitations to all the levels with the values of principle quantum number n up to 10 by using an R-matrix method. And they also calculated the cross sections of photoionizations from valence levels. Yan *et al*[6] calculated the oscillator strengths of all transitions between the C II energy levels with effective quantum numbers $\nu \leq 10$ and total orbital angular momenta $L \leq 3$ using a close-coupling method. However, the calculations of K-shell transitions has been rendered important to the future work.

The experimental study of K-shell transitions has been carried out extensively in recent years. Jannitti *et al*[7] measured the K-shell absorption spectra of C II with a technique using two laser-produced plasmas. Recently, Schlachter *et al*[8] have used a merged-beam technique to measure the absolute cross sections of 1s→2p photoexcitations for the ground-state $1s^22s^22p\ ^2P^o$ and the metastable-state $1s^22s2p^2\ ^4P$ of C II. They also obtained energies, linewidths and lifetimes for the $1s2s^22p^2\ ^2D$, ^2P, ^2S and $1s2s2p^3\ ^4D^o$, $^4P^o$, $^4S^o$ K-shell vacancy states.

On the other hand, the theoretical calculations of K-shell transitions of C II ions are less available to the best of our knowledge, although one might need theoretical values for the analysis of practical plasmas. In this paper, we consider the photoionization and K-shell photoexcitation of a few low-lying states of C II such as the states with configurations $1s^22s^22p$, $1s^22s2p^2$ and $1s^22p^3$ using an R-matrix method.[9] We

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obtain the resonance energies, oscillator strengths and autoionization widths of the 1s−−2p excited states by analysing our results of photoionization cross section.

2. Theoretical methods

The photoionization cross sections are calculated by using the R-matrix program published by Berrington *et al.*[10] Recently, Zeng and Yang [11] and Wu *et al*[12] have calculated the photoionization cross sections for B-like O IV ion and the photodetachment cross section for negative atomic oxygen by employing the same method, respectively. The R-matrix method for electron-atom and photon-atom interactions has been discussed in great detail by Burke *et al.*[13] This method is very effective in considering the resonance structures; the autoionization resonance widths are naturally included in the calculations. In the R-matrix calculation, the wavefunction of the $N+1$ electron system is given by

$$\Psi_k(X_1,\cdots,X_{N+1}) = \hat{A}\sum_{ij} c_{ijk}\,\Phi_i(X_1,\cdots,X_N,\hat{\boldsymbol{r}}_{N+1}\sigma_{N+1})u_{ij} + \sum_j d_{jk}\phi_j(X_1,\cdots,X_{N+1}), \qquad (1)$$

where $\hat{A}$ is the antisymmetrization operator to take into account the exchange effect between the target electrons and the free electron. X_i denotes the spatial ($\boldsymbol{r}_i$) and spin (s_i) coordinates of the ith electron. The functions $u_{ij}(r)$ in the first sum construct the basis sets for the continuum wavefunctions of the free electron, and Φ_i are the coupling between the target states and the angular and spin parts of the free electron. The correlation functions ϕ_j in the second sum are constructed by square integrable orbitals to evaluate the correlation effects not adequately considered because of the cutoff in the first sum. The square integrable orbitals are expressed by a sum of Slater-type orbitals as

$$P_{nl}(r) = \sum_j C_{jnl} r^{I_{jnl}} \exp(-\xi_{jnl} r). \qquad (2)$$

The parameters ξ_{jnl} and coefficients C_{jnl} are optimized variationally for the energy of a particular state, whilst the powers I_{jnl} of r remain fixed.

For the calculations of the photoionization cross sections from the C II low-lying states, six real and five pseudo-orbitals (1s, 2s, 2p, 3s, 3p, 3d, $\overline{4s}$, $\overline{4p}$, $\overline{4d}$, $\overline{5s}$ and $\overline{5p}$) are included in the wavefunction expansion of the target C III ions. The pertinent parameters and coefficients for all orbitals are obtained by using the CIV3 code[14] according to the following rules. The 1s and 2s orbitals are Hartree–Fock orbitals for the C III ground state $1s^2 2s^2\ ^1S$ given by Clementi and Roetti[15], while the 2p, 3s, 3p and 3d orbitals are optimized on the 2s2p $^1P^o$, 2s3s ^1S, 2s3p $^1P^o$, and 2s3d ^1D states, respectively. The pseudo-orbitals $\overline{4s}$ and $\overline{4p}$ are optimized on the $2p^2\ ^1S$ and 2s2p $^1P^o$ states, respectively, while $\overline{4d}$, $\overline{5s}$ and $\overline{5p}$ are optimized on the 1s-hole states $1s2s^2 2p\ ^1P^o$, $1s2p^3\ ^1P^o$ and $1s2s2p^2\ ^3D$, respectively. The R-matrix wavefunctions Ψ_k in Eq.(1) are constructed with 28 target states of C III, for which the differences are listed in Table 1, together with the energy levels we calculated and those from NIST.[16]

Table 1. Calculated energies (in Ry) for the target C III ion relative to the ground state in comparison with the NIST data.[16]

State	NIST	Calc.	Diff/%
$1s^2 2s^2\ ^1S$	0.0	0.0	0.0
2s2p $^3P^o$	0.4777	0.4781	0.08
2s2p $^1P^o$	0.9327	0.9446	1.28
$2p^2\ ^3P$	1.2528	1.2549	0.17
$2p^2\ ^1D$	1.3293	1.3401	0.81
$2p^2\ ^1S$	1.6632	1.6823	1.15
2s3s ^3S	2.1708	2.1743	0.16
2s3s ^1S	2.2524	2.2519	0.02
2s3p $^1P^o$	2.3596	2.3625	0.12
2s3p $^3P^o$	2.3667	2.3665	0.01
2s3d ^3D	2.4605	2.4713	0.44
2s3d ^1D	2.5195	2.5364	0.67
$1s2s^2 2p\ ^3P^o$	21.4060		
$1s2s(^3S)2p^2\ ^5P$	21.5283		
$1s2s^2 2p\ ^1P^o$	21.6360		
$1s2s(^1S)2p^2\ ^3P$	22.0311		
$1s2s2p^2\ ^3D$	22.0359		
$1s2s2p^2\ ^3S$	22.3157		
$1s2s2p^2\ ^1D$	22.3655		
$1s2p^3\ ^5S^o$	22.4255		
$1s2s(^3S)2p^2\ ^3P$	22.4435		
$1s2s(^3S)2p^2\ ^1P$	22.6143		
$1s2s2p^2\ ^1S$	22.6449		
$1s2p^3\ ^3D^o$	22.6956		
$1s2p^3\ ^3S^o$	22.8319		
$1s2p^3\ ^1D^o$	22.9039		
$1s2p^3\ ^3P^o$	22.9657		
$1s2p^3\ ^1P^o$	23.1750		

In Table 1, we can see that the differences between our calculated results and the NIST data are less than 1% for the valence electron excited states

except $1s^22s2p\ ^1P^o$ and $1s^22p^2\ ^1S$ for which the differences are 1.28% and 1.15%, respectively. For core-excited states there are no available NIST data to compare with ours.

In running the R-matrix codes, the R-matrix boundary was chosen to be 19.2 a.u. to ensure that the wavefunctions are completely wrapped within the R-matrix sphere. For each angular momentum, the continuum orbitals are expressed by a linear combination of 50 numerical basis functions. In order to take into account the resonances of K-shell excited states, only one electron is fixed in the 1s orbital, two- or three-electron promotions from specific configurations are used to describe the N or $N+1$ electron wavefunctions.

The resonance oscillator strengths can be obtained from the photoionization cross sections $\sigma_{\rm PI}$ as

$$f(L_iS_i \rightarrow L_jS_j) = \Big(\frac{1}{4\pi^2\alpha a_0^2}\Big)\int_{\Delta E_{\rm r}} \sigma_{\rm PI}(\epsilon; L_iS_i \rightarrow L_jS_j){\rm d}\epsilon, \quad (3)$$

where L_i, S_i, L_j, S_j are the total orbital and spin angular momenta of the initial bound level and the final continuum wavefunction, respectively. Because the cross section $\sigma_{\rm PI}$ is usually calculated in both length and velocity forms, the corresponding resonance oscillator strengths are also given in both length $f_{\rm l}$ and velocity $f_{\rm v}$ forms.

3. Results and discussions

In Table 2, we give the calculated ionization energies of $1s^22s^22p\ ^2P^o$, $1s^22s2p^2\ ^4P$, ^2D, ^2P, ^2S and $1s^22p^3\ ^4S^o$ states of C II. For comparison, the NIST[16] data are also listed. In Table 2, we find the good agreement between the theory and experiment. For the ground state $^2P^o$ and lower excited states ^4P and ^2D, the difference is less than 1%. The largest difference is 2.39% for the $2s2p^2\ ^2P$ excited state.

Table 2. Comparison of the present calculated energies relative to the ground state $1s^22s^2\ ^1S$ of C III with the NIST[16] data (in Ry) for the low lying terms of C II.

Term	NIST	Calc.	Calc.−NIST	Diff/%
$2s^22p\ ^2P^o$	1.7921	1.7843	−0.0078	0.44
$2s2p^2\ ^4P$	1.4000	1.3964	−0.0036	0.26
$2s2p^2\ ^2D$	1.1093	1.0987	−0.0106	0.96
$2s2p^2\ ^2S$	0.9128	0.8917	−0.0211	2.31
$2s2p^2\ ^2P$	0.7838	0.7651	−0.0187	2.39
$2p^3\ ^4S^o$	0.4978	0.4924	−0.0054	1.10

Figure 1 displays the photoionization cross sections from the ground state $1s^22s^22p\ ^2P^o$ in the vicinity of the 1s−−2p resonances, only the length form is given because the relative differences between the length and velocity forms are < 8%. It can easily be seen that three resonances exist in a photon energy range of 287−291 eV. These resonances are caused by the 1s−−2p excited autoionization states $1s2s^22p^2\ ^2D$, ^2P and ^2S. The resonance energies and autoionization widths can be obtained by analysing the resonances using the same method as that in Ref.[17]. From the photoionization cross sections, the oscillator strengths can be determined by using Eq.(3). The results are given in Table 3, together with the results for different transitions. For resonance oscillator strengths, both length and velocity forms are given for comparison. From the inspection of Table 3, one can see that the largest relative difference between the two forms is less than 6%.

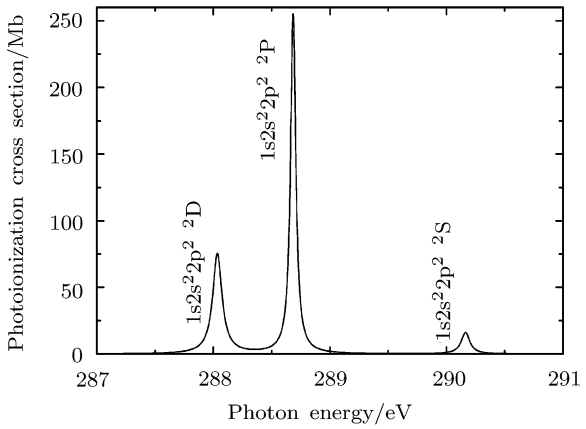


Fig.1. Ground-state photoionization cross section of C II in the vicinity of 1s−2p resonances.

Figure 2 displays the photoionization cross sections from the excited configuration $2s2p^2$ with reference to (a)^{4}P, (b)^{2}D, (c)^{2}S and (d)^{2}P terms. Figure 3 shows the photoionization cross sections from the $2p^3\ ^4S^o$ term. As shown in Fig.1, only the length form is given. The resonance energies, oscillator strengths and autoionization widths are determined from Figs.2 and 3 and the results are listed in Table 3. From the Figs.1–3, we can see that the background cross sections are very small in the whole range of our calculation, which may be attributed to the direct photoionization of the valence shells.

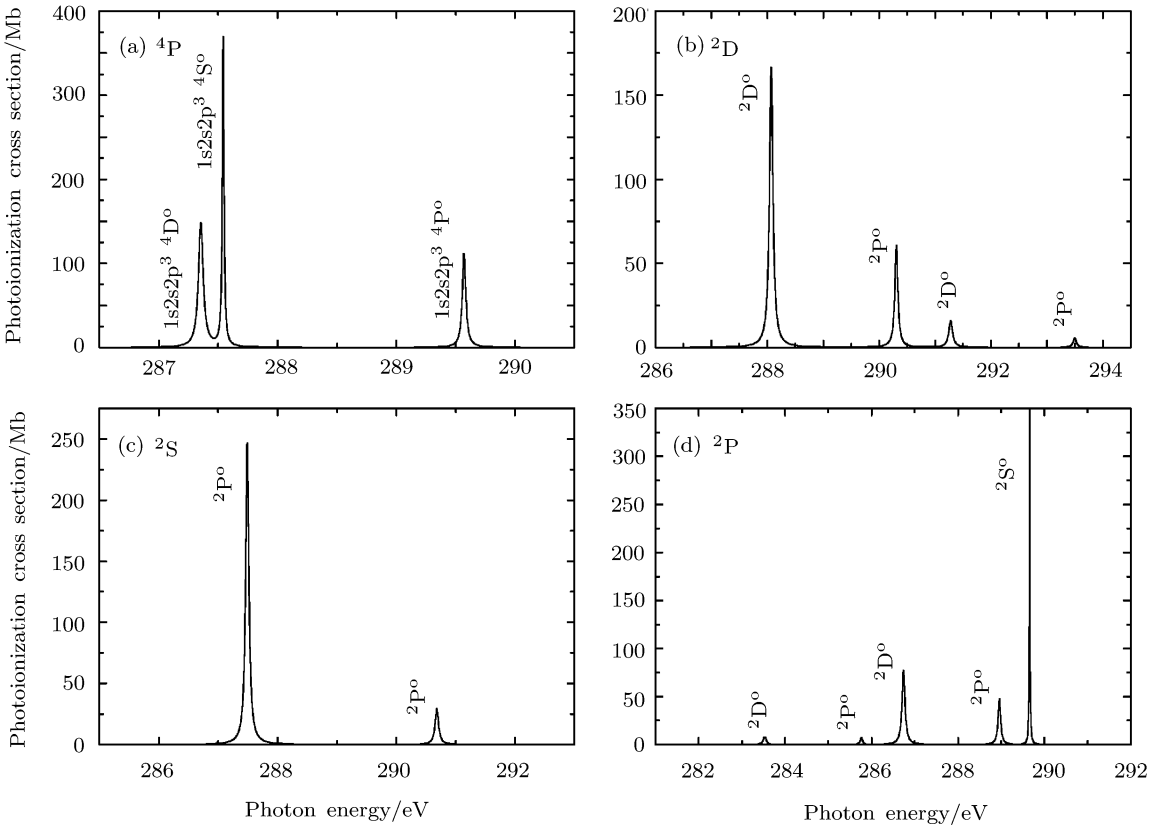


Fig.2. The photoionization cross sections of the configuration $2s2p^2$: (a) ^{4}P, (b) ^{2}D, (c) ^{2}S, and (d) ^{2}P in the vicinity of 1s−−2p resonances.

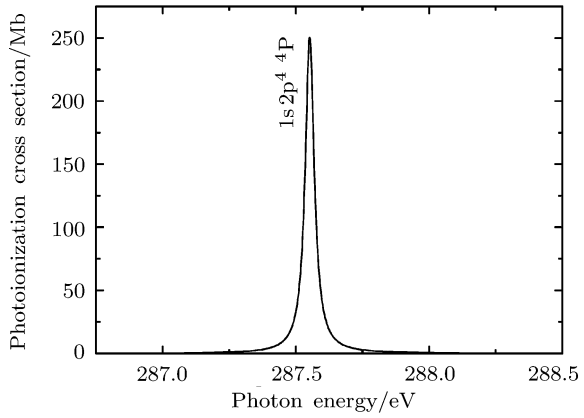


Fig.3. The photoionization cross sections of the configuration $2p^3$ ^{4}S°.

Schlachter *et al*[8] experimentally measured the 1s−2p photoionization cross section of C II. However, in their measurements, the C II ions are a mixture of the ground state (80%) and the metastable state $2s2p^2$ ^{4}P (20%). Figure 4 shows a comparison of our theoretical results with their experimental results; our results are a sum for the two lowest states shown in Figs.1 and 2(a). The experimental resolution (65 meV) has been taken into account. For comparison, other theoretical results[8] and experimental resonance positions[7] are also given.

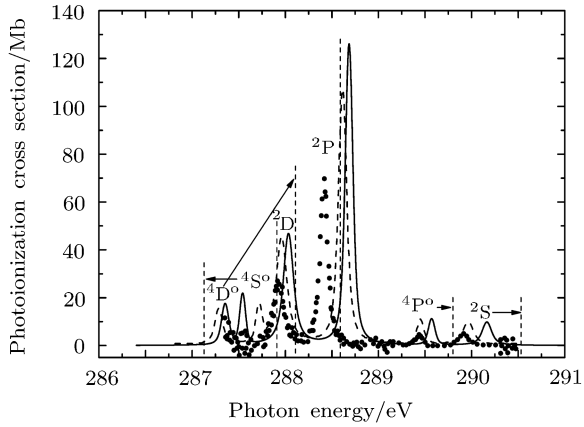


Fig.4. Comparison of different results. The dot refers to the Schlachter *et al*'s[8] experimental results, the solid curve to the present results, the dashed curve to the Schlachter *et al*'s[8] theoretical results and the dashed vertical lines refer to the Jannitti *et al*'s[7] experimental energy positions.

From the inspection of Fig.4, some findings can be pointed out. Both our theoretical resonance peaks and those of Ref.[8] are higher than experimental results in magnitude. At slightly higher energies, our

calculated resonance energies are higher than experimental values of Schlachter *et al*,[8] but lower than Jannitti *et al*'s[7] experimental results. It should be pointed out that in Schlachter *et al*'s[8] experiment the $^4S^o$ resonance peak is missing and in Jannitti *et al*'s[7] experiment the energy order for $^4D^o$ and $^4S^o$ comes opposite to the theoretical one.

In Table 3, we compare our theoretical resonance energies and widths with the experimental results wherever available. For most transitions, our calculated resonance energies are higher than experimental results obtained by Schlachter *et al*[8] but lower than those obtained by Jannitti *et al*.[7] Theoretically, the reasonable agreement is found between our results and those obtained by using the *R*-matrix method including radiation damping[8]. For the autoionization widths, our results show the good agreement with other experimental and theoretical results for the Auger states produced by 1s→2p photoexcitation from the ground state $1s^22s^22p\ ^2P^o$ of C II ion. But for the Auger states of the $1s2s2p^3$ configuration, there exist discrepancies between our results and other results, especially for the state $^4D^o$, where the experimental result is 110±40 meV, the *R*-matrix with radiation damping gives 84 meV and our *R*-matrix value is 47 meV.

Table 3. Resonance energy (E_r), autoionization width (Γ), length (f_l) and velocity (f_v) forms of the oscillator strengths of the 1s−−2p transitions of C II.

	E_r/eV			Γ/meV				
		Theory			Theory			
		Other	This		Other	This	oscillator strengths	
Transition	Expt.	work[c]	work	Expt.	work[c]	work	f_l	f_v
$1s^22s^22p\ ^2P^o - 1s2s^22p^2\ ^2D$	287.93 ± 0.03[a]	287.96	288.034	105 ± 15	103	96	0.1015	0.0977
	287.91 ± 0.2[b]							
$1s^22s^22p\ ^2P^o - 1s2s^22p^2\ ^2P$	288.40 ± 0.03[a]	288.63	288.685	59 ± 6	62	54	0.1927	0.1855
	288.59 ± 0.2[b]							
$1s^22s^22p\ ^2P^o - 1s2s^22p^2\ ^2S$	289.90 ± 0.03[a]	289.97	290.163	112 ± 25	93	88	0.0197	0.0194
	290.53 ± 0.2[b]							
$1s^22s2p^2\ ^4P - 1s2s2p^3\ ^4D^o$	287.25 ± 0.03[a]	287.29	287.354	110 ± 40	84	47	0.0968	0.0931
	288.11 ± 0.2[b]							
$1s^22s2p^2\ ^4P - 1s2s2p^3\ ^4S^o$	287.13 ± 0.2[b]	287.73	287.542		25	16	0.0844	0.0812
$1s^22s2p^2\ ^4P - 1s2s2p^3\ ^4P^o$	289.42 ± 0.03[a]	289.46	289.571	55 ± 25	52	35	0.0547	0.0534
	289.80 ± 0.2[b]							
$1s^22s2p^2\ ^2D - 1s2s(^1S)2p^3\ ^2D^o$	288.45 ± 0.2[b]		288.069			73	0.1716	0.1650
$1s^22s2p^2\ ^2D - 1s2s(^1S)2p^3\ ^2P^o$	290.32 ± 0.2[b]		290.307			63	0.0535	0.0522
$1s^22s2p^2\ ^2D - 1s2s(^3S)2p^3\ ^2D^o$	292.78 ± 0.2[b]		291.279			81	0.0176	0.0169
$1s^22s2p^2\ ^2D - 1s2s(^3S)2p^3\ ^2P^o$	294.59 ± 0.2[b]		293.499			69	0.0053	0.0052
$1s^22s2p^2\ ^2P - 1s2s(^1S)2P^3\ ^2D^o$			283.529			73	0.0099	0.0096
$1s^22s2p^2\ ^2P - 1s2s(^1S)2P^3\ ^2P^o$			285.768			63	0.0066	0.0064
$1s^22s2p^2\ ^2P - 1s2s(^3S)2P^3\ ^2D^o$	288.36 ± 0.2[b]		286.740			81	0.0868	0.0835
$1s^22s2p^2\ ^2P - 1s2s(^3S)2P^3\ ^2P^o$	290.09 ± 0.2[b]		288.960			69	0.0465	0.0452
$1s^22s2p^2\ ^2P - 1s2s(^3S)2P^3\ ^2S^o$	289.95 ± 0.2[b]		289.659			16	0.0862	0.0828
$1s^22s2p^2\ ^2S - 1s2s(^1S)2P^3\ ^2P^o$	287.57 ± 0.2[b]		287.491			63	0.2187	0.2088
$1s^22s2p^2\ ^2S - 1s2s(^3S)2P^3\ ^2P^o$			290.682			69	0.0292	0.0279
$1s^22p^3\ ^4S^o - 1s2p^4\ ^4P$	287.36 ± 0.2[b]		287.552			41	0.1426	0.1384

[a]merged-beam technique[8]; [b]two laser-produced plasmas technique[7]; [c]*R*-matrix method including radiation damping.[8]

4. Conclusion

Close-coupling calculations based on an *R*-matrix formalism have been carried out to investigate the photoionization cross sections from the low-lying states of B-like C II ions. Emphasis is laid on analysing the 1s−−2p resonances and on obtaining the resonance energies, widths of the core-excited states

and the oscillator strengths of the 1s−−2p transitions. Our calculated resonance energies and autoionization widths are compared with existing experimental and theoretical results. Rather good agreement is found between our results and other experimental and theoretical results, but for autoionization widths there remain some differences.

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