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Electron impact ionization of the B-like ion C^+: Resonance enhancement of the single-channel cross section

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Abstract

We have calculated the total and single differential cross sections for electron impact ionization of the B-like ion C^+ in its $(2s^2 2p)^2 P^0$ ground state at 26.2, 28.2, and 33.2 eV incident energies using the R-matrix method of Bartschat and Burke in the single-channel approximation and the three-state close-coupling approximation, respectively. The single differential cross section exhibits the pronounced resonance structure in detail. A list of these resonances is given together with a classification scheme based on quantum defect theory. Our calculated results indicate that autoionization exceeds the direct contribution by about a factor of two. © 1998 Elsevier Science B.V.

For many years, there has been considerable interest in electron impact ionization processes; this is based on the urgent practical need to obtain accurate data for plasma and fusion research. Most of the work in the field has been performed using Born type approximations where no account is taken of the mixing between the excited state and continuum, which is the source of the autoionization. We use the R-matrix method of Bartschat and Burke to calculate electron impact ionization cross sections of the B-like ion C^+, and focus on discussing the contributions of excitation-autoionization [1–5].

It was first suggested by Goldberg that direct ionization in highly ionized atoms might be enhanced by electron impact excitation of an inner-subshell electron to a quasi-bound state lying above the first ionization limit, followed by autoionization [6]. Burgess et al. stressed the importance of these contributions [7]. Some calculations and experiments have shown that these indirect contributions are quite significant in some cases [8–17]. These theoretical works, however, neglected interference effects between the direct and the excitation-autoionization mechanism as well as correlations between the ejected electron and the final ionic state, which lead to a Rydberg series of resonances similar to those occurring in photoionization processes. We use an R-matrix expansion for both these initial atomic and continuum states, consisting of the final ion plus the ejected electron, to take into account interference effects which give rise to the series of resonances [3,4]. One of the assumptions which is implicit in the form of the R-matrix close-coupling wave functions used in our calculation is that all the autoionizing states only decay into the continuum and cannot decay by radiative emission. In order to correct for such effects within the framework of the present formulation it would be necessary to include radiative terms in the Hamiltonian, a procedure which could

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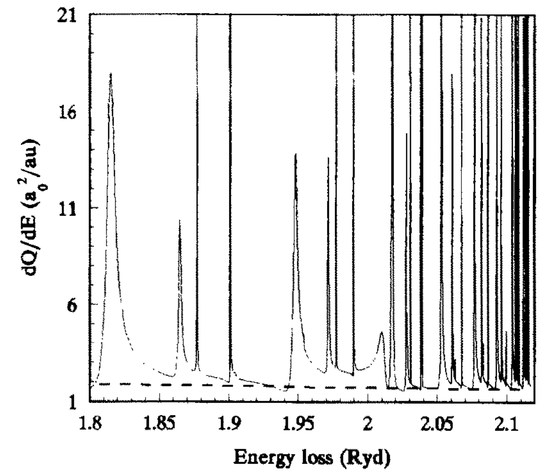

Fig. 1. Single differential cross section for electron impact ionization of C^+ for an impact energy of 33.2 eV. (- - -) Direct ionization, (—) three-state close-coupling approximation.

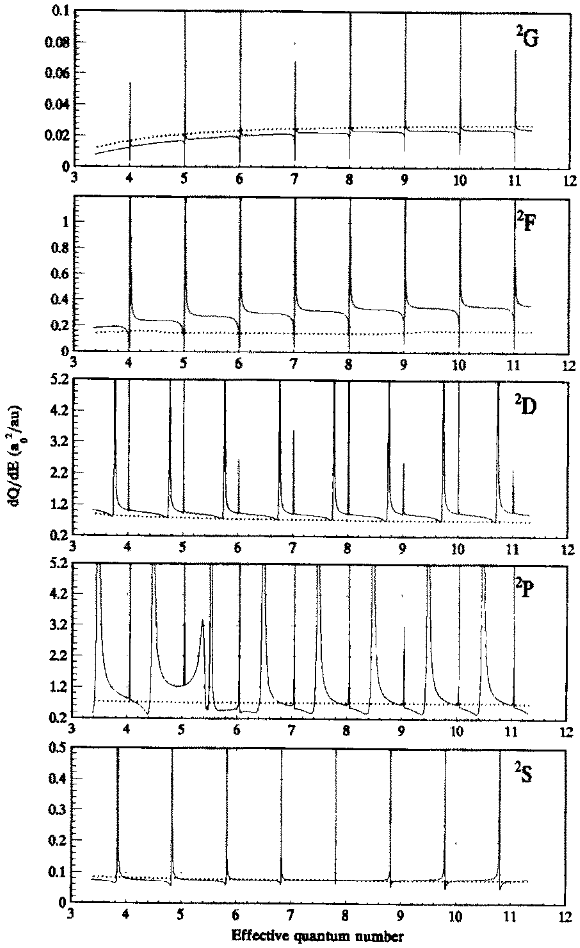

Fig. 2. Contributions to dQ/dE from the various final state symmetries, plotted against the effective quantum number. (- - -) Direct ionization, (—) three-state close-coupling approximation.

rapidly lead to the problem becoming numerically intractable. Radiative decay, on the other hand, which is of little effect for $Z < 10$, need not be included in the calculation of excitation-autoionization cross sections [4,5].

We have considered C^+ in the $(2s^22p)^2P^0$ ground state. Here, we can calculate the following processes,

$$e_f + C^+(2s^22p)^2P^0 \to e_f + C^{2+}(2s^2)^1S + e_s \quad (1)$$

$$\to e_f + C^+(2s2pnl)^2L \quad (2)$$

$$\hookrightarrow C^{2+}(2s^2)^1S + e_s, \quad (3)$$

with ionization potential of 24.4 eV. The "fast" ionizing electron e_f with incident energy E and suffering an energy loss ΔE is described by a distorted wave, while the R-matrix expansion is used to describe the initial target state and the final (ion $+e_s$) continuum state [18]. In the first process, where the $2p$ is removed directly, the "slow" ejected electron e_s has energy $E_s = \Delta E - 24.4$, while in the second process a $2s$ electron is excited to the nl orbit. The interactions between the excited state and the continuum lead to a Rydberg series of resonances. A $2s$ electron can be ionized at the energies of interest here.

In our calculation the states which were included in the R-matrix close-coupling wave functions were of the form ^2L, with L taking values from zero to four. These states were formed by coupling the configuration $2s^2$ to the added electron to give a single free channel of configuration $2s^2kl$ together with bound channels of configurations $2s^22p$, $2s2p^2$, $2p^3$, $2s2p(^3P^0)nl$ and $2s2p(^1P^0)nl$ in the three-state close-coupling approximation, and to obtain only a single free channel of configuration $2s^2kl$ in the single-channel approximation. Partial waves up to $l = 17$ were included to describe the ionizing electron. For the ejected electron six partial waves with 15 continuum functions for each angular momentum were taken into account. The distortion potential was taken to be the static potential of the B-like ion C^+. The bound orbitals used in the calculation were the

Table 1
Rydberg resonances in e-C^+ scattering

ΔE (Ryd)	ν		ΔE (Ryd)	ν	
		$2s2p(^3P)np^2S$			$2s2p(^3P)ns^2P$
1.8771	3.8394	4p	1.8149	3.4630	4s
1.9772	4.8330	5p	1.9479	4.4660	5s
2.0306	5.8272	6p	2.0174	5.5258	6s
2.0625	6.8220	7p	2.0529	6.4719	7s
2.0829	7.8153	8p	2.0768	7.4718	8s
2.0969	8.8089	9p	2.0927	8.4705	9s
2.1068	9.8047	10p	2.1038	9.4704	10s
2.1141	10.8007	11p	2.1119	10.4729	11s
		$2s2p(^3P)nd^2P$			$2s2p(^3P)np^2D$
1.9044	4.0485	4d	1.8644	3.7526	4p
1.9909	5.0387	5d	1.9715	4.7552	5p
2.0390	6.0454	6d	2.0276	5.7532	6p
2.0678	7.0447	7d	2.0606	6.7497	7p
2.0866	8.0433	8d	2.0818	7.7470	8p
2.0995	9.0444	9d	2.0961	8.7413	9p
2.1087	10.0416	10d	2.1062	9.7329	10p
2.1156	11.0416	11d	2.1136	10.7228	11p
		$2s2p(^3P)nf^2D$			$2s2p(^3P)nd^2F$
1.9004	4.0157	4f	1.9011	4.0214	4d
1.9894	5.0157	5f	1.9897	5.0205	5d
2.0379	6.0166	6f	2.0380	6.0193	6d
2.0672	6.0165	7f	2.0672	7.0187	7d
2.0862	8.0161	8f	2.0862	8.0187	8d
2.0992	9.0168	9f	2.0993	9.0214	9d
2.1085	10.0164	10f	2.1086	10.0189	10d
2.1154	11.0148	11f	2.1155	11.0182	11d
		$2s2p(^3P)nf^2G$			
1.8993	4.0068	4f			
1.9888	5.0063	5f			
2.0376	6.0071	6f			
2.0670	7.0079	7f			
2.0860	8.0071	8f			
2.0991	9.0076	9f			
2.1085	10.0064	10f			
2.1154	11.0081	11f			

$1s$ and $2s$ orbitals given by Clementi and Roetti for $C^{2+}(2s^2)^1S$ [19], while the outer $2p$ orbital was re-optimized on the state $C^{2+}(2s2p)^3P^0$, using the program CIV3 of Hibbert [20]. As in the calculation of Bartschat and Burke, the operators $R^{\lambda}_{\ell_0\ell_1}(E,\Delta E,r)$ (here, E is the incident energy, ΔE is the energy loss of the incident electron) are calculated for only a few "key" values of ΔE, say ΔE^k. For each ΔE, the single differential cross section is calculated for a complete range of the ejected electron energy (of course, corresponding to a unique ΔE^k). In the present calculation, three values of the energies ΔE^k were used on integrating the single differential cross section over ΔE; thus, we finally obtain the total cross section.

The single differential cross section for an incident energy of 33.2 eV as a function of the energy loss is shown in Fig. 1. The contribution of excitation-autoionization is given by comparing the three-state close-coupling result with the single-channel result. We can see that autoionizing resonances enhance the cross section. Fig. 2 shows the pronounced resonance structure in detail. These resonances are due to autoionizing states of C^+ with an nl electron bound to $C^{2+}(2s2p)^3P^0$ and $C^{2+}(2s2p)^1P^0$ to form C^+ states of symmetry ^2S, ^2P, ^2D, ^2F or ^2G, which lie in the continuum of $C^{2+}(2s^2)^1S + e_s$. This is illustrated in Fig. 2, where the contributions to the single differential cross section from the ^2S, ^2P, ^2D, ^2F, and ^2G final state symmetries are plotted on a nonlinear scale as a function of the effective quantum number.

It can be seen that the ^2S contribution shows a single series of autoionizing levels due to a p electron bound to $C^{2+}(2s2p)^3P^0$. The ^2P contribution has two series of autoionizing levels, one due to an s electron and the other one due to a d electron. Furthermore, the ^2D contribution has two series of autoionizing levels, one due to a p electron and the other one due to an f electron, and ^2F has a single series of autoionizing levels due to a d electron. Finally, the ^2G contribution exhibits a single series of autoionizing levels due to an f electron. The contributions to the cross section are mainly from the ^2P and ^2D final state symmetries. From the ^2P, ^2D, and ^2G final state symmetries we have seen that the autoionizing resonances enhance the cross section. A list of all these resonances together with a classification based on elementary quantum defect theory is given is Table 1. The assignment for the g and h orbitals is unambiguous because the large radii of these orbits mean that they have very small quantum defects. This also explains the narrowness of these resonances. For the same reason, the resonances involving g or h orbitals would not be expected to be significant, and indeed none were found.

By integrating the single differential cross section over ΔE, we finally obtain the total cross sections at 26.2, 28.2, and 33.2 eV incident energies, respectively. Table 2 gives our calculated results and experimental data [21]. By comparing with the experimental data, we find that our results are too small. This is mainly due to using the close-coupling method and taking no account of the exchange between the ionizing electron and the ejected electron. In our calculation we only take into account the direct ionization and excitation-autoionization processes and neglect other processes, so we can expect to get better results by a calculation including other processes or final states. Furthermore, the impact energies considered are less than 10 eV above threshold, so we cannot expect the distorted wave approach to give accurate results at these energies. Finally, the continuum state consisting of the final ion and a "slow" ejected electron must have the same total spin as the ground state after the collision. So these states for the different total spin as the ground state need not be included in the close-coupling expansion. They can, however, be excited if the ionization process is considered as an excitation of the B-like ion by the ionizing electron, as in a conventional scattering calculation, with only one electron in the continuum in the final state. But we mainly focus on the contribution of excitation-autoionization, and have shown its importance. Our results indicate that the resonance enhancement of the single-channel cross section dominates the direct ionization process by about a factor of two.

Table 2
Ionization cross section (10^{-17} cm^2)

E (eV)	Q_1 [a]	Q_2 [b]	Q_{expt}
26.2	0.224	0.532	1.078
28.2	0.424	1.083	1.714
33.2	0.796	2.291	3.062

[a] Direct ionization.
[b] Three-state close-coupling approximation.

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