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Cross Section Ionization By Electron Impact Of Helium Like Ions

Manel Hariz Belgacem¹, Elhabib Guedda^{1,*}, Haikel Jelassi²

¹LEVRES Laboratory and Faculty of Exact Sciences, University of El Oued, BP.789, El Oued, Algeria.

² Research Laboratory on Energy and Matter for Nuclear Science Development (LR16CNSTN02), National Center for Nuclear Science and Technologies, 2020 Sidi Thabet, Tunis, Tunisia.

Abstract:

In this paper we present our calculation of the cross section ionization by electron impact of C V, N VI and O VII. Using the Flexible Atomic Code (FAC), we obtain the cross sections for the ionization of these ions from the ground state 1^1S , and from the unstable states 2^1S and 2^3S . Our results are in good agreement with those based on the Coulomb Born (CB) approximation and the available measurements.

Keywords: helium like ions, cross section ionization, FAC code, Coulomb Born approximation.

*Corresponding author. E-mail:elh_guedda@yahoo.fr, guedda-elhabib@univ-eloued.dz

1. Introduction

Electron impact ionization (EII) of atoms and molecules was studied during the last hundred years, from the very early days of modern physics [1]. The cross sections and ionization rates are atomic data that have important applications in astrophysics and plasma physics [2, 3]. Several research works have been carried out in the calculation of ionization cross section using different methods [4], including classical methods [5], Coulomb Born approximation [6] and semi-empirical equations [7]. The first classical method was proposed by Burgess [5], in which the cross section of ionization is treated by perturbation theory with a classical orbital motion of a disturbed electron. Calculation of cross section based on CB approximation was summarized by Vanshtein et al. [6]. The third method based on a set of equations presented by Kato et al. [8], Lotz [9] and Arnaud et al. [10] which gives a description to calculate the cross section and the ionization rate with an electron impact. A complete, new set of ground level electron collision ionization rate coefficients has been developed for all atoms and ions of the elements from hydrogen through zinc. These are based on an analysis of measurements of ionization cross sections and theoretical calculations with FAC and other codes [11]. Fontes et al. [12] used the distorted wave (DW) codes of Zhang et al. [13] and Sampson et al. [14] to calculate cross sections for EII from $n=3, 4$ and 5 sub shells of various ions. According to our knowledge and available references, the EII cross sections for the higher sub shells from $n=2$ are considered very rare. Especially with regard to available laboratory measurements. So, this work aims to calculate the cross sections of the ions C V, N VI and O VII using the FAC code in the ground state and in the unstable states 2^1S and 2^3S . We compare our results obtained by the relativistic distorted wave (DW) method implemented in FAC code with those obtained by CB approximation [15] and the available measurements [16, 17].

2. Theoretical background

The process of impact ionization occurs when an electron hits an ion and knocks out one bound electron into the continuum following this equation:

$$A^{Z+}(i) + e(\varepsilon) \rightarrow A^{(Z+1)+}(j) + e(\varepsilon') + e(\varepsilon'') \quad (1)$$

With the ion initially in state i and the struck electron directly entering the continuum of the residual ion of charge state $(z+1)$ which is left in the state j . This is often considered as, in effect, ionization from the ground state of the ion A^{z+} to the ground state of the ion $A^{(z+1)+}$ [18]. The quantities ε , ε' and ε'' are energies. Coulomb Born approximation method depends on the calculation of the cross section by electron impact of the helium like ions in the ground state 1^1S in the unstable singlet state 2^1S and in the unstable triplet state 2^3S [15]. The equation (2) is used to describe of the initial wave function's state of the system:

$$\Psi_i(r_0, r_1, r) = \psi_{c,K_0}(Z_A, r_0) \phi_i(r_1, r_2) \quad (2)$$

Where $\psi_{c,K_0}(Z_A, r_0)$ is a Coulomb wave function with outgoing spherical wave behavior, normalized to a delta function in momentum space, describing the incident electron of momentum k_0 moving in a Coulomb field corresponding to an effective charge Z_A which is such that $Z_A = Z - 2a$, according to the CB approximation. $\phi_i(r_1, r_2)$ representing the wave function of the target initial state, describing respectively the singlet state, the unstable singlet state 2^1S and the unstable triplet state 2^3S . We use the equation (3), for the description of the final state of the system; the wave function is as follows [19]:

$$\Psi_f(r_0, r_1, r) = \psi_{c,K_A}(Z_A, r_0) \phi_f(r_1, r_2) \quad (3)$$

Where $\psi_{c,K_A}(Z_A, r_0)$ is a Coulomb wave function which describes the scattered electron with momentum k_A , while the wave function $\phi_f(r_1, r_2)$ describes the final target state consisting of an ion $A^{(q+i)} 1^1S$ plus an outgoing electron. As for the total Coulomb Born cross section, including exchange between the scattered and ejected electrons is then given by the following equation (4):

$$\sigma_{CB} = \int_0^{K_B^{\max}} dk_B \frac{K_A K_B^2}{K_0} \int d\Omega_A d\Omega_B |f_{CB}(K_A, K_B)|^2 \quad (4)$$

Where $f_{CB}(K_A, K_B)$ the direct amplitude in the CB approximation, $K_B^{\max} = [2(E - I)]^{1/2}$, E is the electron incident energy and I is the ionization energy. We used the CB approximation method results of ionization cross section by electron impact to compare with FAC code calculation of the ions C V, N VI and O VII. The Flexible Atomic Code [20] has been used to compute the EII cross sections by the relativistic DW method. In this method, the total EII cross section $\sigma_{ij}(\epsilon)$ (in atomic unit) from the initial fine-structure state ψ_i to the final ionized fine-structure state ψ_j at the incident electron kinetic energy ϵ is expressed in terms of the EII collision strength from the initial fine-structure state ψ_i to the final ionized.

$$\sigma_{ij}^{EII} = \frac{1}{k^2(2J_i + 1)} \int_0^{\frac{\epsilon - I_{ij}}{2}} \Omega_{ij}^{EII}(\epsilon, \epsilon') d\epsilon' \quad (5)$$

$$\Omega_{ij}^{EII} = 2 \sum_{kk_i k_j} \sum_{JJ_T} (2J_T + 1) \times \left| \left\langle \psi_i k_i J_T M_T \left| \sum_{n < m} \frac{1}{r_{nm}} \right| (\psi_j k) J k_j J_T M_T \right\rangle \right|^2 \quad (6)$$

k represents the electron kinetic momentum, J_i is the total angular momentum of the target state ψ_i , ϵ' the kinetic energy of the scattered electron, I_{ij} expresses the threshold energy of the fine-structure transition $\psi_i \rightarrow \psi_j$, k_i , k_j , and k is the relativistic angular quantum numbers of respectively the incident, the scattered and the ejected electrons, J the total angular momentum that results from the coupling of the final ionized state ψ_j and the ejected electron momentum k , J_T the total angular momentum that results from the

coupling of J and the scattered electron momentum k_j which must be equal to the coupling of the initial state ψ_i with the incident electron momentum k_i , M_T the corresponding projection of J_T , i.e. the total magnetic quantum number [21].

Several DW programs have been developed for the calculation of cross sections in the past decades, in either non-relativistic [22] or relativistic approximations [14, 23]. The FAC code is similar to that of Sampson and Zhang [14] in particular, which extends the efficient factorization-interpolation method of Bar-Shalom et al. [24] to the calculation of cross sections, and leads to great simplifications for ions. The essence of the factorization method is the separation of the angular and radial parts in the formula of cross sections. The angular part depends on the angular momentum coupling of the target states, while the radial part only depends on the one-electron radial orbitals, without explicit reference to the initial and final states involved in the process. Different initial and final states affect the radial part only implicitly through the ionization energy due to the energy conservation. Such a separation enables the rapid calculation of the radial integrals on a few ionization energy points, the integrals at actual ionization energies are obtained by interpolation [25].

3. Results and Discussions

We use FAC code to calculate the ionization cross section by electron impact for C V, N VI and O VII ions in the ground state 1^1S , unstable states singlet 2^1S and triplet 2^3S . The energy range [0-10000 eV] of the incident electron was selected to calculate all the respective cross sections. In the FAC code, we involve several excited levels to take into account the effects of coupled configuration (1snl, n=1,10).

Figure 1 shows our results for the cross sections of C V, N VI and O VII ions, calculated by the FAC program in the ground state and compared to CB approximation results and available measurements [16, 17]. The EII cross sections and relative differences for the C V ion are presented in table 1.1. The comparison with CB approximation results gives good agreement where the relative error is between 4 and 9% in the electron impact energy interval (400-450 eV). For larger energies (1000-2000 eV), the relative error does not exceed 20%. This seems acceptable to us since these energies are far from the ionization energy for C V ion, which is about 392 eV [26]. On the other hand, the comparison with the experimental available data of Crandall et al. [16] and Donets et al. [17] gives an excellent agreement less than 6% within the experimental errors. The same analysis can be done for the N VI ion in table 1.2. The relative error is between (4-7%) for the energies range (575-700 eV) for CB approximation data. This result can be considered as good for this interval, which also contains the ionization energy of this ion (about 552 eV [26]). The relative error is about 15% in the energies range (1000-2600 eV). A good agreement was observed with the experimental measurements [16, 17]. In this case the relative error does not exceed 15% within the experimental errors. For the O VII ion and referring to the table 1.3, the relative error for CB approximation cross sections is estimated to 10% for the energies range (750-800 eV) which contains the ionization energy (739.32 eV [26]). For the rest of the energies the relative error does not exceeds 10% also. The relative comparison with available measurements of Donets et al. [17] are

below 10% in the range of experimental errors, which gives also excellent agreement.

Table 1.1 EII cross sections and relative differences for the ground state (1^1S) of C V.

σ in unit of 10^{-20}cm^2 , (*) The second value after comma represents value within the experimental error.

E(eV)	σ_{FAC}	σ_{CB} [15]	$\sigma_{crandall}$ [16]	σ_{donets} [17]	$\frac{\Delta\sigma}{\sigma_{CB}}$	$\frac{\Delta\sigma}{\sigma_{crandall}}$	$\frac{\Delta\sigma}{\sigma_{donets}}$
400.00	0.89	0.94			0.05		
437.19	4.09		3.00±1.90			0.36,0.00*	
450.00	5.10	4.88			0.04		
475.00	6.89	6.42			0.07		
500.00	8.52	7.75			0.09		
588.15	13.14		11.70±1.80			0.12,0.00*	
600.00	13.66	11.76			0.16		
686.17	16.69		16.30±2.60			0.02,0.00*	
700.00	17.09	14.40			0.18		
780.27	18.95		17.70±0.80			0.07,0.02*	
900.00	20.70	17.41			0.18		
980.25	21.39		23.30±2.00			0.08,0.00*	
1000.00	21.51	18.19			0.18		
1180.22	22.00		22.00±1.10			0.00,0.00*	
1300.00	22.03	18.96			0.16		
1478.21	21.60		23.40±1.00			0.07,0.03*	
1750.00	20.75	17.97			0.15		
2116.27	19.30			18.00±2.90			0.07,0.00*
2250.00	18.80	16.04			0.17		
3828.80	13.90			16.20±2.15			0.14,0.01*
4844.90	11.86			12.10±1.31			0.01,0.00*
5632.95	10.64			12.20±1.38			0.12,0.01*
6639.14	9.41			10.70±1.20			0.12,0.01*
7391.11	8.67			10.40±1.17			0.16,0.06*
8170.63	8.02			9.43±1.30			0.14,0.01*

Table 1.2 EII cross sections and relative differences for the ground state (1^1S) of N VI.

σ in unit of 10^{-20}cm^2 , (*) The second value after comma represents value within the experimental error.

E(eV)	σ_{FAC}	σ_{CB} [15]	$\sigma_{crandall}$ [16]	σ_{donets} [17]	$\frac{\Delta\sigma}{\sigma_{CB}}$	$\frac{\Delta\sigma}{\sigma_{crandall}}$	$\frac{\Delta\sigma}{\sigma_{donets}}$
575.00	0.84	0.91			0.07		
789.50	6.06		8.50±1.60			0.29,0.13*	
900.00	7.73	6.95			0.11		
966.17	8.50		12.00±2.00			0.29,0.15*	
1000.00	8.84	7.82			0.13		
1187.01	10.17		13.70±1.90			0.25,0.13*	
1300.00	10.62	9.30			0.14		
1463.06	11.01		10.60±1.80			0.03,0.00*	
1700.00	11.18	9.83			0.13		
2065.21	10.90			12.20±1.30			0.10,0.00*
2200.00	10.82	9.59			0.12		

2675.72	10.18			10.70 ± 1.10			0.04,0.00*
3683.80	8.79			9.26 ± 0.77			0.05,0.00*
4669.98	7.67			8.10 ± 0.74			0.05,0.00*
5465.11	6.93			7.49 ± 0.80			0.07,0.00*
6526.23	6.14			7.46 ± 0.79			0.17,0.07*
7398.76	5.62			7.43 ± 0.88			0.24,0.14*
8293.79	5.16			6.69 ± 0.84			0.22,0.11*

Table 1.3 EII cross sections and relative differences for the ground state (1^1S) of O VII.

σ in unit of 10^{-20} cm^2 , (*)The second value after comma represents value within the experimental error.

E(eV)	σ_{FAC}	σ_{CB} [15]	σ_{donets} [17]	$\frac{\sigma\Delta}{\sigma_{CB}}$	$\frac{\sigma\Delta}{\sigma_{donets}}$
750.00	0.18	0.21		0.15	
775.00	0.54	0.60		0.10	
800.00	0.87	0.96		0.09	
1000.00	2.96	2.91		0.01	
2189.95	6.24		5.54 ± 0.57		0.12,0.02*
2400.00	6.23	5.60		0.11	
2796.95	6.11		5.65 ± 0.57		0.08,0.00*
3000.00	6.01	5.38		0.11	
3780.10	5.56		4.86 ± 0.58		0.14,0.02*
4792.46	4.96		4.42 ± 0.60		0.12,0.00*
5605.83	4.55		4.20 ± 0.53		0.08,0.00*
6610.79	4.11		3.41 ± 0.38		0.20,0.08*
7379.59	3.83		3.10 ± 0.37		0.23,0.10*
8356.14	3.51		3.25 ± 0.44		0.08,0.00*

Fig 1. Ionization cross sections of the C V, N VI and O VII in the ground state (1^1S).

Figure 2 shows the results of the cross sections of C V, N VI and O VII ions in the unstable singlet state that was calculated by the FAC code and compared to the results of CB approximation. For the C V ion, it gives very good results as the error relative was estimated between 3-18% in the field of impact electron energies 90-500 eV, these are good results because they are close to the ionization energy of C V which is at about 87.77 eV [15]. As for the N VI ion, the comparison results for the cross sections are generally good, as in the energy range of impact electron close to the ionization energy 250-400 eV, the error rate is between 8-17%. Incident-electron energies ranging between 500-850 eV, the relative error is between 10-19%. Regarding the comparison results of O VII ion, good results were presented in the various incoming electron energies, the relative error was estimated between 9-16% in the impacting electron energy range 175-800 eV. These can be considered as good results because the ionization energy of O VII is estimated at 170.33 eV [15] which belong to this energy field. All results are listed in Table 2.

Table 2. EII cross sections and relative differences for the unstable singlet state (2¹S).

σ in unit of 10⁻²⁰ cm².

$E(eV)$	$\sigma_{FAC}(C\ V)$	$\sigma_{CB}(C\ V)$ [15]	$\frac{\Delta\sigma}{\sigma_{CB}}(C\ V)$	$E(eV)$	$\sigma_{FAC}(N\ VI)$	$\sigma_{CB}(N\ VI)$ [15]	$\frac{\Delta\sigma}{\sigma_{CB}}(N\ VI)$	$E(eV)$	$\sigma_{FAC}(O\ VII)$	$\sigma_{CB}(O\ VII)$ [15]	$\frac{\Delta\sigma}{\sigma_{CB}}(O\ VII)$
90.00	14.79	14.23	0.03	250.00	72.26	64.90	0.17	175.00	3.80	4.19	0.09
100.00	54.15	66.63	0.18	280.00	80.43	72.23	0.11	180.00	7.05	8.21	0.14
110.00	83.32	100.66	0.17	300.00	82.13	75.00	0.09	200.00	17.59	20.80	0.15
120.00	106.01	125.05	0.15	320.00	83.18	76.66	0.08	240.00	31.58	35.50	0.11
150.00	150.18	164.28	0.08	380.00	83.74	77.75	0.07	280.00	40.26	42.96	0.06
175.00	170.06	177.63	0.04	420.00	82.79	76.31	0.08	320.00	45.74	46.82	0.02
200.00	180.90	182.67	0.01	480.00	80.39	73.26	0.09	360.00	49.12	48.70	0.01
250.00	187.57	180.91	0.03	520.00	78.44	70.87	0.10	400.00	51.08	49.41	0.03
300.00	184.60	172.42	0.07	580.00	75.33	67.14	0.12	440.00	52.08	49.40	0.05
335.00	180.06	165.00	0.09	600.00	74.28	65.90	0.12	480.00	52.42	48.94	0.07
365.00	175.29	158.24	0.10	640.00	72.18	63.44	0.13	540.00	52.12	47.74	0.09
400.00	169.70	150.38	0.12	700.00	69.11	59.90	0.15	640.00	50.47	45.07	0.11
450.00	161.38	139.34	0.15	780.00	65.25	55.51	0.17	720.00	48.68	42.72	0.13
500.00	153.32	128.94	0.18	850.00	82.12	51.97	0.19	850.00	45.55	38.94	0.16
680.00	128.41			975.00	57.11			970.00	42.74		
855.00	110.45			1450.00	43.40			1064.00	40.68		
1040.00	96.02			2400.00	29.25			1925.00	27.66		
2000.00	57.39			3200.00	23.00			2690.00	21.45		
3000.00	40.73			4600.00	16.80			3850.00	16.05		
4500.00	28.57			5300.00	14.82			4390.00	14.38		
6000.00	23.25			6650.00	12.10			5100.00	12.66		
6500.00	19.73			7000.00	11.55			6680.00	10.02		
8000.00	17.02			8220.00	9.98			8010.00	8.53		
10000.00	13.87			9545.00	8.71			9990.00	7.00

Fig. 2. Ionization cross sections of the C V, N VI and O VII (2^1S).

The figure 3 shows the results of a comparison of the cross sections between our results calculated by the FAC code and those obtained by the CB approximation of C V, N VI, O VII ions in the unstable triplet state. For the C V ion, good results were generally obtained, as shown in Table 3, where the relative error of this ion is estimated between 7% and 27% in the impact electron energies range between 95-600 eV. These energies are within the C V ionization domain. For the N VI ion, the results of the relative error between the FAC program and CB approximation for this ion were estimated from 9 to 25% in incident-electron energies ranging between 140-760 eV. The last results could be considered as good. As for the comparison of O VII, where it showed good agreement in the various energies of the electron impact, especially at the energy close to the ionization energy O VII in the unstable state 2^3S as shown in table 3.

Table 3. EII cross sections and relative differences for the unstable triplet state (2^3S).

σ in unit of 10^{-20} cm^2 .

E(eV)	$\sigma_{\text{FAC}}(\text{C V})$	$\sigma_{\text{CB}}(\text{C V})$ [15]	$\frac{\Delta\sigma}{\sigma_{\text{CB}}}(\text{C V})$	E(eV)	$\sigma_{\text{FAC}}(\text{N VI})$	$\sigma_{\text{CB}}(\text{N VI})$ [15]	$\frac{\Delta\sigma}{\sigma_{\text{CB}}}(\text{N VI})$	E(eV)	$\sigma_{\text{FAC}}(\text{O VII})$	$\sigma_{\text{CB}}(\text{O VII})$ [15]	$\frac{\Delta\sigma}{\sigma_{\text{CB}}}(\text{O VII})$
95.00	8.84	7.08	0.24	140.00	11.81	9.41	0.25	180.00	1.26	1.21	0.04
100.00	28.64	22.47	0.27	160.00	34.32	28.25	0.21	200.00	12.54	10.33	0.21
105.00	45.61	36.27	0.25	180.00	50.15	41.97	0.19	220.00	20.91	17.55	0.15
200.00	168.71	143.77	0.17	280.00	85.00	71.42	0.19	320.00	42.65	36.35	0.15
300.00	177.86	156.28	0.07	340.00	90.04	77.45	0.16	400.00	48.74	41.70	0.16
400.00	165.67	149.72	0.10	440.00	89.61	78.41	0.14	480.00	50.61	43.62	0.16
600.00	137.05	127.85	0.07	560.00	84.19	74.70	0.12	560.00	50.45	43.85	0.15
800.00	114.91			760.00	73.64	67.00	0.09	640.00	49.33	43.22	0.14
1000.00	98.60			920.00	66.22			720.00	47.76	42.15	0.13
2370.00	50.19			1100.00	59.24			840.00	45.11	40.17	0.12
3690.00	34.42			2300.00	34.51			1040.00	40.77	36.79	0.10
4700.00	27.68			3740.00	23.14			2040.00	26.48		
5600.00	23.85			4600.00	19.39			3600.00	17.03		
6200.00	21.78			5010.00	18.00			4600.00	13.90		
7530.00	18.29			6300.00	14.73			5460.00	12.02		
8780.00	16.04			9000.00	11.91			7770.00	8.85		

9000.00	10.72			10000.00	09.74			9990.00	7.07		
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Fig. 3. Ionization cross sections of the C V, N VI and O VII (2^3S).

Regarding the variation of the cross sections with z , it is clear that for the three levels 1^1S , 2^1S and 2^3S the maximum values of the cross sections are inversely proportional to the values of z for the three helium like ions, as also indicated by the shapes of the figures 1, 2 and 3. The maximum values for the cross-sections of $(22.08, 11.18, 6.27) \times 10^{-20} \text{ cm}^2$ have been calculated successively for the three ions C V, N VI and O VII for the ground state 1^1S . For the 2^1S level the values are successively $(187.57, 83.89, 53.47) \times 10^{-20} \text{ cm}^2$, whereas for the level 2^3S the maximum cross sections take successively the values $(174.14, 90.71, 50.71) \times 10^{-20} \text{ cm}^2$. These values show that the maximum cross sections are divided by almost half depending on the increase in the value of Z for the 1^1S level. No periodicity that can be drawn for the other cross sections. A rigorous quantitative study can be done on enlarged data for all helium like ions.

4. Conclusion

In this contribution, we have presented our performed calculation of EII cross sections for the C V, N VI and O VII ions by FAC code. These results are in good agreement compared by those of CB approximation and available measurements. The relative errors for these helium like ions do not exceed 15% for the ground state. The same relative errors are in the order of 20% for the unstable singlet state and not exceed 30% for the unstable triplet state compared to CB approximation results.

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