Recommended Cross Section Data for Carbon Ions and Atoms: Electron-Impact Excitation, Ionization and Charge Exchange

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Abstract

Cross section data have been compiled for electron-impact excitation and ionization of carbon ions C^{n+}, as well as charge-exchange process between carbon ions and hydrogen atoms. A large amount of theoretical and experimental cross section data have been collected from the litterature, and we have critically assessed their accuracy. The recommended cross sections, the best values for use, are expressed in the form of simple analytical functions. These are also presented in graphical form. In this work, we have treated 76 electron-impact excitation processes for C^{n+} ($n = 5, 4, \ldots, 0$), electron-impact ionization processes for all of them, and 26 total and state-selective charge exchange processes in H+C^{n+} processes.

Keywords:

electron-impact excitation, electron-impact ionization, charge exchange

1. Introduction

Electron-impact excitation and ionization of atomic carbon ions are important processes in plasma diagnostics and energy-loss calculations in fusion plasmas. Charge-exchange process of carbon ions with hydrogen atoms also provides a useful plasma diagnostics. In this report, we present a complete set of cross sections for these processes. As a basis for this cross section set we have used the available experimental and theoretical data from the literature and critically assessed their accuracy.

2. Electron-impact excitation

There exist numerous theoretical cross section data for electron-impact excitation of carbon ions. Previously, Itikawa *et al.* [1] compiled cross sections reported before 1985, assessed them for carbon ions ($C^+ - C^{5+}$) as well as oxygen ions ($O^+ - O^{8+}$), and fitted their recommended values to an analytical formula. Theoretical cross sections were reported by McDowell *et al.* [2], Aggarwal *et al.* [3], and Zou *et al.* [4] for C^{5+}. Fisher *et al.* [5] have also carried out cross section calculations. Callaway [6] have reported theoretical rate coefficient data. There also exist results on electron-impact excitation cross sections for the other ionic states. Except for optically allowed transitions, all electron-impact excitation cross sections are scattered, and it has been sometimes difficult to determine the recommended data. However, the close-coupling method and *R*-matrix method provide more reliable results at lower collision energies, so can the distorted wave method and Coulomb-Born method at high energies. Our recommended cross sections are chosen following this criterion.

Electron-impact excitation cross sections σ are expressed in terms of collision strengths Ω. For the excitation from a state i to f, the cross section is given by

$$\sigma_{if}\,[\pi a_0{}^2] = \frac{\Omega_{if}}{\omega_i E_e[Ry]} = \frac{1}{\omega_i V_{if}[Ry]}\frac{\Omega_{if}}{X}, \qquad (1)$$

where E_e is the energy of the incident electron, ω_i is the statistical weight of the initial state, V_{if} is the excitation energy, and Ω_{if} is the collision strength. Here, the cross section is in units of $\pi a_0{}^2$, where a_0 is the Bohr radius and X is the reduced electron energy defined by

$$X = E_e/V_{if}. \qquad (2)$$

When the cross section and energy are given respectively in units of cm^2 and eV, we have

$$\sigma_{if}\,[\mathrm{cm}^2] = 11.969 \times 10^{-16} \times \frac{\Omega_{if}}{\omega_i E_e\,[\mathrm{eV}]} = 11.969 \times 10^{-16} \times \frac{\Omega_{if}}{\omega_i V_{if}\,[\mathrm{eV}]X}. \qquad (3)$$

With the Maxwellian distribution of electron velocity for temperature T_e, the rate coefficient is calculated by

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$$R_{if}\,[\mathrm{cm^3s^{-1}}] = \frac{8.010\times10^{-8}}{\omega_i\sqrt{T_e\,[\mathrm{eV}]}}\,y\int_1^\infty dX\Omega_{if}(X)e^{-yX}, \tag{4}$$

where

$$y = V_{if}/T_e. \tag{5}$$

We have carefully chosen reliable electron-impact data from the above mentioned references. Once the recommended cross sections were determined, a fit was made, which facilitates their applications. Unless otherwise stated, we used the formula:

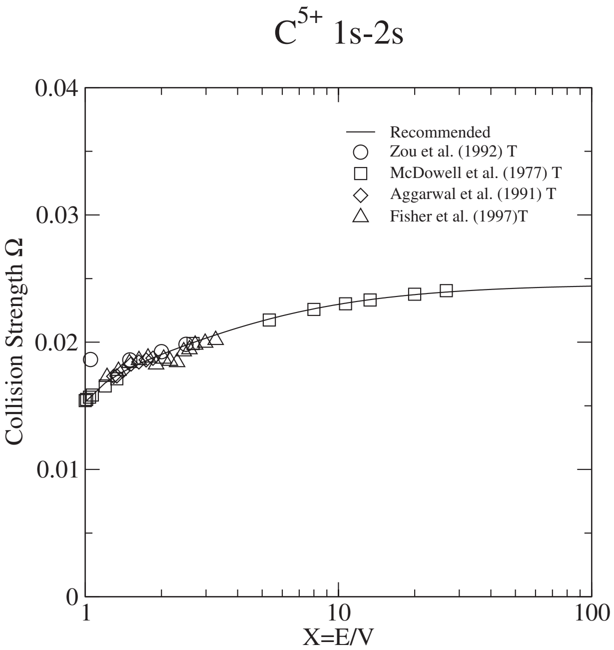

Fig. 1 Collision strengths for the electron-impact excitation 1s → 2s of C^{5+}.

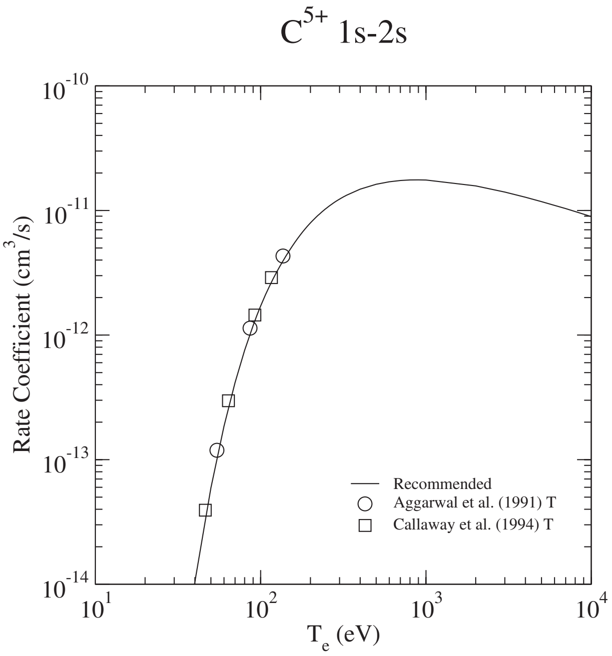

Fig. 2 Rate coefficients for the electron-impact excitation 1s → 2s of C^{5+}.

$$\Omega_{if}(X) = A + \frac{B}{X} + \frac{C}{X^2} + \frac{D}{X^3} + E\ln X, \tag{6}$$

where A, B, C, D and E are adjustable coefficients. However, we should note that we can not use such a simple formula when resonant effects dominate. In such a case, we need to indicate the boundary of the energy region where resonances dominate. The expression for the rate coefficient can be obtained analytically by using eq.(4). For example, we have obtained $A = 2.446\times10^{-2}$, $B = -1.567\times10^{-2}$, $C = 1.010\times10^{-2}$ and $D = E = 0$ for the 1s→2s transition of the C^{5+} ion. The recommended collision strength and the original ones from the references are graphically shown in Fig. 1. The rate coefficients are shown in Fig. 2. In this work, we have treated 76 electron-impact excitation processes for $C^{5+} - C^{0+}$, as shown in Table 1. These results will be published in Atomic Data and Nuclear Data Tables.

3. Electron-impact ionization

Electron-impact ionization of carbon ions has been extensively studied both experimentally and theoretically. Expetimental measurements of C^{n+} were carried out by Donets and Ovsyamnikov [7] for ionic states $n = 1, 2, 3, 4$ and 5, in the energy range above 0.1 keV. Cross sections were obtained semi-empirically by Pattard and Rost [8] for C^{5+}. Experimental measurements were also performed by Aichele *et al.* [9] for the same species. Theoretical calculation cross sections were alsoreported by Younger [10], Kao *et al.* [11], and Fang *et al.* [12].

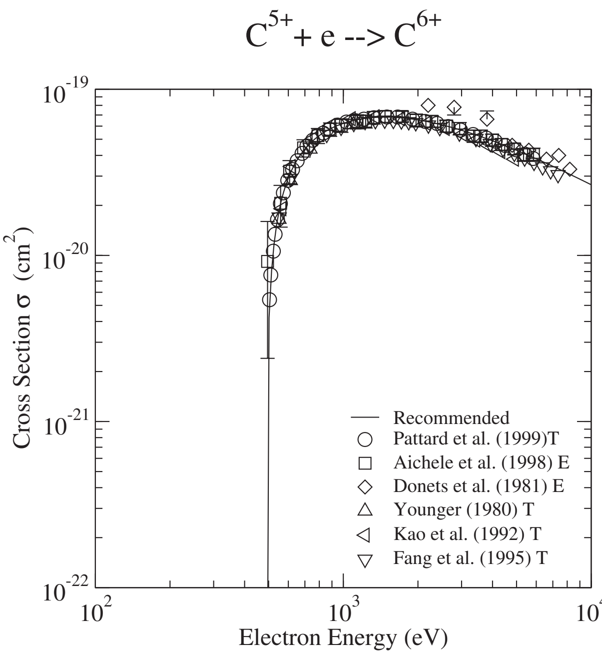

Fig. 3 Cross sections for the electron-impact ionization of C^{5+}.

Table 1 List of processes treated in the work.

excitation	C^{5+} (H-like): 1s→2s, 1s→2p, 1s→3s, 1s→3p, 1s→3d, 1s→4s, 1s→4p, 1s→5p C^{4+} (He-like): $1s^2\ {}^1S$→1s2s ^3S, $1s^2\ {}^1S$→1s2s ^1S, $1s^2\ {}^1S$→1s2p ^3P, $1s^2\ {}^1S$→1s2p ^1P, $1s^2\ {}^1S$→1s3d ^3D, $1s^2\ {}^1S$→1s3p ^1P, 1s2s ^3S→1s2s ^1S, 1s2s ^3S→1s2p ^3P, 1s2s ^3S→1s2p ^1P, 1s2s ^3S→1s3p ^3P, 1s2s ^1S→1s2p ^3P, 1s2s ^1S→1s2p ^1P, 1s2p ^3P→1s2p ^1P, 1s2p ^3P→1s3s ^3S C^{3+} (Li-like): 2s ^2S→2p ^2P, 2s ^2S→3s ^2S, 2s ^2S→3p ^2P, 2s ^2S→3d ^2D, 2s ^2S→4p ^2P, 2p ^2P→3s ^2S, 2p ^2P→3d ^2D, 2p ^2P→4s ^2S C^{2+} (Be-like): 2s2p ^3P→$2p^2\ {}^3P$, 2s2p ^3P→$2p^2\ {}^1D$, 2s2p ^3P→$2p^2\ {}^1S$, 2s2p ^3P→2s3s ^1S, 2s2p ^3P→2s3p ^1P, 2s2p ^3P→2s3p ^3P, 2s2p ^3P→2s3d ^3D, 2s2p ^3P→2s3s ^1D, 2s2p ^1P→$2p^2\ {}^3P$, 2s2p ^1P→$2p^2\ {}^1D$, 2s2p ^1P→$2p^2\ {}^1S$, $2p^2\ {}^3P$→$2p^2\ {}^1D$, $2p^2\ {}^3P$→$2p^2\ {}^1S$, $2p^2\ {}^1D$→$2p^2\ {}^1S$ C^+ (B-like): $2s^22p\ {}^2P$→$2s2p^2\ {}^4P$, $2s^22p\ {}^2P$→$2s2p^2\ {}^2D$, $2s^22p\ {}^2P$→$2s2p^2\ {}^2S$, $2s^22p\ {}^2P$→$2s2p^2\ {}^2P$, $2s^22p\ {}^2P$→$2s^23s\ {}^2S$, $2s^22p\ {}^2P$→$2s^23p\ {}^2P$, $2s^22p\ {}^2P$→$2s^23d\ {}^2D$ C: $2s^22p^2\ {}^3P$→$2s^22p^2\ {}^1D$, $2s^22p^2\ {}^3P$→$2s^22p^2\ {}^1S$, $2s^22p^2\ {}^3P$→$2s2p^3\ {}^5S$, $2s^22p^2\ {}^3P$→$2s^22p3s\ {}^3P$, $2s^22p^2\ {}^3P$→$2s^22p3s\ {}^1P$, $2s^22p^2\ {}^3P$→$2s2p^3\ {}^3D$, $2s^22p^2\ {}^3P$→$2s^22p3p\ {}^1P$, $2s^22p^2\ {}^3P$→$2s^22p3p\ {}^3D$, $2s^22p^2\ {}^3P$→$2s^22p3p\ {}^3S$, $2s^22p^2\ {}^3P$→$2s^22p3p\ {}^3P$, $2s^22p^2\ {}^3P$→$2s^22p3p\ {}^1D$, $2s^22p^2\ {}^3P$→$2s^22p3p\ {}^1S$, $2s^22p^2\ {}^3P$→$2s2p^3\ {}^3P$, $2s^22p^2\ {}^3P$→$2s^22p3d\ {}^1D$, $2s^22p^2\ {}^3P$→$2s^22p3d\ {}^3F$, $2s^22p^2\ {}^3P$→$2s^22p3d\ {}^3D$, $2s^22p^2\ {}^3P$→$2s^22p3d\ {}^1F$, $2s^22p^2\ {}^3P$→$2s^22p3d\ {}^3P$, $2s^22p^2\ {}^3P$→$2s2p^3\ {}^1D$, $2s^22p^2\ {}^3P$→$2s2p^3\ {}^3S$, $2s^22p^2\ {}^3P$→$2s2p^3\ {}^1P$, $2s^22p^2\ {}^1D$→$2s^22p^2\ {}^1S$, $2s^22p^2\ {}^1D$→$2s2p^3\ {}^3D$, $2s^22p^2\ {}^1D$→$2s^22p3s\ {}^3P$, $2s^22p^2\ {}^1D$→$2s^22p3s\ {}^1P$
ionization	C^{5+} →C^{6+}, C^{4+} →C^{5+}, C^{3+} →C^{4+}, C^{2+} →C^{3+}, C^+ →C^{2+}, C^+ →C^{3+}, C→C^+
charge exchange	C^{6+}+H→C^{5+}(*nl*)+H^+ (*nl*=1s,2s,2p,3s,3p,3d,4s,4p,4d,4f,5s,5p,5d,5f,5g), C^{6+}+H→C^{5+}(*n*)+H^+ (*n*=1,2,3,4,5), C^{6+}+H→C^{5+}+H^+, C^{5+}+H→C^{4+}+H^+, C^{4+}+H→C^{3+}+H^+, C^{3+}+H→C^{2+}+H^+, C^{2+}+H→C^++H^+, C^++H→C+H^+

The recommended cross section for electron-impact ionization is parametrized by the expression

$$\sigma\,[\mathrm{cm}^2] = \frac{10^{-13}}{IE}\left\{A_1 \ln(E/I) + \sum_{i=2}^{N} A_i\left(1-\frac{I}{E}\right)^{i-1}\right\}, \tag{7}$$

where the collision energy E and ionization potential I are expressed in eV units and A_i are fitting coefficients. The coefficient A_1 can be related to the continuum oscillator strength $df/d\epsilon$ by

$$A_1 = 8.39\times10^{-2} I\,[\mathrm{eV}]\int_0^\infty \frac{1}{E+\epsilon}\frac{df}{d\epsilon}d\epsilon \tag{8}$$

where ϵ is the energy of ejected electrons. For example, we have obtained $I = 490.0$, $A_1 = 2.489\times10^{-1}$, $A_2 = 1.847\times10^{-1}$, $A_3 = 4.475\times10^{-2}$, $A_4 = -9.432\times10^{-2}$ and $A_5 = 5.122\times10^{-1}$ for the C^{5+} →C^{6+} transition. The recommended cross section is shown graphically in Fig. 3, together with the cross sections from the literature. In this work, we have treated the electron-impact ionization processes for all ionic species $C^{5+} - C^{0+}$ as well as the electron-impact double ionization processes of C^+.

4. Charge exchange in collisions between carbon ions and hydrogen atoms

There exist numerous theoretical and experimental results for charge exchange processes in collisions of carbon ions with hydrogen atoms. The C^{6+}+H collision is the most studied process: theoretical cross sections for charge exchange were reported by Panov *et al.* [13], Fritsch *et al.* [14], Kimura *et al.* [15], Janev *et al.* [16], Fritsch [17], Olson *et al.* [18] and Belkic [19]. The recommended cross sections are fitted to the following analytic functions:

$$\sigma\,[\mathrm{cm}^2] = 10^{-16}\times\begin{cases} \dfrac{a_1\exp[-(a_2/E)^{a_3}]}{1+(E/a_4)^{a_5}+(E/a_6)^{a_7}} \\ \dfrac{a_1\exp[-(a_2/E)^{a_3}]}{1+(E/a_4)^{a_5}+(E/a_6)^{a_7}+(E/a_8)^{a_9}} \\ \dfrac{a_1\exp[-(a_2/E)^{a_3}]}{1+(E/a_4)^{a_5}+(E/a_6)^{a_7}+(E/a_8)^{a_9}} \\ \quad+\dfrac{a_{10}\exp[-(a_{11}/E)^{a_{12}}]}{1+(E/a_{13})^{a_{14}}} \end{cases}, \tag{9}$$

where the collision energy E is expressed in eV/amu units and a_i, $i = 1-14$ are fitting parameters. For example, we have found $a_1 = 2.301\times10^2$, $a_2 = 5.983\times10^3$,

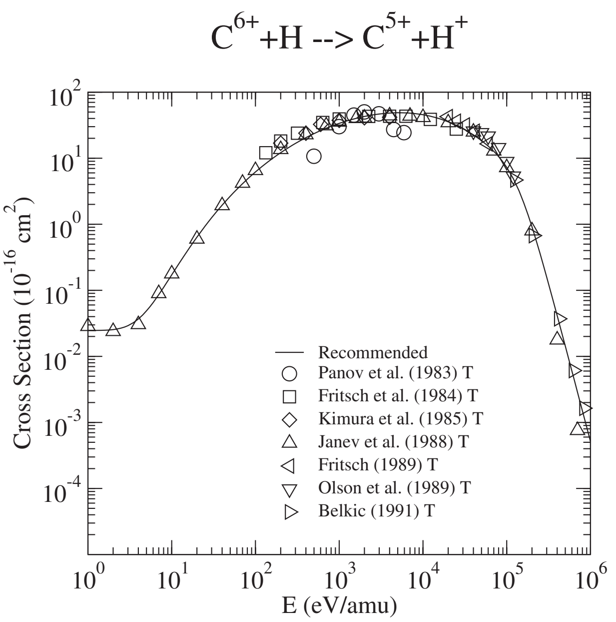

Fig. 4 Cross sections for the charge exchange process $C^{6+} + H \rightarrow C^{5+} + H^{+}$.

$a_3 = 3.117 \times 10^{-1}$, $a_4 = 1.300 \times 10^4$, $a_5 = 6.613 \times 10^{-1}$, $a_6 = 7.299 \times 10^4$, $a_7 = 4.985$, $a_8 = 2.100 \times 10^4$, $a_9 = 1.557$, $a_{10} = 3.355 \times 10^{-2}$, $a_{11} = 1.800 \times 10^{+5}$, $a_{12} = -9.768 \times 10^{-2}$, $a_{13} = 4.500 \times 10^3$ and $a_{14} = 3.584$ for the $C^{6+} + H \rightarrow C^{5+} + H^{+}$ transition. The fitted cross section as well as the original cross sections form the literature are graphically shown in Fig. 4. In this work, we have treated 26 total and state-selective charge exchange processes in H+C^{n+} processes, as shown in Table 1. These results will be published in Atomic Data and Nuclear Data Tables.

5. Summary

We have compiled and critically assessed the cross sections for electron-impact excitation and ionization of atomic carbon ions, as well as charge exchange in collisions between carbon ions and hydrogen atoms. The recommended cross sections are expressed in terms of simple analytic fit functions. These can immediately lead to applications in fusion science. In this paper, we have shown only examples of our results. All our results will be published in Atomic Data and Nuclear Data Tables.

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