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Calculation of total cross sections for electron capture in collisions of Carbon ions with H(D,T)(1s)

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Abstract. The calculations of total cross sections of electron capture in collisions of C^{q+} with H(1s) are reviewed. At low collision energies, new calculations have been performed, using molecular expansions, to analyze isotope effects. The Classical Trajectory Monte Carlo method have been also applied to discuss the accuracy of previous calculations and to extend the energy range of the available cross sections.

1. Introduction

Carbon ions are one of the main impurities in present tokamak plasmas, where carbon composites are used in first wall tiles, specially in the divertor. It is known that these materials are not appropriate for D-T plasmas because of the tritium deposition problem, and it is planned that ITER first wall will be completely made of Be and W tiles. However, small amounts of carbon impurities will be present in ITER, and it is possible that future devices will include materials which will release C^{q+} ions. The importance of carbon impurities has stimulated many theoretical and experimental works on collisions of these ions with Hydrogen. In particular, the electron capture reactions (EC) were reviewed in 2006 by Suno and Kato [1]; they reviewed the bibliography and proposed a set of recommended data for both total and state-selective electron capture cross sections.

The aim of the present work is to discuss the existing calculations on the EC reactions:

$$C^{q+} + H(1s) \rightarrow C^{(q-1)+} + H^{+}. \quad (1)$$

The collisions involving the fully stripped projectile C^{6+} have been studied in many works because their relevance in charge exchange diagnostics [2] and also because, being a one-electron system, it is relatively easier to describe theoretically than the collisions with other Carbon ions, which require the use of sophisticated quantum chemistry techniques to obtain accurate results. The collision C^{4+} + H, can also be treated as a one-electron system, where the interaction of the active electron with the C^{4+} core is described by means of an effective potential.

In order to discuss the accuracy of previous calculations and to fill up some gaps of the existing database, we have carried out new calculations employing classical trajectory Monte Carlo (CTMC) methods for energies above 10 keV/u. We have applied the CTMC method to H collisions with partially stripped projectiles by employing a model potential to represent the


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interaction of the active electron with the ionic core, as previously employed in the classical calculations of Stancil *et al* [3].

At low energies, we have employed the molecular-functions-close-coupling (MFCC) method[1]. our calculations aim to extend the energy range of the computed EC total cross sections and to discuss the isotopic effect. These two aspects have been less studied because they are not relevant in core plasma diagnostics, but can be important in passive diagnostics and in plasma modeling. For collisions of low charged (q=1,2) Carbon ions, the EC reaction is endothermic, the EC channels $C^{(q-1)+}$ are closed at low energies, and the total cross section decreases rapidly as the collision energy, E, decreases. However, for q=3-6, the reaction (1) is exothermic for some EC channels and, consequently, there is not a threshold in the EC total cross sections, which increase approximately as $E^{-1/2}$ as E decreases, as predicted by the Langevin model [4, 5], leading to large cross sections at energies below $E \approx 10$ eV/u. Another relevant aspect of low-energy EC is the presence of shape resonances, found in several theoretical works [6, 7, 8, 9], although the precision of the experimental techniques has precluded to observe them hitherto.

2. Computational methods

2.1. The MFCC method

The MFCC calculations have been carried out using the method described ion detail in previous publications [8, 10]. In this method, the scattering wave function Ψ^J is solution of the stationary Schrödinger equation:

$$\widehat{H}\Psi^J = E\Psi^J \tag{2}$$

where E is the collision energy and $\widehat{H}$ is the total Hamiltonian of the system given by

$$\widehat{H} = -\frac{1}{2\mu}\nabla_R^2 + \widehat{H}_{\rm el} \tag{3}$$

with μ the reduced mass of the nuclei and $\widehat{H}_{\rm el}$ the Born-Oppenheimer electronic Hamiltonian. Ψ^J is expanded in a molecular basis set, $\{\phi_j\}$:

$$\Psi^J(\boldsymbol{r},\boldsymbol{\xi}) = \sum_j \chi_j^J(\boldsymbol{\xi})\phi_j(\boldsymbol{r};\xi) \tag{4}$$

In this expression, J is the total angular momentum and $\boldsymbol{r}$ are the electronic coordinates. $\boldsymbol{\xi}$ is a common reaction coordinate [11], a linear combination of the internuclear vector $\boldsymbol{R}$ and the electronic coordinates that ensures that a truncated expansion fulfills the boundary conditions. We have employed a common reaction coordinate based on the switching function of reference [12] for the many-electron systems, while for C^{4+} and C^{6+} + H collisions the common reaction coordinate is defined by means of the switching function of references [13, 14]. The molecular functions ϕ_j are (approximate) eigenfunctions of $\widehat{H}_{\rm el}$:

$$\widehat{H}_{\rm el}\phi_j(\boldsymbol{r};R) = \epsilon_j(R)\phi_j(\boldsymbol{r};R) \tag{5}$$

For a N-electron system, $\widehat{H}_{\rm el}$ has the form:

$$\widehat{H}_{\rm el} = -\frac{1}{2}\sum_{k=1}^{N}\nabla_k^2 + V(\boldsymbol{r},R) \tag{6}$$

[1] Since in this method the collision wave function is expanded in terms of many-electron wave functions, we name these basis functions "molecular functions" instead of the commonly-used "molecular orbitals" name.

Table 1. Values of the parameter α of equation (8) for $C^{(q-1)+}$.

	C	C^{2+}	C^{3+}	C^{4+}
α	1.18	1.85	3.72	5.67

where $V(\boldsymbol{r}, R)$ is the potential that includes electron-nuclei and electron-electron interactions.

Substitution of the expansion (4) into the Schrödinger equation leads to system of differential equations for the nuclear functions χ_j^J, which is solved numerically. The asymptotic behavior of these functions allows us to evaluate the **S**-matrix, as explained in detail in [15], and the total cross section for the transition between two states $\phi_i \to \phi_j$, σ_{ij}, is computed from the **S**-matrix elements using the equation:

$$\sigma_{ij} = \frac{\pi}{k_i^2} \sum_J (2J+1) \left| \delta_{ij} - S_{ij}^J \right|^2 \tag{7}$$

The molecular orbitals of the one-active electron systems CH^{4+} and CH^{6+} were obtained using the method of Power [16]. For the many-electron systems we have computed the molecular wave functions, the potential energy curves and non-adiabatic couplings by applying the multi-reference configuration interaction (MRCI) methods. In the present work we have employed the package MOLPRO [17] for calculating the molecular functions of the four-active electron system CH^+, and the package MELD [18] for the three- and two-active electron quasimolecules CH^{2+} and CH^{3+}.

2.2. The CTMC method

At $E > 10$ keV/u, we have employed the CTMC method. In our treatment the nuclei follow rectilinear trajectories ($\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$) and the electronic motion is described by means of a classical distribution function $\rho(\boldsymbol{r}, \boldsymbol{p}, t)$ for an ensemble of $\mathcal{N}$ ($\mathcal{N} \approx 10^5$ in our calculations) independent electron trajectories, $(\boldsymbol{r}(t), \boldsymbol{p}(t))$, which are obtained by integration of the Hamilton equations determined by the electronic Hamiltonian. The standard CTMC method [19] is restricted to one-electron systems, but it can be applied to one-effective electron systems by employing an effective potential. In our calculations we have used the model potential:

$$V(r_C) = -\frac{6 - N_c}{r_C} - \frac{N_c}{r_C}(1 + \alpha\, r_C) \exp\left(-2\alpha\, r_C\right) \tag{8}$$

to represent the interaction of the active electron with the C^{q+} ion. In equation (8), r_C is the electron distance to the C nucleus, N_c the number or core electrons and the parameter α (see table 1) has been obtained by fitting the ionization energy of the $C^{(q-1)+}$ ion.

The total EC cross section is given in this method by:

$$\sigma^{\mathrm{EC}}(E) = 2\pi \int_0^\infty b P^{\mathrm{EC}}(b) \mathrm{d}b \tag{9}$$

where the EC transition probability is calculated as:

$$P^{\mathrm{EC}} = \frac{\mathcal{N}^{\mathrm{EC}}}{\mathcal{N}}, \tag{10}$$

being $\mathcal{N}^{\mathrm{EC}}$ the number of trajectories where the electron is bound to the projectile at the end of the collision ($vt_{\mathrm{fin}} = 500$ a.u. in our calculation); i.e., those with negative energy with respect to the projectile and positive energy with respect to the target.

Table 2. Total cross sections in 10^{-16} cm^2 for C^{q+} + H(1s) $\rightarrow$ $C^{(q-1)+}$ + H^+ as functions of the impact energy in keV/u.

E	$q=1$	$q=3$	$q=4$	$q=5$	$q=6$
10	5.23	21.4	31.1	40.3	49.2
25	2.73	17.0	25.8	34.3	42.6
50	0.946	7.71	13.2	19.4	26.3
100	0.266	1.59	3.09	5.02	7.37
200	0.0565	0.173	0.341	0.599	0.926
300	0.0186	0.0396	0.0714	0.126	0.209

At low collision energies, the accuracy of the CTMC method is determined by the quality of the initial distribution, $\rho^i(\boldsymbol{r},\boldsymbol{p})$, that, in our case, is the classical distribution for the ground state of the Hydrogen atom. The standard CTMC treatment employs a microcanonical distribution, where all electron trajectories have the energy -0.5 a.u. of the quantal level. In order to compare with the quantal distributions, one can introduce the radial and momentum distributions:

$$\rho_r^i(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{p}\rho^i(\boldsymbol{r},\boldsymbol{p});\ \rho_p^i(\boldsymbol{p}) = \int \mathrm{d}\boldsymbol{r}\rho^i(\boldsymbol{r},\boldsymbol{p}) \tag{11}$$

It is well known (e.g. [20]) that, although the microcanonical distribution leads to a momentum distribution identical to the quantal one, it is unable to describe the tail of the radial quantal distribution, which includes electron-nucleus distances in the classically forbidden region. At low collision energies, this limitation is specially relevant because the EC probability is high for the initially loosely bound electron trajectories. Some alternatives have been suggested in order to solve this limitation of the microcanonical distribution. In particular, we have employed the so-called hydrogenic distribution [21, 22], which is a linear combination of several (ten in our calculations) microcanonical distributions with different energies; the coefficients of the combination are obtained by fitting the quantal radial distribution with the restriction that the mean energy of this distribution is approximately equal to -0.5 a.u.. In practice, it is found that the hydrogenic spatial and momentum distributions agree with their quantal counterparts.

Previous calculations on collisions Hydrogen atoms and fully stripped ions with $q \geq 6$ have shown that the CTMC EC cross sections at high impact energy ($E \gtrsim 500$ keV/u) are larger than those obtained with perturbative treatments, which are expected to be accurate in this energy range. Therefore, we present in table 2 our CTMC cross sections for $E < 300$ keV/u.

3. C^+ + H collisions

Janev *et al* [23] deduced a recommended total cross section for the reaction

$$C^+(1s^2 2s^2 2p\ ^2P) + H(1s) \rightarrow C + H^+ \tag{12}$$

based on the experimental data of references [24, 25] and [26]. Stancil *et al* [3] have performed a combined experimental and theoretical study of this process. In order to cover a wide energy range, they reported merged-beam experiments and calculations with several methods: MFCC, CTMC, multielectron hidden crossing and the decay model. Although the new results agree with the high-energy measurements of references [24] and [26], they disagree with those of [25] at collision energies between 0.3 and 1 keV/u. However, the MFCC results of Stancil *et al* [3] agree with the merged-beam experimental cross sections reported in the same paper, which lead to the authors to suggest a new recommended cross section for reaction (12) that clearly differs from that of reference [23] for energies below 1 kev/u. As explained in reference [3],

the potential energy curves of the CH^+ system do not show any avoided crossing between the potential energy curves of the entrance channels and those of the molecular states leading to EC. The main mechanism of reaction (12) involves transitions from the state $a^3\Pi$ to $2^3\Pi$, with a energy difference of about 0.2 a.u., that yield a cross section that decays rapidly as E decreases.

We have performed a MRCI calculation with an aug-cc-pVQZ basis set [27]. The molecular orbitals were obtained by a 5-state CASSCF procedure, and the ensuing MRCI calculation included up to 5×10^5 configuration state functions. We have employed these molecular wave functions to calculate the EC total cross section, which is practically identical to that of reference [3]. Moreover, the merged-beams experiment of Stancil et al. [3] was carried out with Deuterium, while that of Nutt et al. [25] was performed with Hydrogen. We have checked that the isotopic dependence of the calculated cross section for the reaction (12) is negligible above $E = 10$ eV/u and does not explain the difference between both measurements.

On the other hand, the CTMC results of Stancil *et al* [3] underestimate the experimental data for energies between 1 and 25 keV/u. These can be due to the inadequacy of the microcanonical classical distribution for H(1s) [19, 20], which leads to a decrease of the EC total cross section at low energies (see e.g. reference [28]). The use of a model potential, whose functional form is not shown in the paper of reference [3], might also limit the validity of that calculation. For $E < 1$ keV the CTMC calculation overestimates the experiment, which is explained by the authors as due to the trajectories leading to capture with energies below those in the phase space bin associated to the 2p level and that would correspond to the electron capture into quantum levels that are already occupied. The above-mentioned difficulties are probably not important at $25 < E < 200$ keV/u, where the CTMC calculation agrees with the available experiments [24, 26]. The recommended data are not supported by either calculations or experiments at $E > 200$ keV/u. To further study the workings of the CTMC method we have calculated the total cross section with the eikonal CTMC method and with the model potential of equation (8). A hydrogenic distribution [22] has been used to represent the initial distribution of the H(1s). The comparison of the present calculation with the recommended data of Stancil *et al* [3] and the CTMC data from the same reference (figure 1) indicates that the underestimation of the total cross section for energies below 25 keV/u is reduced by using the hydrogenic distribution; our results with the microcanonical distribution, not shown in figure 1, are indistinguishable from those from reference [3]. In the energy range of figure 1 we have not found a sizable effect of trajectories leading to nonphysical EC.

4. C^{2+} + H collisions

The system has been studied theoretically by Gu *et al* [29] and Errea *et al* [30], both calculations used a MFCC method within a semiclassical treatment. This system was studied experimentally by Nutt *et al* [31], Phaneuf *et al* [24], Goffe *et al* [26], Gardner *et al* [32] and Voulot *et al* [33]. The calculation of reference [30] tabulated total and state-selective cross section for the EC reaction:

$$C^{2+}(1s^2 2s^2\,{}^1S) + H(1s) \rightarrow C^+ + H^+ \tag{13}$$

From the experimental point of view, the main difficulty to study this system is the presence of unknown quantities of metastable ions $[C^{2+}(1s^2 2s 2p^3P)]$ in the beams. However, references [33] and [30] pointed out that the experimental total cross sections are not modified by a contamination of the beam as high as 20% for energies above 0.1 keV/u. Nonetheless, the calculated cross sections overestimate the experimental ones at $E < 1$ keV/u (see figure 2). Errea *et al* [30] suggested that the discrepancies could be due to a normalization problem of the experiment, but neither new experiments nor calculations have been performed. At $E > 1$ keV/u, target ionization is not negligible, and the molecular close-coupling treatment, which does not include continuum wave functions, is not applicable. To our knowledge, no other theoretical methods have been applied to this particular reaction.

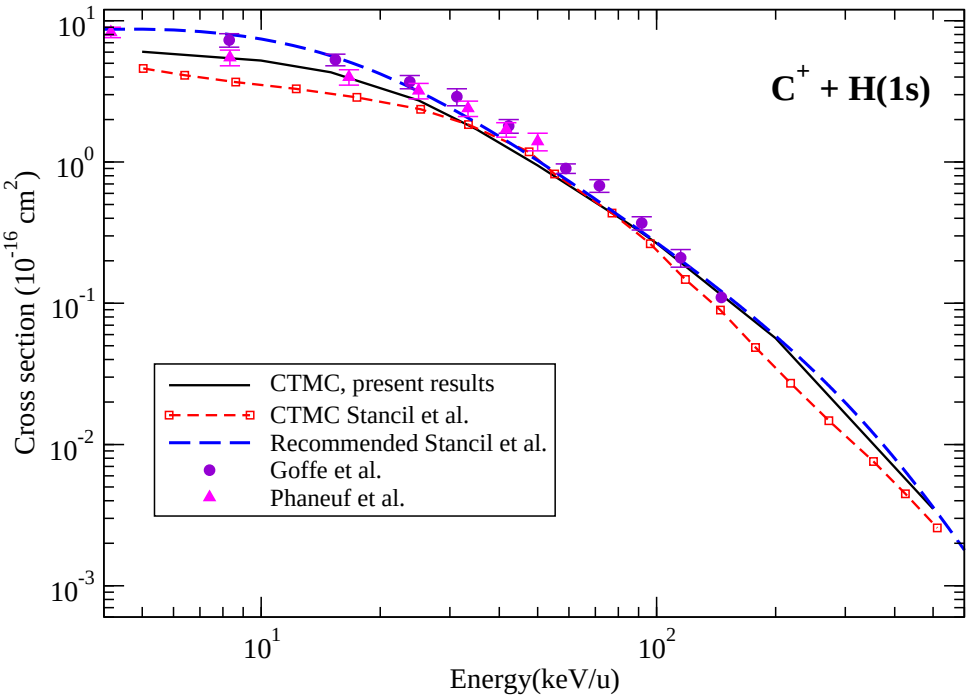


Figure 1. Total cross section for reaction (12) as a function of the impact energy. CTMC results are compared with previous calculations of Stancil *et al* [3], recommended data of reference Stancil *et al* [3] and experimental data [24, 26].

At low energies ($E < 100$ eV/u), the eikonal approximation employed in references [29] and [30] is not accurate, and we have carried out a fully quantal calculation. Since energy differences are critical in low-energy calculations, we have recalculated the potential energy curves and dynamical couplings of the doublet molecular states of the CH^{2+} quasimolecule. In our calculation, the asymptotic energy difference between the states dissociating into $C^{2+}(1s^2 2s^2\,{}^1S)$ + H(1s) (the entrance channel) and $C^{+}(1s^2 2s 2p^2\,{}^2D)$ (the main exit channels) is 0.0577 a.u., which has to be compared to the value 0.0384 a.u. reported in [30] and the experimental value 0.0547 a.u. [34]. The cross sections for reaction (13) are shown in figure 2. It is clear that the new MFCC calculation with rectilinear trajectories reproduces the results of Errea *et al* [30], and the difference with the experiment of Nutt *et al* [31] is essentially due to the population of the state $C^{+}(2s^2 2p^2\,{}^2S)$. In fact, the 3-state calculation, including the entrance channel and the most populated $^2\Sigma^+$ states [those dissociating into $C^{+}(2s^2 2p\,{}^2P)$ + H^+ and $C^{+}(2s 2p^2\,{}^2D)$ + H^+], yields a cross section practically identical to the experimental one and to that reported by Gu *et al* [29], who only included the populations of ^2P and ^2D exit channels.

At energies below 0.1 keV/u, the trajectory effects are sizable, but a relatively simple 2-state calculation can be carried out, as can be deduced from the comparison of 2- and 3-state cross sections. The two-state quantal calculation leads to the cross sections for different isotopes shown in figure 2. As for C^+ + H collisions, the EC cross section of figure 2 shows a threshold at low E, as expected for a endothermic reaction. The isotope effect is small but noticeable, and with a behavior ($\sigma_T > \sigma_D > \sigma_H$) already observed in other systems (see [35, 36]). This isotopic dependence is typical of systems where the electron capture reaction takes place at short internuclear distances where the ion-atom interaction potential that defines the trajectory is positive. We do not present CTMC results for reaction (13) because this collision is not accurately described by means of a single electron treatment given that two-

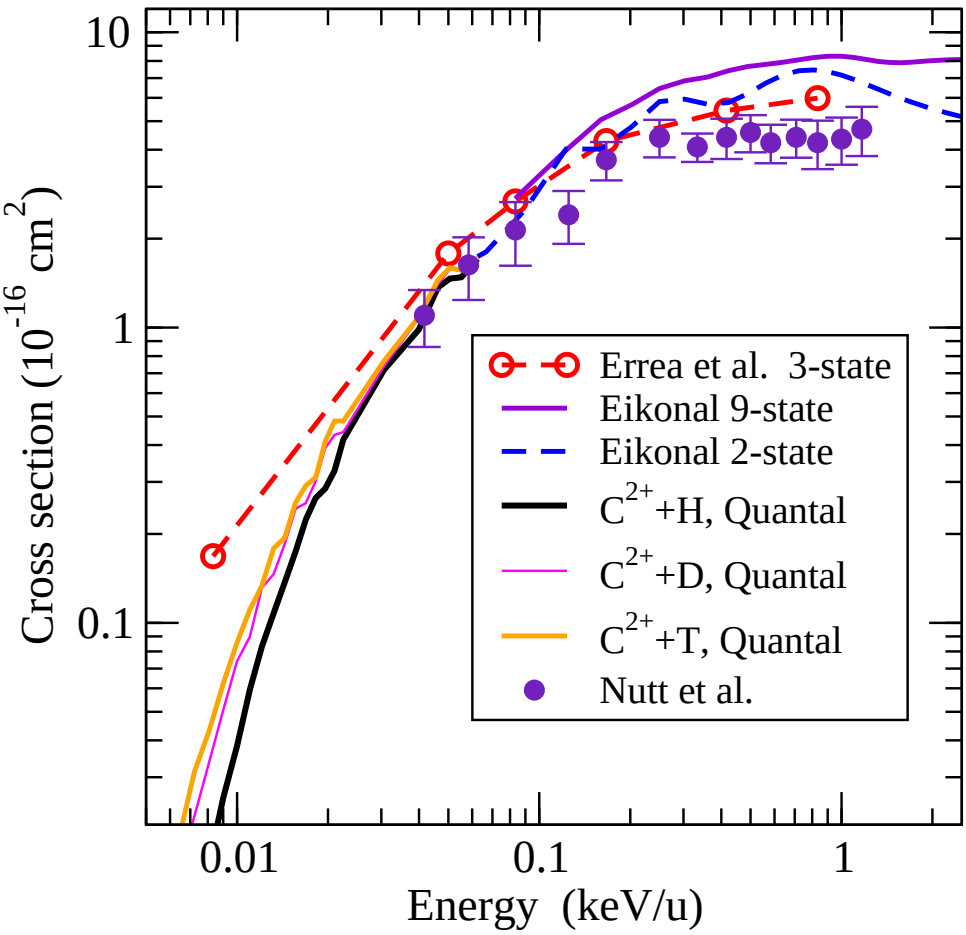


Figure 2. Total cross section for electron capture in C^{2+} + H(D,T)(1s) collisions, reaction (13), as function of the impact energy. Semiclassical results with 9- and 2-state basis are compared to 2-state quantal calculations for collisions with H, D and T. Also included are the eikonal result of Errea *et al* [30] and the experimental results of Nutt *et al* [31].

electron processes are known to play a significant role. In particular, the formation of the main exit channel $C^+(1s^2 2s 2p^2\ ^2D)$ of the EC reaction involves a two-electron process from the initial state, $C^{2+}(1s^2 2s^2\ ^1S)$ + H(1s), in which one electron is captured and another one excited.

5. C^{3+} + H collisions

Total cross sections for electron capture in C^{3+} + H collisions were measured by Phaneuf *et al* [24, 37], Goffe *et al* [26], Crandall *et al* [38], Gardner *et al* [32], Ćirić *et al* [39] and Havener *et al* [40]. Previous calculations have been carried out using MFCC treatments within semiclassical [41] and quantal formalisms [42, 43, 44], atomic orbital close-coupling (AOCC) treatments [45] and the so-called Electron-Nuclear-Dynamics method [46]. The results of previous works are plotted in figure 3. In the present work we have performed a MFCC calculation with MRCI wave functions. As a confirmation of the quality of the molecular wave functions, the asymptotic energy differences between the most important channels differ in about 0.01 a.u. from the spectroscopic values, which is a significant improvement with respect to those employed by Errea *et al* [41] and Herrero *et al* [44].

In the present work, we have evaluated the EC cross section by using an improved set of 33

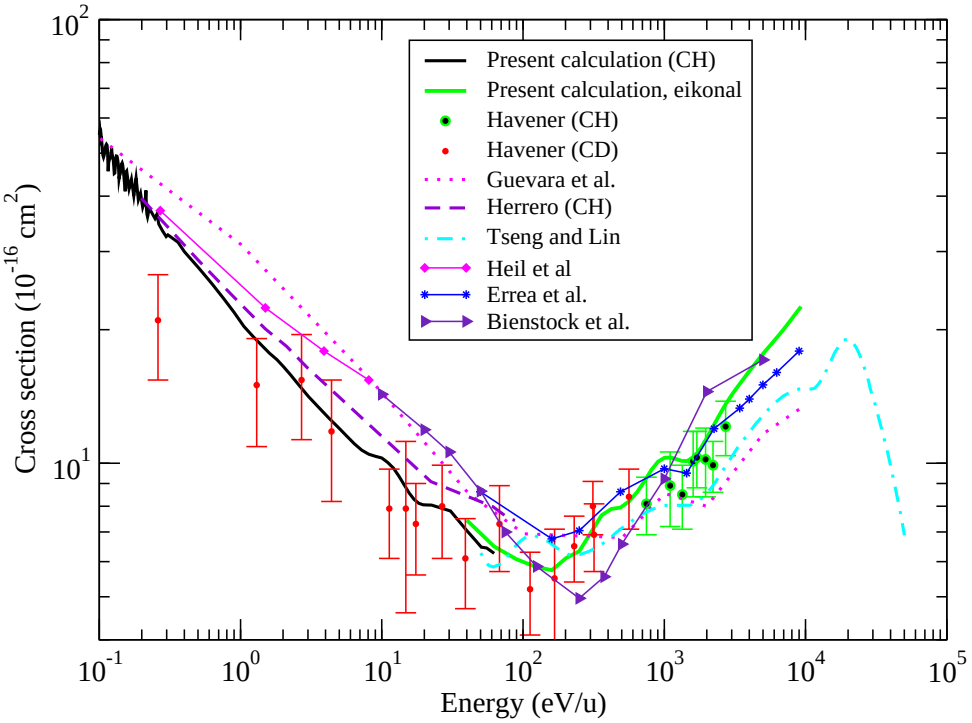


Figure 3. Total cross section for electron capture in C^{3+} + H(1s) collisions as function of the impact energy. Full lines: present quantal (thin line) and eikonal (thick line) results. Previous calculations of references [42, 43, 41, 44, 45, 46] and experiments [40] are also included, as indicated in the figure.

molecular functions (15 singlets and 18 triplets) in the eikonal calculation and 10 functions (5 singlets and 5 triplets) in the quantal one. Our quantal total cross section is lower than that of Herrero *et al* [44] and the eikonal one is somewhat lower than that of Errea *et al* [41]; the differences are due to the changes in the potential energy curves and couplings with respect to those of the valence bond calculation [47] used in previous MFCC calculations. The new results show very good agreement with the merged-beams experiment [40]. At energies above $E \approx 2$ keV the molecular expansion converges slowly, and the AOCC results of Tseng and Lin [45] are probably more accurate. Moreover, the AOCC calculation agrees with the experimental data and the cross section computed by Guevara *et al* [46].

At low velocities, the EC cross section (see figure 4) increases rapidly as E decreases, following approximately the Langevin model [4], where the cross section is proportional to $E^{-1/2}$. As already pointed out by Herrero *et al* [44], the isotopic dependence is small in the triplet subsystem, which leads to a small but noticeable isotopic dependence of the total cross section for $v < 2 \times 10^{-3}$ a.u. ($E < 0.1$ eV/u). One can also note the spikes in the cross sections due to the presence of quasi-stationary vibrational states in the effective potential of the initial molecular state. This effective potential is obtained by adding the centrifugal term and the electronic energy, whose asymptotic behavior:

$$\epsilon \sim -\frac{q^2\alpha}{2R^4}, \tag{14}$$

corresponds to the ion-induced-dipole interaction, with α the atom polarizability. One can also note the oscillations of the EC cross section for $0.1 < E < 0.3$ eV/u, caused by the interferences

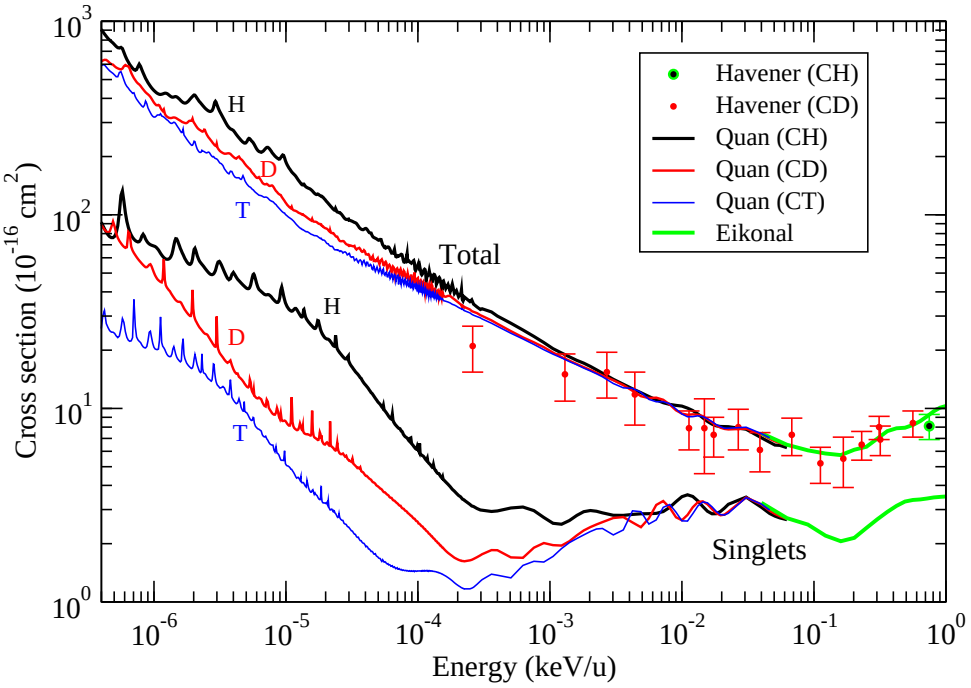


Figure 4. Total cross section for electron capture in C^{3+} + H(D,T)(1s) collision as function of the collision energy. Present results corresponding to different isotopes are plotted with solid lines. The contributions of the singlet subsystem to the total cross sections are also shown. Experimental data by Havener *et al* [40] are included.

between the nuclear wave functions in two avoided crossings between the potential energy curves of the entrance and the main exit channel in the triplet subsystem.

At high energy (see figure 5), there are no theoretical data available, and we have performed a calculation similar to that for C^+ + H (figure 1). The calculation employs the eikonal-CTMC method with the hydrogenic initial distribution and the model potential of equation (8). At $E > 30$ keV/u, our cross section shows good agreement with the experiments and the recommended data. For $E < 30$ keV/u the calculation agrees with the experimental results of Goffe *et al* [26], but these energies are probably too low to employ the CTMC method to asses the accuracy of the experimental values.

6. C^{4+} + H collisions

Several calculations have been carried out of EC total cross sections in C^{4+} + H collisions. In particular, MFCC calculations of [48, 49], expansions in terms of atomic orbitals [50], wave-packet treatments [51] and the hyperspherical close coupling method [52]. The low-energy behavior of the cross section has been studied in reference [9]. The EC cross sections is almost constant for collision energies between 100 eV/u and 10 keV/u. For $E > 10$ keV/u, target ionization is the dominant process and the EC cross section decreases rapidly as E increases. The cross section at high energies was measured by Phaneuf *et al* [24] and Goffe *et al* [26], but there is no theoretical counterpart of these measurements.

At $E < 10$ keV/u, there is a remarkable good agreement between different calculations, but the agreement with the experiments [53, 54] is less satisfactory. In this respect, Liu *et al* [52] concluded that the low-energy measurements are not supported by the theories, and that further experimental work is needed. In our opinion, the calculated cross sections are more accurate

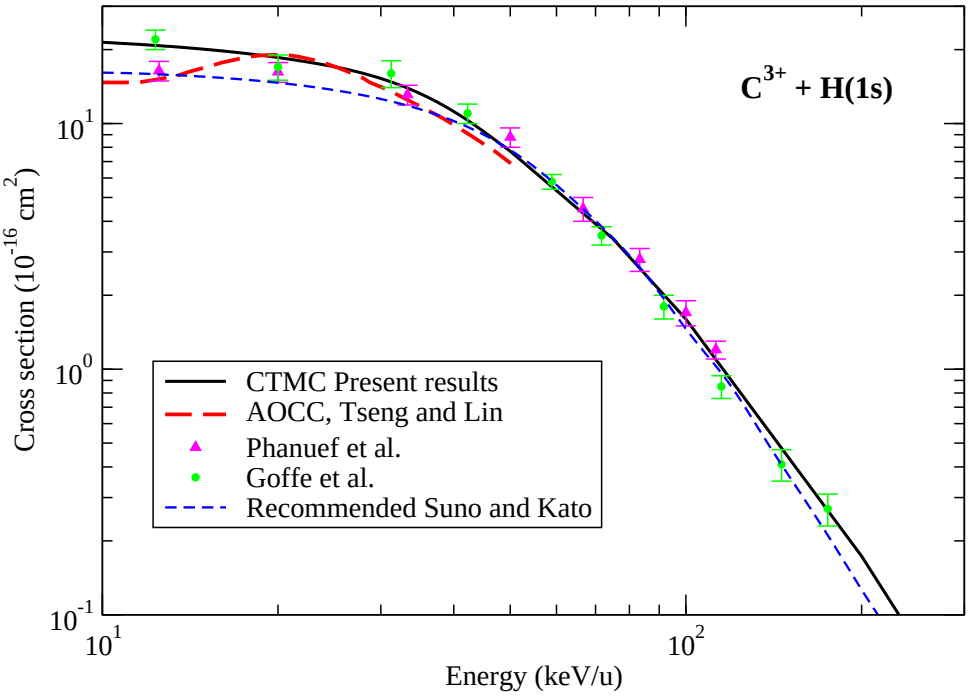


Figure 5. Total cross section for electron capture in C^{3+} + H (1s) collisions as function of the impact energy. Our CTMC results are compared to the experimental results of references [24, 26], the AOCC calculation of Tseng and Lin [45] and the recommended data of Suno and Kato [1].

than the experimental ones for this particular system, in contrast with the recommended values of reference [1] that follow the experimental data at $E < 100$ eV/u. One should also note the excellent agreement between different calculations (see reference [52]) for the partial cross sections for populating $C^{3+}(3l)$ states.

In this work we have recalculated the total EC cross section at very low energies using the molecular basis set of Barragán *et al* [9] to study the isotope effect. Our results are displayed in figure 6. In contrast with the dependence illustrated in figure 2, characteristic of reactions that take place at internuclear distances where the interaction potential is repulsive, the isotopic dependence ($\sigma_T > \sigma_D > \sigma_H$) shown in figure 6 is similar to that found for C^{3+} + H and comes from trajectory effects for the relative motion in the attractive ion-induced dipole interaction potential [36]. Our CTMC results are compared to the experimental results in figure 7, where one can note the excellent agreement between experiments and calculations.

7. C^{5+} + H collisions

C^{5+} + H collisions have been considered in MFCC calculations within both quantal [55, 56] and semiclassical [57, 56] formalisms. CTMC calculations have been reported in reference [57]. Total cross sections have been measured in references [38, 58, 26]. Recently, Draganić *et al* [59] have performed merged-beams experiments. The MFCC calculations lead to a Langevin-type cross section in satisfactory agreement with the experimental data, although the energy grid of the calculation does not allow to observe the spikes due to shape resonances.

We have applied the CTMC method with the corresponding model potential to evaluate the EC total cross section (figure 8), which shows a general good agreement with experiments [26] and the calculation of reference [57], although our calculation extends over a larger energy

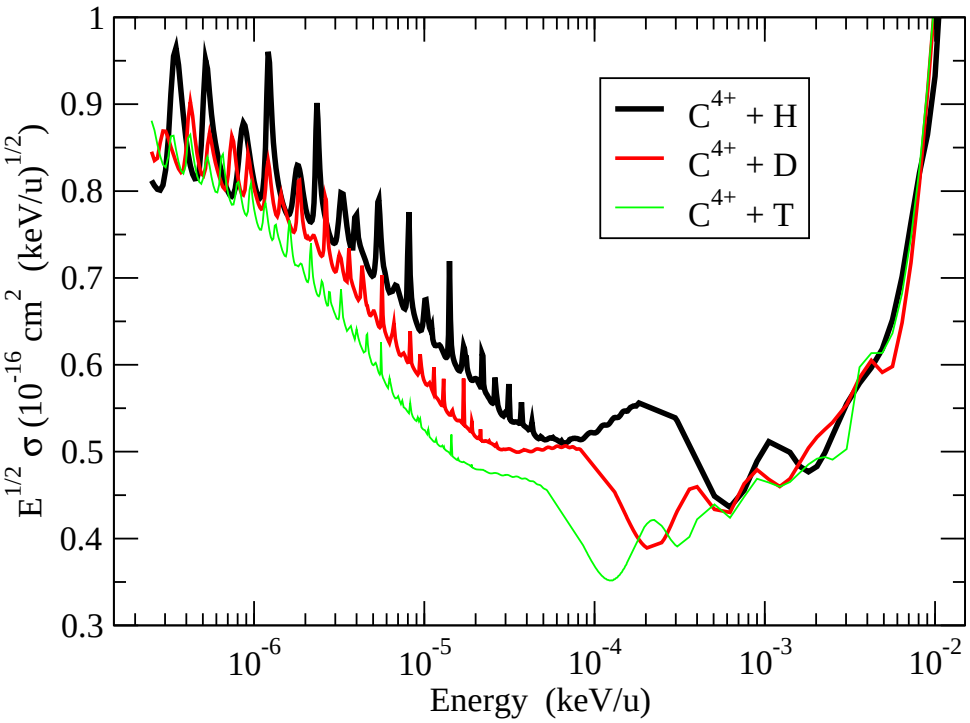


Figure 6. Total cross section for electron capture in C^{4+} + H(D,T)(1s) collisions, multiplied by $E^{1/2}$, as function of E.

range than the previous one, It can be noted that the energy dependence of our cross section is identical to that of the recommended data of Suno and Kato.

8. C^{6+}+ H collisions

As already mentioned, EC in C^{6+} + H(1s) collisions has been studied in several publications. Experimental data have been reported in references [26], [58] and [60]. High-energy calculations include the first Born approximation [61] and the eikonal impulse approximation [62]. The AOCC method has been employed in references [63, 64, 65, 66] and [67]. CTMC calculations have been carried out in references [22, 67, 68] and [69]. MFCC calculations were performed in references [70, 71] and [72]. The hyperspherical-close-coupling method was applied in the reference [73]. The mentioned calculations provide accurate values of the EC total cross section for energies above 10 eV/u together with state-selective cross sections. At E <10 eV/u, the work of Liu *et al* [73] has pointed out the relevance of the EC into $C^{5+}(n = 5)$ and the Langevin-type behavior of the total cross section, but values of this cross section have not been reported. The EC reaction at low energies takes place via transitions between the molecular orbitals 650 and 450 (in the united atom notation), at the avoided crossing at large internuclear distances ($R \approx 21.3$ bohr). In the present work, we have calculated the EC total cross section by using a molecular basis set that includes the entrance channel and the exit channels dissociating into $C^{5+}(n = 5)$ + H^+; the cross section is shown in figure 9. We have also checked that EC into $C^{5+}(n = 4)$ + H^+ is negligible for the collision energies of figure 9. We have also plotted in figure 9 the total cross section for collisions with H, D and T to show that the isotope effect is almost unnoticeable for this collision system, in accordance with the fact that, at the large internuclear distances where the transitions take place, the trajectory effects that give rise to the isotopic dependence are very small.

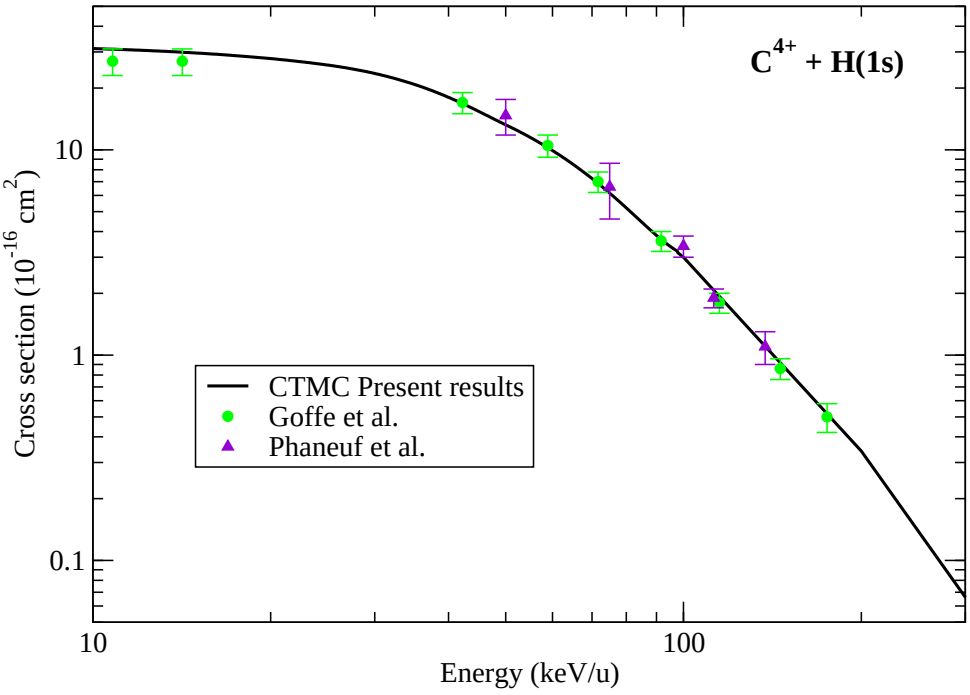


Figure 7. Total cross section for electron capture in C^{4+} + H(1s) collisions as function of the collision energy. Our CTMC results are compared to the experimental results of Goffe *et al* [26] and Phaneuf *et al* [24].

Recently, we have carried out CTMC calculations for this collision [68], and the results are displayed in figure 10, which also contains previous calculations and experimental data. Our results agree satisfactorily with the available experimental data. We also find a good agreement with the AOCC calculation of Igenbergs *et al* [67] for $E < 100$ keV/u. At higher energies, the CTMC calculation agrees with the first Born approximation [61], but it overestimates the results of the reference [62] (eikonal impulse approximation), which may be due to a limitation of the CTMC method to describe the EC into low n shells in the high-velocity limit.

9. Concluding remarks

In this work we have reviewed the calculations of electron capture total cross sections in collisions of Carbon ions with H(D,T)(1s). Although there exist several calculations for C^{6+} + H(1s) with different methods, few calculations have considered collisions of partially stripped ions, and the recommended data are based on experimental data, with the exception of C^{4+}+ H(1s); this system can be accurately described by employing a one-active electron treatment, and the agreement between different calculations is conspicuous. For the other collision systems, molecular calculations have been carried out systematically, employing multireference-configuration-interaction wave functions. The atomic expansion is difficult to apply to many-electron systems and the CTMC method has not been employed routinely until now to evaluate the EC total cross sections.

The new calculations presented in this work are focused on two points. First, the low-energy behavior of the EC cross section. It has been shown that the cross sections for Hydrogen collisions with the ions with $q \geq 3$ show the Langevin-type energy dependence, and the isotopic effect can be explained as due to trajectory effects. In the particular case of C^{6+}+ H(1s), the isotopic effect is negligible. Although the EC cross section at $E < 20$ eV/u for the collision

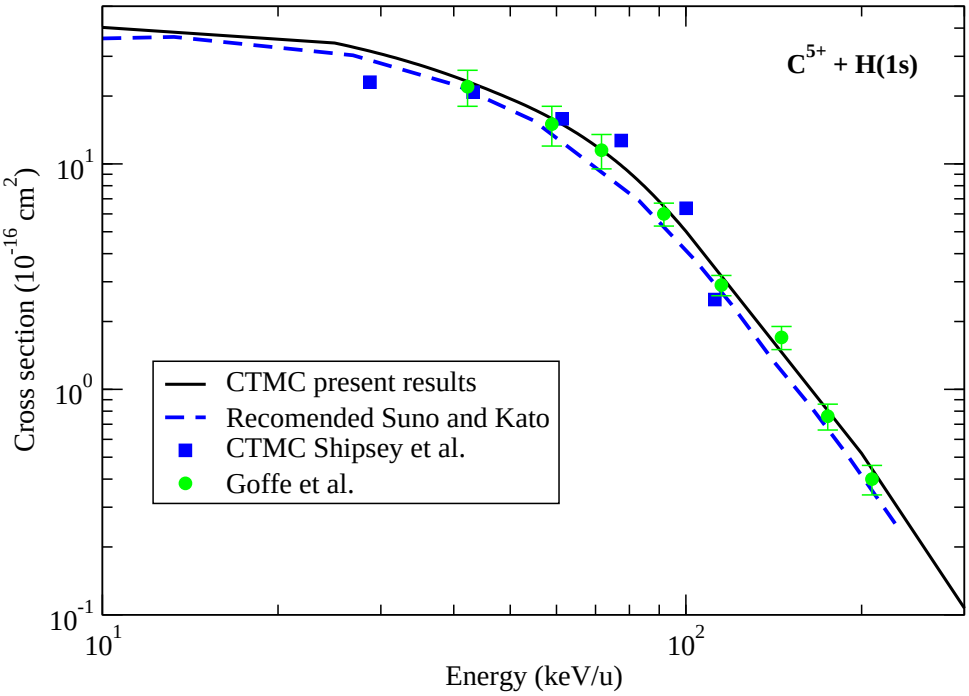


Figure 8. Total cross section for electron capture in C^{5+} + H(1s) collisions as function of the collision energy. Our CTMC results are compared to the experimental results [26], the CTMC calculation of Shipsey *et al* [57] and the recommended data of Suno and Kato [1].

C^{2+}+ H(1s) is small, its isotopic dependence is noticeable.

The second aspect covered by our work is the calculation of EC cross sections at energies $E \gtrsim 25$ keV/u. We present CTMC calculations for $q = 1$, 3, 4, 5 and 6, with an excellent agreement with experiments. Our results support the usefulness of CTMC method and show that the one-electron approximation, with the model potential of equation (8), provides a remarkably good representation of EC in these collisions at high energies. In particular, the comparison with the experimental data indicates that capture into occupied shells is not significant. The method is not applicable to treat C^{2+}+ H(1s) collisions, and new calculations are required for this system, for instance using a many-electron AOCC expansion, to compute the EC cross section for energies above 1 keV/u.

Acknowledgments

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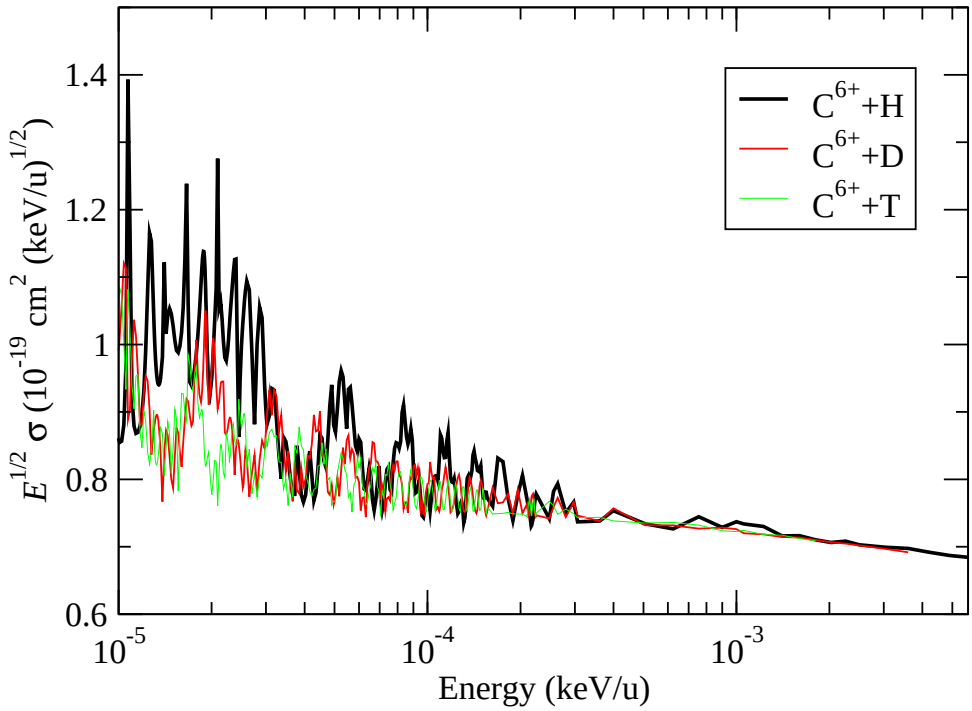


Figure 9. Total cross section for electron capture in C^{6+} + H(D,T)(1s) collisions multiplied by $E^{1/2}$, as function of E.

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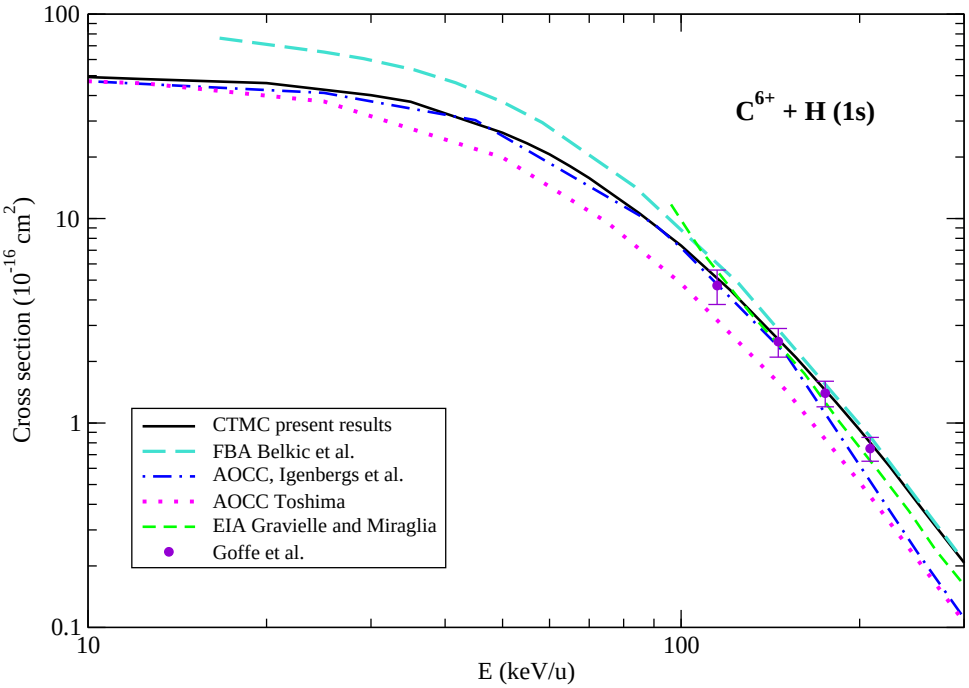


Figure 10. Total cross section for electron capture in C^{6+} + H(1s) collisions as function of the collision energy. Our CTMC results are compared to the experimental results [26], the AOCC calculations of Toshima [65] and Igenbergs *et al* [67], the eikonal impulse approximation (EIA) [62] and first Born approximation (FBA) [61].

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