Recommended partial cross sections for electron capture in $C^{6+} + H(1s)$ collisions

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Abstract. We report $n\ell$-selective capture cross sections for the C^{6+}– $H(1s)$ collision system at low and intermediate impact energies. The present converged results take into account important trajectory effects for $C^{5+}(n=5)$ capture channels and allow for the extension of the analytical fits proposed by Janev *et al.* in *At. Data Nucl. Data Tables* **55** 201 in the 0.1 – 60 keV amu^{-1}energy range.

An important limitation to the heating of fusion plasmas arises from the presence of non-negligible impurity ions in the medium [1, 2]. Among others, plasma modeling and diagnostics require the knowledge of accurate cross sections of electron transfer from atomic hydrogen to fully stripped carbon and oxygen ions. For both systems Janev *et al.* [2] proposed analytical fits of capture cross sections based on reliable theoretical and experimental data, when available in the 0.1 – 1000 keV amu^{-1} impact energy range.

Since the seventies, the C^{6+}– $H(1s)$ collision system has been widely studied which makes it a benchmark system for atomic collisions involving highly charged ions [3]. The two main capture channels are the C^{5+} $(n=4)$ and C^{5+} $(n=5)$ manifolds,

$$C^{6+} \ + \ H(1s) \ \rightarrow \ C^{5+}(4\ell) \ + \ H^{+}$$

$$C^{6+} \ + \ H(1s) \ \rightarrow \ C^{5+}(5\ell) \ + \ H^{+}$$

For the dominant C^{5+} $(n=4)$ capture cross sections, experimental data and theoretical predictions were found to be in good agreement and the fits covered the entire energy domain of interest, cf. figure 1. However, severe discrepancies were reported for electron capture to the $C^{5+}(n=5)$ shell at low impact energies (0.1 – 10 keV amu^{-1}). These disagreements, as well as the lack of data for minor channels, prevented Janev *et al.* to extend their fits to the low energy range [2].

We have recently reported new results for that system [4, 5] with special emphasize in the low energy range where the above mentioned discrepancies were observed. By a detailed analysis of the mechanisms responsible for the capture processes and of the inter nuclear trajectory effects [4], we have proposed a set of cross sections reliable in this range. These data are reported in the present paper.

We use a non-perturbative semi-classical approach, within the straight-line inter nuclear trajectory approximation. The electron wave function is expanded on a set of target- and projectile-centered atomic orbitals. The projectile orbitals are furthermore

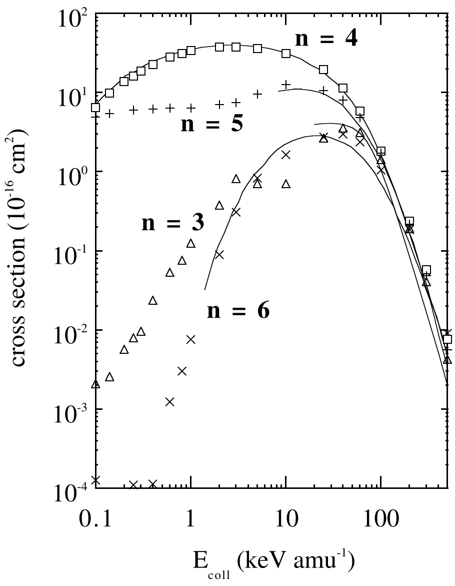

FIG. 1. Electron capture cross sections from H(1s) to C^{5+}(n=3–6). Our results: △, n=3; □, n=4; +, n=5; ×, n=6. Recommended data [2]: ___, n=3–6.

modified with Electron Translational Factors in order to take into account the relative motion of the two atomic centers. Inserting this expansion in the time-dependent Schrödinger equation leads to a set of coupled differential equations for the coefficients c. These coupled equations are solved numerically for given impact energies E_{coll} and a well chosen set of trajectories, characterized by the impact parameter b. From the expansion coefficients after collision the probabilities and cross sections for transition from initial atomic state i to final atomic states f can be evaluated, respectively

$$P_{i \to f}\left(E_{coll}, b\right) = \left|c_f\left(t \to \infty, E_{coll}, b\right)\right|^2 \tag{1}$$

$$\sigma_{i \to f}\left(E_{coll}\right) = 2\pi \int_0^\infty b\, db\, P_{i \to f}\left(E_{coll}, b\right) \tag{2}$$

However, for $C^{5+}(n = 5)$ capture, the small impact parameter range (b $\leq$ 4 a.u.) is very dominant in the integration of eq. 2, and trajectory effects due to the strong repulsive interaction between the collision partners in the final channel were found very important [4]. To take into account the departure from straight-line trajectory, we have performed Classical Trajectory Monte Carlo (CTMC) [9] calculations to obtain realistic deflection functions. The trajectory effects were then introduced in the semi-classical results by replacing the impact parameter b in $P_{i \to f}\left(E_{coll}, b\right)$ (eq. 2) by an averaged closest approach distance evaluated from the CTMC results [4].

Table 1. Electron transfer cross sections (in 10^{-16} cm^2) from H(1s) to C^{5+}($n\ell$), n = 3–6 at low collision energies E_{coll} (in keV amu^{-1}). For transfer to C^{5+}(5ℓ) the trajectory modified cross sections are shown by "→" and pure straight-line results are reported underneath in smaller font

E_{coll}	0.05	0.0625	0.1	0.14	0.2*	0.25	0.3*	0.4	0.6	0.81*
3s	1.88^{-6}	2.32^{-6}	1.46^{-5}	5.06^{-5}	2.30^{-5}	2.13^{-5}	1.85^{-5}	1.37^{-5}	4.12^{-4}	7.28^{-4}
3p	3.00^{-6}	7.83^{-6}	2.91^{-5}	2.13^{-5}	2.99^{-5}	4.49^{-5}	4.74^{-5}	3.92^{-5}	2.67^{-4}	1.21^{-3}
3d	5.93^{-6}	5.08^{-6}	8.23^{-5}	1.24^{-5}	3.58^{-5}	4.41^{-5}	6.30^{-6}	6.00^{-5}	5.61^{-4}	1.09^{-3}
n=3	1.08^{-5}	1.52^{-5}	1.26^{-4}	8.42^{-5}	8.88^{-5}	1.10^{-4}	7.22^{-5}	1.13^{-4}	1.24^{-3}	3.02^{-3}
4s	3.70^{-1}	3.72^{-1}	4.90^{-1}	6.48^{-1}	8.94^{-1}	1.05^{+0}	1.34^{+0}	1.61^{+0}	2.12^{+0}	2.07^{+0}
4p	8.38^{-1}	9.51^{-1}	1.46^{+0}	1.97^{+0}	2.79^{+0}	3.30^{+0}	4.01^{+0}	4.69^{+0}	6.42^{+0}	7.23^{+0}
4d	9.95^{-1}	1.15^{+0}	1.87^{+0}	2.22^{+0}	3.01^{+0}	3.93^{+0}	4.91^{+0}	7.06^{+0}	9.49^{+0}	1.12^{+1}
4f	1.13^{+0}	1.43^{+0}	2.67^{+0}	5.06^{+0}	7.07^{+0}	7.93^{+0}	8.42^{+0}	9.29^{+0}	1.00^{+1}	1.07^{+1}
n=4	3.34^{+0}	3.90^{+0}	6.49^{+0}	9.90^{+0}	1.38^{+1}	1.62^{+1}	1.87^{+1}	2.26^{+1}	2.80^{+1}	3.13^{+1}
5s →	1.83^{-1}	1.87^{-1}	5.46^{-1}	5.79^{-1}	5.59^{-1}	3.15^{-1}	2.55^{-1}	3.34^{-1}	6.58^{-1}	7.51^{-1}
	5.44^{-1}	4.39^{-1}	8.53^{-1}	7.83^{-1}	6.81^{-1}	3.66^{-1}	2.88^{-1}	3.64^{-1}	6.89^{-1}	7.71^{-1}
5p →	1.98^{-1}	3.75^{-1}	5.16^{-1}	8.76^{-1}	1.12^{+0}	1.09^{+0}	8.36^{-1}	6.78^{-1}	1.29^{+0}	1.59^{+0}
	5.89^{-1}	8.78^{-1}	8.06^{-1}	1.19^{+0}	1.37^{+0}	1.26^{+0}	9.45^{-1}	7.39^{-1}	1.35^{+0}	1.63^{+0}
5d →	3.26^{-1}	5.68^{-1}	5.05^{-1}	6.72^{-1}	1.17^{+0}	1.12^{+0}	1.12^{+0}	1.45^{+0}	1.77^{+0}	1.83^{+0}
	9.71^{-1}	1.33^{+0}	7.89^{-1}	9.10^{-1}	1.43^{+0}	1.30^{+0}	1.27^{+0}	1.59^{+0}	1.85^{+0}	1.88^{+0}
5f →	8.67^{-1}	1.12^{+0}	1.68^{+0}	1.26^{+0}	1.32^{+0}	1.69^{+0}	2.09^{+0}	2.28^{+0}	1.74^{+0}	1.51^{+0}
	2.58^{+0}	2.62^{+0}	2.63^{+0}	1.70^{+0}	1.61^{+0}	1.97^{+0}	2.36^{+0}	2.49^{+0}	1.82^{+0}	1.55^{+0}
5g →	9.65^{-1}	1.10^{+0}	1.69^{+0}	2.08^{+0}	1.64^{+0}	1.78^{+0}	1.79^{+0}	1.45^{+0}	8.77^{-1}	6.96^{-1}
	2.87^{+0}	2.57^{+0}	2.64^{+0}	2.81^{+0}	2.00^{+0}	2.07^{+0}	2.02^{+0}	1.59^{+0}	9.17^{-1}	7.15^{-1}
n=5 →	2.54^{+0}	3.35^{+0}	4.94^{+0}	5.46^{+0}	5.82^{+0}	6.00^{+0}	6.09^{+0}	6.21^{+0}	6.34^{+0}	6.37^{+0}
	7.55^{+0}	7.84^{+0}	7.72^{+0}	7.39^{+0}	7.10^{+0}	6.97^{+0}	6.89^{+0}	6.77^{+0}	6.64^{+0}	6.54^{+0}
6s	6.03^{-5}	1.13^{-5}	4.91^{-5}	1.22^{-4}	5.71^{-4}	1.04^{-3}	8.54^{-4}	1.32^{-3}	3.14^{-3}	4.74^{-3}
6p	7.77^{-5}	1.71^{-5}	9.23^{-5}	3.51^{-4}	1.07^{-3}	1.03^{-3}	2.65^{-3}	3.06^{-3}	8.01^{-3}	1.21^{-2}
6d	2.03^{-4}	3.81^{-5}	1.79^{-4}	2.77^{-4}	6.03^{-4}	2.16^{-3}	2.01^{-3}	4.32^{-3}	1.31^{-2}	1.20^{-2}
6f	2.33^{-4}	1.13^{-4}	3.50^{-4}	3.99^{-4}	8.52^{-4}	1.31^{-3}	1.43^{-3}	5.91^{-3}	1.48^{-2}	2.16^{-2}
6g	4.26^{-4}	1.93^{-4}	5.41^{-4}	5.08^{-4}	1.01^{-3}	1.23^{-3}	1.58^{-3}	5.56^{-3}	9.62^{-3}	1.65^{-2}
6h	6.58^{-4}	2.52^{-4}	8.93^{-4}	9.33^{-4}	1.60^{-3}	1.22^{-3}	1.18^{-3}	3.61^{-3}	4.73^{-3}	9.19^{-3}
n=6	1.66^{-3}	6.24^{-4}	2.10^{-3}	2.59^{-3}	5.70^{-3}	8.00^{-3}	9.70^{-3}	2.38^{-2}	5.34^{-2}	7.62^{-2}

The basis set used in the calculations consists of the H(1s) initial state and of all the states spanning the C^{5+}($n = 1-6$) shells. This basis set does not include hydrogen excitation and ionisation channels so that it is not expected to give very accurate cross sections above 60 keV amu^{-1}[7]. Indeed Figure 1 shows that the capture cross sections are slightly overestimated (typically 50% at 200 keV amu^{-1}) in our model compared to the recommended data [2]. However in the low energy range the basis set is adequate and describes correctly the (CH)$^{6+}$ molecular curves and the important avoided crossings [4]. Our results are in excellent agreement with recent molecular-orbital calculations of Harel *et al.* [6]: for example at 0.3 keV amu^{-1}, differences between the two data sets are less than 5% for the important channels and below 50% for the minor C^{5+}($n = 3$) and C^{5+}($n = 6$) channels.

The $n\ell$-partial and n-partial ($n = 1-6$) capture cross sections are reported in table for 10 impact energies from .05 keV amu^{-1} to .81 keV amu^{-1} and in table for 10 impact energies from 1 keV amu^{-1} to 200 keV amu^{-1}. As concluded in [4] for electron

Table 2. Electron transfer cross sections (in 10^{-16} cm^2) from H($1s$) to $C^{5+}(n\ell)$, n = 3–6 at medium collision energies E_{coll} (in keV amu^{-1})

E_{coll}	1.0	2.0	3.0	5.0	10.0	25.0	40.0	60.0	100.	200.
$3s$	1.07^{-3}	1.40^{-2}	7.23^{-2}	2.34^{-1}	3.32^{-1}	3.58^{-1}	3.52^{-1}	1.06^{-1}	5.09^{-2}	1.29^{-2}
$3p$	4.05^{-3}	4.66^{-2}	1.45^{-1}	3.94^{-1}	7.54^{-1}	1.07^{+0}	1.16^{+0}	8.98^{-1}	1.99^{-1}	1.82^{-2}
$3d$	2.47^{-3}	2.88^{-2}	9.07^{-2}	2.03^{-1}	5.56^{-1}	1.31^{+0}	1.48^{+0}	1.37^{+0}	7.97^{-1}	1.56^{-1}
n=3	7.60^{-3}	8.94^{-2}	3.08^{-1}	8.31^{-1}	1.64^{+0}	2.74^{+0}	2.99^{+0}	2.38^{+0}	1.05^{+0}	1.87^{-1}
$4s$	3.13^{+0}	2.40^{+0}	2.52^{+0}	1.80^{+0}	1.04^{+0}	3.99^{-1}	1.56^{-1}	9.54^{-2}	6.88^{-2}	1.15^{-2}
$4p$	8.21^{+0}	9.03^{+0}	8.54^{+0}	7.31^{+0}	4.22^{+0}	1.66^{+0}	1.04^{+0}	5.96^{-1}	1.27^{-1}	1.69^{-2}
$4d$	1.15^{+1}	1.37^{+1}	1.36^{+1}	1.39^{+1}	1.06^{+1}	5.44^{+0}	2.16^{+0}	8.62^{-1}	4.43^{-1}	1.10^{-1}
$4f$	1.11^{+1}	1.29^{+1}	1.28^{+1}	1.31^{+1}	1.55^{+1}	1.20^{+1}	8.15^{+0}	4.26^{+0}	1.18^{+0}	9.91^{-2}
n=4	3.40^{+1}	3.80^{+1}	3.74^{+1}	3.61^{+1}	3.13^{+1}	1.95^{+1}	1.15^{+1}	5.82^{+0}	1.81^{+0}	2.37^{-1}
$5s$	6.98^{-1}	2.60^{-1}	2.26^{-1}	1.81^{-1}	1.54^{-1}	1.30^{-1}	8.05^{-2}	1.02^{-1}	6.51^{-2}	9.80^{-3}
$5p$	1.55^{+0}	7.21^{-1}	6.26^{-1}	6.16^{-1}	6.58^{-1}	5.51^{-1}	5.53^{-1}	3.31^{-1}	9.17^{-2}	1.42^{-2}
$5d$	1.79^{+0}	1.20^{+0}	1.04^{+0}	1.29^{+0}	1.53^{+0}	1.36^{+0}	7.75^{-1}	5.64^{-1}	3.36^{-1}	8.08^{-2}
$5f$	1.60^{+0}	2.46^{+0}	2.17^{+0}	2.72^{+0}	3.17^{+0}	2.61^{+0}	2.36^{+0}	1.76^{+0}	7.26^{-1}	8.50^{-2}
$5g$	7.89^{-1}	2.39^{+0}	3.41^{+0}	4.79^{+0}	7.27^{+0}	5.98^{+0}	4.26^{+0}	2.10^{+0}	4.93^{-1}	2.69^{-2}
n=5	6.42^{+0}	7.03^{+0}	7.47^{+0}	9.61^{+0}	1.28^{+1}	1.06^{+1}	8.04^{+0}	4.86^{+0}	1.71^{+0}	2.17^{-1}
$6s$	4.46^{-3}	1.60^{-2}	3.20^{-2}	1.65^{-2}	2.21^{-2}	4.22^{-2}	5.64^{-2}	8.76^{-2}	6.09^{-2}	9.19^{-3}
$6p$	2.16^{-2}	4.60^{-2}	9.25^{-2}	5.30^{-2}	5.15^{-2}	1.88^{-1}	2.51^{-1}	2.16^{-1}	8.89^{-2}	1.25^{-2}
$6d$	3.41^{-2}	9.44^{-2}	1.28^{-1}	8.64^{-2}	1.11^{-1}	3.33^{-1}	3.40^{-1}	3.81^{-1}	2.65^{-1}	6.34^{-2}
$6f$	2.66^{-2}	4.72^{-2}	2.19^{-1}	8.65^{-2}	1.42^{-1}	5.52^{-1}	8.67^{-1}	9.16^{-1}	5.04^{-1}	7.15^{-2}
$6g$	2.31^{-2}	5.29^{-2}	2.24^{-1}	2.67^{-1}	1.44^{-1}	7.46^{-1}	1.18^{+0}	1.01^{+0}	3.89^{-1}	3.10^{-2}
$6h$	1.56^{-2}	1.23^{-1}	1.23^{-1}	2.00^{-1}	2.35^{-1}	7.94^{-1}	8.84^{-1}	5.20^{-1}	1.24^{-1}	5.15^{-3}
n=6	1.25^{-1}	3.80^{-1}	8.19^{-1}	7.09^{-1}	7.06^{-1}	2.66^{+0}	3.58^{+0}	3.13^{+0}	1.43^{+0}	1.93^{-1}

capture to $C^{5+}(n\ell)$ we recommend the use of the trajectory modified cross sections, in good agreement with the data of Green *et al.* [8] (for information pure impact-parameter results are also reported in smaller font).

Trajectory effects were interpolated from figure 4 in [4] for 3 impact energies (.2, .3 and .81 keV amu^{-1}) marked by "*" in table (CTMC predictions not available). These effects were considered identical for the different ℓ states in the $C^{5+}(n=5)$ shell. Note finally that trajectory effects are not significant for all other channels ($C^{5+}(n=3,4,6)$) compared to the uncertainty of the data. Thus trajectory-modified cross sections are not reported in these cases.

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