Electron capture from excited hydrogen atoms by highly charged beryllium and carbon ions

N Shimakura¹, N Kobayashi¹, M Honma¹, T Nakano² and H Kubo³

¹ Faculty of Science, Niigata University, Niigata 950-2181, Japan
² Naka Fusion Institute, Japan Atomic Energy Agency, 801-1 Mukoyama, Naka, Ibaraki, Japan
³ E-mail: shima@shimakura.gs.niigata-u.ac.jp

Abstract. The cross sections for electron capture in collisions of bare and helium-like ions of Be and C with excited H atoms \( (n = 2) \) have been calculated by a molecular-state close-coupling method in a collision energy range of 60 eV/amu–6 keV/amu. Calculated results show that these cross sections are remarkably larger than those for collisions with ground-state H atoms. For example, for collisions of Be \(^2\)+, Be \(^4\)+, C \(^4\)+, and C \(^6\)+ ions with H(2s) atoms at ~1 keV/amu, the cross sections are 190 \( \times 10^{-16} \) cm\(^2\), 610 \( \times 10^{-16} \) cm\(^2\), 920 \( \times 10^{-16} \) cm\(^2\), and 720 \( \times 10^{-16} \) cm\(^2\), respectively. In contrast, the cross sections for collisions with ground-state H atoms are 25 \( \times 10^{-16} \) cm\(^2\), 35 \( \times 10^{-16} \) cm\(^2\), 30 \( \times 10^{-16} \) cm\(^2\), and 40 \( \times 10^{-16} \) cm\(^2\), respectively.

1. Introduction
Thus far, a number of experimental and theoretical studies have been conducted on electron capture in collisions of highly charged ions with ground-state hydrogen atoms. However, despite the known importance of such processes in understanding the impurity behaviour in tokamak divertors, very few studies have been conducted on electron capture cross sections of electronically excited hydrogen atoms. To our knowledge, only two theoretical estimations of such processes have been carried out in the case of C \(^4\)+ + H(\(n = 2\)) collisions. One is the classical trajectory Monte Carlo calculation carried out by Zaniol et al. [1] at a collision energy of 1 eV/amu; the other is the molecular-state close-coupling (MSCC) calculation carried out by Shimakura et al. [2].

Macek and Ovchinnikov [3] have developed a simple model for electron capture from high-\(n\) states of H atoms by multiply charged ions and have predicted that the cross sections depend on \(n\) as \(n^5\). They have concluded that this high-\(n\) dependence explains why a small fraction (less than 0.1\%) of H atoms in high-\(n\) states contribute 30\% of the capture yield at 50 eV/amu during the O\(^5\)+ + H collisions. Combining this model with the cross sections for ground-state H atoms, we can estimate the cross sections for excited H atoms.

In this study, the cross sections for electron capture in collisions of Be \(^2\)+, Be \(^4\)+, C \(^4\)+, and C \(^6\)+ ions with electronically excited H(\(n = 2\)) atoms are calculated in the range of 60 eV/amu–6 keV/amu using an MSCC method [4].

2. Calculation method
Since details of the theoretical treatment in this paper have already been described elsewhere [4], only specific information used for the present calculation is given below.

2.1. Electronic states and couplings
The electronic structures were calculated by a modified valence-bond configuration-interaction methods. In order to represent the Be\(^{2+}\)(1s\(^2\)) and C\(^{4+}\)(1s\(^2\)) cores, an \(l\)-dependent Gaussian-type pseudopotential was employed; hence, only one active electron was treated explicitly in all collision systems considered in this paper. The pseudopotential parameters for Be\(^{2+}\)(1s\(^2\)) and C\(^{4+}\)(1s\(^2\)) ions were taken from papers by Wetmore et al. [5] and Kimura and Olson [6]. The orbital exponents of the Slater-type orbitals were obtained by optimizing the energies of the respective electronic states. The accuracy of the electronic state calculations performed in this study with respect to spectroscopic values [7] is better than 0.05 eV, except for the states whose contribution to the electron capture processes was insignificant.

We calculated radial and rotational couplings with atomic-type electron translation factors (ETFs) to solve the MSCC equations. The ETFs were included to the first order in velocity.

2.2. Collision dynamics
A semi-classical MSCC method was employed. The coupled equations were solved numerically under the assumption of straight-line trajectories of the heavy particles. By squaring the resulting amplitude, the transition probability was obtained as a function of collision energy and impact parameter. The cross sections were obtained by integrating the impact-parameter-weighted transition probability over the impact parameter.

3. Results and discussion

3.1. Be\(^{2+}\) + H collision system
The total cross sections for the Be\(^{2+}\) + H(1s) collisions depend weakly on the collision energy; their maximum value is \(\sim 20 \times 10^{-16}\) cm\(^2\) at 1.68 keV/amu. The electron in H(1s) is dominantly captured into the Be\(^{+}\)(2s) state.

The calculated cross sections for electron capture in the Be\(^{2+}\) + H(2s) collisions are shown in figure 1. The total cross sections are ten times larger than those for collisions with H(1s) at \(\sim 1\) keV/amu. At the lowest and the highest ends of the collision energy region covered in this work, the electron is mainly captured into the Be\(^{+}\)(4\(l\)) states (\(\sim 90\%\)). At intermediate energies, the contribution of the Be\(^{+}\)(3\(l\)) states increases.

The total cross sections for the Be\(^{2+}\) + H(2p) collisions are approximately five times larger than those for collisions with H(1s) targets at \(\sim 1\) keV/amu. At the lowest and the highest collision energies, the electron is mainly captured into the Be\(^{+}\)(3\(l\)) (\(\sim 80\%\)) and Be\(^{+}\)(4\(l\)) states (\(\sim 70\%\)), respectively.

3.2. Be\(^{4+}\) + H collision system
The cross sections for the Be\(^{4+}\) + H(2s) collisions are shown in figure 2. The calculations were carried out for values of \(\Lambda\) from 0 to 3, namely, for \(\Sigma\), \(\Pi\), \(\Delta\), and \(\Phi\) symmetries, where \(\Lambda\) is the electronic angular momentum of the total system projected onto the internuclear axis. The solid curves in figure 2 represent the cross sections including all the symmetries up to \(\Lambda = 3\), whereas the broken curves
include only up to $\Lambda = 2$. This figure proves that the contributions from $\Lambda = 3$ and above too, perhaps, are negligibly small. The total cross sections are $500 \times 10^{-16} \text{cm}^2 \sim 700 \times 10^{-16} \text{cm}^2$. The $n = 6$ states are the most dominant over the collision energy range covered in this study; at the lowest and highest collision energies, the contributions of the $n = 6$ states are ~85% and ~65%, respectively. The second dominant are the $n = 7$ states. The cross sections for electron capture into these states increase with the collision energy.

The total cross sections for the $\text{Be}^{4+} + \text{H}(2p)$ collisions are smaller than those for the $\text{Be}^{4+} + \text{H}(2s)$ collisions. At the lowest and the highest collision energies, the cross sections are $200 \times 10^{-16} \text{cm}^2$ and $500 \times 10^{-16} \text{cm}^2$, respectively. The electron is mainly captured into the $\text{Be}^{3+}(6l)$ states ($200 \times 10^{-16} \text{cm}^2 \sim 330 \times 10^{-16} \text{cm}^2$). The second dominant at the lowest and the highest collision energies are the $\text{Be}^{3+}(5l)$ and $\text{Be}^{3+}(7l)$ states, respectively. The cross section for capture into $\text{Be}^{3+}(7l)$ takes the largest value of $100 \times 10^{-16} \text{cm}^2$ at the highest energy.

### 3.3. $C^{4+} + H$ collision system

Experimental and theoretical cross sections for the $C^{4+} + \text{H}(1s)$ collisions are found in the literature. All have a maximum value of $\sim 30 \times 10^{-16} \text{cm}^2$ at $\sim 250 \text{eV/amu}$. The total cross section for the $C^{4+} + \text{H}(2s)$ collisions obtained by the CTMC method [1] is $\sim 380 \times 10^{-16} \text{cm}^2$ at 1 eV/amu. Our calculated cross sections for the latter collisions are shown in figure 3. The solid curves are for the calculations including the $\Lambda = 0 \sim 3$ symmetries and the broken curves only up to $\Lambda = 2$. The total cross sections are $800 \times 10^{-16} \text{cm}^2 \sim 930 \times 10^{-16} \text{cm}^2$. The electron is mainly captured into the $C^{3+}(6l)$ states.

The total cross sections for the $C^{4+} + \text{H}(2p)$ collisions ($580 \times 10^{-16} \text{cm}^2 \sim 650 \times 10^{-16} \text{cm}^2$) are smaller than those for the $C^{4+} + \text{H}(2s)$ collisions. Capture into the $n = 6$ states ($550 \times 10^{-16} \text{cm}^2 \sim 600 \times 10^{-16} \text{cm}^2$) is the most dominant over the collision energy range covered in this study; its contribution is ~80%. The second dominant are the $n = 7$ states, except at low collision energies; their maximum contribution is ~10%.

### 3.4. $C^{6+} + H$ collision system

Thus far, two theoretical and one experimental reports are found in the literature for the $C^{6+} + \text{H}(1s)$ collisions. We have also calculated the electron capture cross sections using the MSCC method. Our results are similar to the previously reported ones; the cross sections increase with the collision energy.
Our calculated cross sections for the C$_{6}^{+}$ + H(2s) collisions are shown in figure 4. The total cross sections are $550 \times 10^{-16}$ cm$^2$ $\sim 750 \times 10^{-16}$ cm$^2$. The electron is mainly captured into the C$_{5}^{+}(8l)$ states; the cross sections are in a range of $450 \times 10^{-16}$ cm$^2$ $\sim 490 \times 10^{-16}$ cm$^2$. The contribution is 82% at the lowest collision energies. The C$^{5+}(9l)$ and C$^{5+}(7l)$ states are the second dominant states at the lowest and highest energies, respectively; the cross sections for capture into the C$^{5+}(9l)$ states are $77 \times 10^{-16}$ cm$^2$ $\sim 107 \times 10^{-16}$ cm$^2$.

The total cross sections for the C$_{6}^{+}$ + H(2p) collisions are $430 \times 10^{-16}$ cm$^2$ $\sim 560 \times 10^{-16}$ cm$^2$. The $n = 8$ states are the most dominant, the cross section being $310 \times 10^{-16}$ cm$^2$ $\sim 360 \times 10^{-16}$ cm$^2$; their contribution is $\sim 80\%$ at the lowest collision energies. The second dominant are the $n = 7$ states; their contribution is $10\%$ $\sim 18\%$.

3.5. Test of the $n^5$ rule on the MSCC cross sections

Table 1 shows the calculated cross sections for the Be$^{2+}$, Be$^{4+}$, C$^{4+}$, and C$^{6+}$ + H(1s, 2s) collisions at $\sim$1keV/amu along with the H(2s) cross sections estimated from the $n^5$ rule as $2^5$ times the H(1s) cross sections. A good agreement is found for the C$^{6+}$ + H system, but a large discrepancy is seen for the Be$^{2+}$ + H collisions.

|       | Be$^{2+}$ | Be$^{4+}$ | C$^{4+}$ | C$^{6+}$ |
|-------|-----------|-----------|----------|----------|
| H(1s) | 25        | 35        | 30       | 40       |
| H(2s) | 190       | 610       | 920      | 720      |
| $2^5$$\times$H(1s) | 800       | 1100      | 960      | 1300     |

4. Summary and conclusion

Our calculations show that the electron capture cross sections for collisions with electronically excited hydrogen atoms are remarkably larger than those for collisions with ground-state hydrogen atoms. This can be explained in terms of the effective distances at which electron capture occurs. The H(2l) states are more diffusely distributed than the H(1s) state, and hence, the Be$^{2+}$, Be$^{4+}$, C$^{4+}$, and C$^{6+}$ ions can capture the electron in H(2l) at longer distances than that in H(1s).

Acknowledgment

This study was supported in part by the Japan Atomic Energy Agency.

References

[1] Zaniol B, Isler R C, Brooks N H, West W P and Olson R E 2001 Phys. Plasmas 8 4386
[2] Shimakura N, Honma M and Kubo H 2006 J. Plasma Fusion Res. Ser. 7 199
[3] Macek J and Ovchinnikov S Y 1992 Phys. Rev. Lett. 69 2357
[4] Kimura M and Lane N F 1989 Advances in Atomic, Molecular, and Optical Physics vol 26, ed by Bates D R and Bederson B (New York :Academic) pp 79
[5] Wetmore A E, Cole H R and Olson R E 1986 J. Phys. B: At. Mol. Phys. 19 1515
[6] Kimura M and Olson R E 1984 J. Phys. B: At. Mol. Phys. 17 L713
[7] Bashkin S and Stoner J R Jr 1975 Atomic Energy levels and Grotrian Diagrams vol I (Amsterdam: North-Holland)