Charge transfer in collisions of Be\textsuperscript{q\thinspace +} (q=2-4) and B\textsuperscript{q\thinspace +} (q=3-5) ions with H

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Abstract. The charge transfer reactions in collisions of Be\textsuperscript{q\thinspace +}(q=2-3) and B\textsuperscript{q\thinspace +}(q=3-4) ions and atomic hydrogen are investigated by using the quantal molecular orbital close-coupling (QMOCC) and the two-center atomic-orbital close-coupling (TC-AOCC) methods. Total and sub-shells state-selective cross sections are calculated for low and intermediate energy region and compared with other data available. Sets of recommended cross sections, based on the QMOCC and TC-AOCC calculations, are deduced and tabulated for Be\textsuperscript{2,3+} + H and B\textsuperscript{3,4+} + H collisions, which provide important atomic data needed in the charge-exchange-recombination spectroscopy diagnostics in magnetic fusion plasmas investigation.

1. Introduction

Charge transfer processes in atom – multi-charged ion collisions play an important role in magnetic fusion plasmas investigation and the radiation following the charge transfer processes has been widely used as a plasma diagnostic tool, namely the charge-exchange-recombination spectroscopy (CXRS) diagnostics [1]. The electron capture processes of multiply charged impurity ions in magnetic fusion plasma with the neutral hydrogen species are also important in the studies of impurity transport in the edge and divertor plasma regions [2]. In the past three years, as one of the participants in the IAEA Coordinated Research Program on data for light ions, we have studied the collision processes between some basic edge/divertor plasma constituents (H\textsuperscript{+}, H, He, H\textsubscript{2}) and the light element atomic and molecular plasma impurities including Li, Be, B, C, N, O ions [3-19] by using the quantal molecular orbital close-coupling (QMOCC) and the two-center atomic orbital close-coupling (TC-AOCC) methods over a large energy region.

In the present paper, the collisions of Be\textsuperscript{2,3,4+} and B\textsuperscript{3,4,5+} ions with atomic hydrogen have been investigated by using the QMOCC and TC-AOCC methods. Beryllium is the adopted first wall material for the International Thermonuclear Experimental Reactor (ITER) [4]. The charge transfer cross sections for Be\textsuperscript{4+}+H and B\textsuperscript{5+}+H collisions are calculated by using the TC-AOCC method and sets
of recommended charge transfer cross sections are proposed for the \( \text{Be}^{2,3,+} + \text{H}, \text{B}^{3,4,+} + \text{H} \) collisions based on our previous work on \( \text{Be}^{2+}, \text{Be}^{3+}, \text{B}^{3+}, \text{B}^{4+} \) ions collisions with atomic H [6,7].

The QMOCC and TC-AOCC methods are only outlined here. In QMOCC calculations, a coupled set of second-order differential equations is solved and matched to the plane-wave boundary conditions at a large internuclear distance [20-21]. The molecular structure data (potential curves, radial and rotational couplings matrix elements) required in the QMOCC has been calculated by using the multireference single- and double-excitation configuration interaction (MRD-CI) method [22-23]. Note that the translation effects have been considered by using appropriate reaction coordinates [24, 25] and the modified radial and rotational coupling matrix elements [26]. In the TC-AOCC calculations [27], the total scattering wave function is expanded over the electronic states centered on the target and on the projectile which are determined by using the variational method with the even-tempered trial functions [27, 28]. One-active electron approximation and model potential are applied in our TC-AOCC calculation and a sufficiently large expansion basis, including a large number of pseudostates, has been used to ensure the convergence of the cross sections for each of collision systems. For the relative nuclear motion, the straight-line approximation has been applied. Due to the limitation of the model potential and the straight-line approximation adopted, the present TC-AOCC method is more applicable in treating the collision processes where the electron-correlation effects are not important and the collision velocity not too slow (larger than a few hundred eV/u ). The charge transfer cross sections with different spin-manifolds (\( S \)- resolved) become especially important in CXRS simulations when different manifold electronic molecular states evolved in the charge transfer processes. The present QMOCC calculations can provide reliable \( n, \ell, S \)-resolved cross sections. For example, the state-resolved cross sections presented in the Fig. 8 of the paper of Liu and Wang [7] are comparable for singlet and triplet manifold for the charge transfer in \( \text{Be}^{3+} + \text{H} \) collisions. Only \( n, \ell \)-resolved cross sections are presented in this paper and the QMOCC partial cross sections are obtained by statistically averaging different spin-manifolds contributions.

For the convenience of applications in CXRS diagnostics in magnetic fusion plasmas investigation and other related fields, total and state-selective charge transfer cross sections in \( \text{Be}^{2,3,4,+} + \text{H} \) and \( \text{B}^{3,4,5,+} + \text{H} \) collisions have been calculated and presented by using the QMOCC and TC-AOCC methods. Sets of total and state-selective cross sections have been recommended over a large energy region based on our calculations, and as parts of the recommended data, the state-resolved cross sections are tabulated for \( \text{Be}^{2,3,+} + \text{H} \) and \( \text{B}^{3,4,+} + \text{H} \) collisions for energies less than 100eV/u.

2. Results and Discussions

In this section, the total and state-resolved cross section for \( \text{Be}^{2,3,4,+} + \text{H} \) and \( \text{B}^{3,4,5,+} + \text{H} \) Collisions are presented and compared with the available data. Recommended cross sections for \( \text{Be}^{2,3,+} + \text{H} \) and \( \text{B}^{3,4,+} + \text{H} \) Collisions are deduced based on our previous work on these systems. For \( \text{Be}^{4,+} + \text{H} \) and \( \text{B}^{5,+} + \text{H} \) collisions, the total and state-resolved cross sections are computed by using the TC-AOCC and excellent agreements have been obtain in comparison with the available data.

2.1. Total charge transfer cross sections for \( \text{Be}^{2,3,+} + \text{H} \) and \( \text{B}^{3,4,+} + \text{H} \) Collision Systems

In Figure 1-4, the total QMOCC and TC-AOCC cross sections for \( \text{Be}^{2,3,+} + \text{H} \) and \( \text{B}^{3,4,+} + \text{H} \) collisions are presented and compared with the theoretical and experimental data available. It can be found that there are good agreements between our QMOCC and TC-AOCC calculations and the data available in a large energy range, and good agreements have been achieved in the overlapping energy region between the QMOCC and TC-AOCC calculations. Combining the QMOCC results with the TC-AOCC data, reliable cross sections can be obtained over a large energy range from 0.1 eV/u to 100 keV/u. Note that the QMOCC and TC-AOCC results in Fig.1-4 have been reported in the papers of Liu et al. [6, 7] and the detail of the methods applied can be found there. The good consistence between the QMOCC and TC-AOCC calculations provides a good foundation to deduce the recommended data over a larger collision energy region.
Figure 1. (Color online) The total charge-transfer cross sections for the $\text{Be}^{2+} (1s2) + \text{H}(1s)$ collision. The QMOCC calculation of Liu et al. [3] (solid line with filled circles); The TC-AOCC results of Liu et al. [6] (solid line); The perturbed stationary state (PSS) results of Wetmore et al. [29] (solid line with filled squares); The classical trajectory Monte Carlo (CTMC) results of Schultz et al. [30] (solid line with open squares).

Figure 2. Total charge-transfer cross sections for the $\text{Be}^{3+} + \text{H}$ collision. The QMOCC calculation of Liu et al. (solid line with filled circles) [7]; The TC-AOCC calculation of Liu et al. (solid line) [6]; SCMOCC results of Shimakura [31] (solid line with open circles); and CTMC results of Schultz et al. [30] (open squares).
Figure 3. (Color online) Total charge-transfer cross sections for $\text{B}^{3+}(1s^2) + \text{H}(1s)$ collisions. The QMOCC results of Liu et al. (solid line with filled circles) [3]; The TC-AOCC results of Liu et al. (solid line) [6]; AOCC results of Hansen et al. [32] (solid line with open squares); PSS results of Wetmore et al. [29] (solid line with open circles); SC-MOCC results of Shimakura et al. [33] (solid line with downward triangle); SC-MOCC results of Olson et al. [34] (solid line with upward triangle); and experiment results of Crandall et al. [35] (stars).

Figure 4. (Color online) The total charge transfer cross sections for $\text{B}^{4+}-\text{H}(1s)$ collisions as functions of collision energy. Theory: (—) The TC-AOCC results of Liu et al [6]; (----) AOCC results of Tseng and Lin, [36], (○) The quantal molecular orbital close-coupling (QMOCC) results of Gargaud and McCarroll, [37], (.....) The Semi-classical molecular...
orbital close-coupling (SCMOCC) results of Shimakura et al., [38] (●) The boundary corrected continuum intermediate state approximation results of Das et al., [39]. Experiment: (●) Goffe et al.,[40] (□) Gardner et al., [41] (□) Crandall et al.,[35], (○) Pieksma and Havener, [42].

2.2. Recommended cross sections for $\text{Be}^{2,3+}+\text{H}$ and $\text{B}^{3,4+}+\text{H}$ Collisions

In Figure 5-8, the state selective cross sections of QMOCC and TC-AOCC calculations are presented for $\text{Be}^{2,3+}+\text{H}$ and $\text{B}^{3,4+}+\text{H}$ collisions. Only $n, l$ - resolved cross sections are presented in the present paper and the QMOCC partial cross sections are obtained by statistically averaging different spin-manifolds contributions. It can be found that there are good agreements between the QMOCC and TC-AOCC calculations even for the sensitive $n,l$-resolved cross sections, which provides a good foundation for deducing the $n,l$-resolved cross sections.

For the convenience of application, the state-selective cross sections for $\text{Be}^{2,3+}+\text{H}$ and $\text{B}^{3,4+}+\text{H}$ collisions are evaluated and recommended data are proposed based on the two close-coupling calculations and the data available. In our evaluation, the QMOCC results are preferred for the energy less than about 1keV/u and the TC-AOCC results are chosen for energy larger than a few keV/u. While discrepancies appear in the overlapping energy region, usually the smooth connection between two sets of calculations is preferred in our deduction. If experimental data is available, it serves as the benchmark data in our evaluation. Based on such a criterion, recommended charge transfer cross sections are deduced for $\text{Be}^{2,3+}+\text{H}$ and $\text{B}^{3,4+}+\text{H}$ collisions. As shown in the figures 5-8, the recommended data are represented by the red solid lines. For the dominant reaction channels, there are excellent agreements between two close coupling calculations and the deduction is straightforward, for example the 2s cross sections in $\text{Be}^{2,3+}+\text{H}$ collisions and 3s, 3p cross section in $\text{B}^{3,4+}+\text{H}$ collisions. However, for the 3s capture cross sections presented in the first panel of figure 7, the TC-AOCC results merge to the QMOCC data around the energy of 300eV/u and the TC-AOCC results are adopted to about 300eV/u in the recommendation due to the good agreement between our TC-AOCC results and the data of Hansen and Dubois [32]. In Figure 7 and 8, only the $n, l$-resolved cross sections are proposed for the dominant $n=3$ channels and $n$-resolved cross sections are presented for the less important channels of $n=2$ and $n=4$. For the clarity of Figures 5-8, the recommended cross sections are only presented for energy larger than 10eV/u. For lower energy region, the QMOCC calculations are more reliable and chosen as recommended data. In table 1-4, the QMOCC cross section for $\text{Be}^{2,3+}+\text{H}$ and $\text{B}^{3,4+}+\text{H}$ collisions are presented. Note that the recommended data in the whole energy range and the $S$-resolved cross sections can be obtained when required.
Figure 5. (Color online) The \( n, l \)-resolved charge-transfer cross sections for the Be\(^{2+}\)(1s\(^3\)) + H(1s) collision. The QMOCC results: black solid lines with unfilled squares; The TC-AOCC results: black solid lines with unfilled circles. Recommended data: red solid lines.

Figure 6. (Color online) The \( n, l \)-resolved charge-transfer cross sections for the Be\(^{3+}\)(1s\(^3\)) + H(1s) collision. The QMOCC results: black solid lines with unfilled squares; The TC-AOCC results: black solid lines with unfilled circles. Recommended data: red solid lines.
where the CB approximation is expected to be reasonable. For continuum intermediate state approximation (CB) calculations of Das et al \[43, 44\], as shown in figure 9 and figure 10. For Be \(4^+\) collisions, as shown in figure 9. The present TC-AOCC results converge to the boundary corrected total and state-resolved cross sections are compared with the late work of Das et al. \[43\] at higher energy where the CB approximation is expected to be reasonable. For B\(^{3+}\) + H collisions, excellent agreements

**Figure 7.** (Color online) The \(n, l\)-resolved charge-transfer cross sections for the B\(^{3+}(1s^2) + H(1s)\) collision. The QMOCC results: black solid lines with unfilled squares; The TC-AOCC results: black solid lines with unfilled circles. Recommended data: red solid lines.

**Figure 8.** (Color online) The \(n, l\)-resolved charge-transfer cross sections for the B\(^{4+}(1s) + H(1s)\) collision. The QMOCC results: black solid lines with unfilled squares; The TC-AOCC results: black solid lines with unfilled circles. Recommended data: red solid lines.

### 2.3. Total and state-resolved cross sections for Be\(^{4+}+H\) and B\(^{5+}+H\) Collisions

The TC-AOCC method has been applied to investigate Be\(^{4+}\) + H and B\(^{5+}\) + H collisions and the obtained total and state-resolved cross sections are compared with the late work of Das et al \[39\] and Errea et al \[43, 44\], as shown in figure 9 and figure 10. For Be\(^{4+}\) + H collisions, there are excellent agreement between the present TC-AOCC calculations and the semi-classical MOCC results of Errea et al \[43\] for total cross sections and for the \(n, l\)-resolved cross sections available for the dominant \(n=3,4,5\) channels, as shown in figure 9. The present TC-AOCC results converge to the boundary corrected continuum intermediate state approximation (CB) calculations of Das et al. \[39\] at higher energy where the CB approximation is expected to be reasonable. For B\(^{3+}\) + H collisions, excellent agreements
are also achieved over a large energy region between the present TC-AOCC calculations and the recommended data of Errea et al [44]. In Errea’s evaluation, the Semi-classical MOCC results are preferred for low energy side and the classical CTMC results are used for high energy side. The present TC-AOCC results and the recommended data of Errea et al. [44] both converge to the CB results of Das et al. [39] at energy larger than 100keV/u. For the energies less than a few hundred eV/u, the QMOCC method becomes more applicable. The QMOCC calculations will be performed in the near future and recommended data can be proposed over a larger energy region.

**Figure 9.** (Color online) The total and n-resolved charge transfer cross sections for Be\(^{4+}\) - H(1s) collisions as functions of collision energy.

**Figure 10.** (Color online) The total and n-resolved charge-transfer cross sections for the B\(^{5+}\) + H(1s) collision.
3. Conclusions
In the present work, the Be$^q$-H (1s) (q=2, 3, 4) and B$^q$-H (1s) (q=3, 4, 5) collision have been investigated by using QMOCC and TC-AOCC methods. Good agreements have been obtained between the present QMOCC and TC-AOCC calculations and the experiment and theoretical data available. For Be$^3$, 4$^+$-H and B$^3$, 4$^+$-H collisions, recommended cross sections are deduced over a large energy region, as shown in figure 5-8 and Table 1-4. For Be$^q$-H and B$^q$-H collisions, TC-AOCC calculations are performed and excellent agreements have been achieved in comparison with the data available.

Table 1. State-selective charge transfer cross sections (in units of $10^{-16}$cm$^2$) for Be$^{2+}$-H calculated by using QMOCC method at selected collision energies. (a (b) stands for a×10$^b$).

| Be$^{2+}$ state | 0.1eV/u | 0.5eV/u | 1.0eV/u | 5.0eV/u | 10eV/u | 50eV/u | 100eV/u |
|----------------|---------|---------|---------|---------|--------|--------|---------|
| 1s$^2$2s       | 4.09(-4)| 6.50(-3)| 2.80(-2)| 8.15(-1)| 2.611  | 12.28  | 17.23   |
| 1s$^2$3p       | 8.80(-5)| 1.623   | 3.76(-4)| 4.86(-4)|        |        |         |
| 1s$^2$3s       | 1.33(-4)| 3.76(-4)|        |         |        |        |         |
| 1s$^2$3p       | 1.12(-4)| 4.86(-4)|        |         |        |        |         |
| 1s$^2$3d       | 0       | 1.62(-4)|        |         |        |        |         |

Table 2. State-selective charge transfer cross sections (in units of $10^{-16}$cm$^2$) for Be$^{3+}$-H calculated by using QMOCC method at selected collision energies. (a (b) stands for a×10$^b$).

| Be$^{3+}$ state | 0.1eV/u | 0.5eV/u | 1.0eV/u | 5.0eV/u | 10eV/u | 50eV/u | 100eV/u |
|----------------|---------|---------|---------|---------|--------|--------|---------|
| 1s$^4$         | 4.69(-3)| 1.95(-3)| 1.52(-3)| 1.16(-3)| 1.04(-3)| 7.25(-4)| 5.43(-4)|
| 1s2s           | 5.74(-4)| 2.33(-4)| 1.69(-4)| 1.07(-4)| 9.67(-5)| 1.06(-4)| 1.09(-4)|
| 1s2p           | 4.05(-4)| 1.64(-4)| 1.11(-4)| 5.38(-5)| 3.86(-5)| 5.57(-4)| 7.21(-3)|
| 1s3s           | 2.00(-3)| 3.70(-2)|        |         |        |        |         |
| 1s3p           | 2.52(-3)| 0.227   |        |         |        |        |         |
| 1s3d           | 7.69(-4)| 0.135   |        |         |        |        |         |

Table 3. State-selective charge transfer cross sections (in units of $10^{-16}$cm$^2$) for B$^{3+}$-H calculated by using QMOCC method at selected collision energies. (a (b) stands for a×10$^b$).

| B$^{3+}$ state | 0.1eV/u | 0.5eV/u | 1.0eV/u | 5.0eV/u | 10eV/u | 50eV/u | 100eV/u |
|----------------|---------|---------|---------|---------|--------|--------|---------|
| 1s$^2$2s       | 3.08(-4)| 1.38(-4)| 9.98(-5)| 5.58(-5)| 5.79(-5)| 7.25(-5)| 6.41(-5)|
| 1s$^2$2p       | 6.74(-4)| 2.85(-4)| 1.91(-4)| 9.77(-5)| 7.78(-5)| 1.15(-4)| 2.13(-3)|
| 1s$^3$3s       | 8.38(-5)| 4.79(-5)| 3.95(-5)| 3.81(-5)| 4.22(-5)| 0.021  | 0.218   |
| 1s$^3$3p       | 0       | 0       | 0       | 0       | 0       | 3.77(-3)| 0.462   |
| 1s$^3$3d       | 0       | 0       | 0       | 0       | 0       | 2.48(-5)| 0.031   |
Table 4. State-selective charge transfer cross sections (in units of $10^{-16}$ cm$^2$) for B$^{4+}$-H calculated by using QMOCC method at selected collision energies. (a (b) stands for $a \times 10^b$).

| B$^{3+}$ state | 0.1eV/u | 0.5eV/u | 1.0eV/u | 5.0eV/u | 10eV/u | 50eV/u | 100eV/u |
|---------------|--------|--------|--------|--------|--------|--------|--------|
| 1s2s          | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 1s2p          | 0      | 0      | 0      | 0      | 0      | 0      | 0      |
| 1s3s          | 1.00(-4)| 1.67(-4)| 9.21(-5)| 5.70(-3)| 0.052  | 1.778  | 4.078  |
| 1s3p          | 21.2   | 7.52   | 6.226  | 9.721  | 14.82  | 19.70  | 18.26  |
| 1s3d          | 25.95  | 14.97  | 11.77  | 9.206  | 7.168  | 6.731  | 7.044  |
| 1s4p          | 0      | 0      | 0      | 0      | 0      | 8.34(-3)| 0.020  |
| 1s4p          | 0      | 0      | 0      | 0      | 0      | 0.045  | 0.082  |
| 1s4d          | 0      | 0      | 0      | 0      | 0      | 4.78(-3)| 0.038  |
| 1s4f          | 0      | 0      | 0      | 0      | 0      | 0.052  | 0.306  |

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