Theoretical investigation of electron capture processes in slow \(O^{7+}-H\) collisions

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ABSTRACT

Aims. The total and n-, l-, and S-resolved single-electron-capture cross sections for the collisions of \(O^{7+}\) with atomic hydrogen are studied in the energy region from \(10^{-3}\text{eV/u} - 5\text{keV/u}\).

Methods. These state-selective cross sections were calculated by employing the full quantum-mechanical molecular-orbital close-coupling (QMOCC) method. The ab initio multireference single- and double-excitation configuration interaction approach, with optimized atomic basis sets to accurately describe the highly excited states, was used to obtain the adiabatic potentials and the radial and rotational coupling matrix elements that are required in the QMOCC calculation.

Results. Our results are compared with other available theoretical and experimental data. The n = 5 manifold is the dominant reaction channel for the charge-transfer process for this collision system over the entire energy range, and our results agree better with the experimental data than the other theoretical results in the energy region in which they overlap because we included the necessary highly excited states in the expansion basis set. These charge-exchange cross-section data are useful for understanding and modeling the X-ray emission in astrophysical environments.

Key words. charge transfer process, full quantum-mechanical molecular-orbital close-coupling (QMOCC) method, cross section

1. Introduction

Collisions between highly charged ions and neutral species have been extensively studied in various fields, such as astrophysics and fusion-plasma diagnostics. In an astrophysical environment, electron-capture processes resulting from highly charged ions colliding with the neutral atoms or molecules are very important for explaining the celestial phenomena (Zhang et al. 2023, 2022; Wu et al. 2012; Lin et al. 2019). For example, the formation of solar wind X-rays and the extreme ultraviolet can be attributed to the electron-capture collisions of fast solar wind ions with neutral ambient gases (Wu et al. 2012). The solar wind is composed of electrons, protons, alpha particles, and a large number of other highly charged ions, such as \(C^{q+}\), \(N^{q+}\), \(O^{q+}\), \(S^{q+}\), \(Ne^{q+}\), \(Mg^{q+}\), \(Al^{q+}\), \(Si^{q+}\), and \(Ar^{q+}\). The types of neutral particles are different in different astrophysical environments. For instance, the atmosphere of a comet contains \(H_2O\), \(CO\), \(HO_2\), and their dissociation products \(H_2\), \(H\), \(O\), and so on, the heliosphere mainly contains \(H\) and \(He\), the geocorona mainly contains \(H\) and the halo of Mars mainly contains \(H\) and \(O\). Therefore, it is crucial to investigate highly charged solar wind ions colliding with these neutral particles. Moreover, the obtained cross-section data and rate coefficients can also provide insights into the research of X-ray simulations of the solar wind.

With the continuous advancement of science and technology, various space equipments have appeared in succession, such as the Chandra X-ray Observatory, the XMM-Newton detector, the far-ultraviolet spectroscopic detector (FUSE), and the Suzaku satellite. The soft x-ray and extreme-ultraviolet emission of the objects from the Solar System have been observed using these space equipments. For example, in 2006, Chandra detected X-rays from Venus, which revealed that the Venusean halo X-rays originated from a charge-exchange mechanism of the solar wind (Dennerl 2009). Moreover, the XMM-Newton detector has observed soft X-rays (0.2-2 keV) from the auroral region of Jupiter, and it was found that these X-rays originated from the charge-transfer processes between highly charged solar wind ions (\(O^{q+}\), \(C^{q+}\), and \(Ne^{q+}\)) and neutral particles from the Jupiter atmosphere (Krasnopolsky & Mumma 2001; Cravens 1997). Similarly, the soft X-rays from Mars have been observed by XMM-Newton (Bhardwaj et al. 2009), and it was confirmed that the charge-exchange process of highly charged solar wind ions (\(C^{q+}\), \(N^{q+}\), \(O^{q+}\), \(Ne^{q+}\)) colliding with neutral particles in the atmosphere or outer atmosphere are the origin of this emission. These X-rays are important for diagnosing the composition, evolution, velocity, and distribution of the neutral gas density in the solar wind.

We study the electron-capture process in collisions of \(O^{7+}\) ions with atomic hydrogen in the energy region 0.001 eV/u-5 keV/u using the full quantum-mechanical molecular-orbital close-coupling (QMOCC) method. To the best of our knowledge, the available experimental and theoretical data for this collision system have been very limited so far. Total charge-transfer cross sections have been measured by R. T. Zhang et al. (Zhang et al. 2022), Meyer et al. (Meyer et al. 1985), Panov et al. (2001), and Meyer et al. (2009). Furthermore, the available theoretical results are compared with our results. The present investigation is of significant importance for understanding and modeling the X-ray emission in astrophysical environments.
wave functions can be expanded in terms of adiabatic electronic transfer cross sections for O- ions in the energy range 875 - 350 eV. The potentials curves established so far. The main motivation of our work is to investigate electron-capture dynamics of O- - H collisions in the energy region 0.001eV/u - 5keV/u and provide the accurate total and state-selective electron-capture cross-section data in a wide energy region for this collision system. The QMOC method is employed to calculate the total, n-resolved, nl-resolved, and nls-resolved charge-transfer cross sections. The potentials curves and matrix elements that are required in the scattering calculation are obtained by the ab initio multifrference single- and double-excitation configuration interaction (MRDCI) method.

2. Theoretical methods
2.1 Scattering theory
We employed the QMOC method, which has been described in the literature (Lin et al. 2019; Nolte et al. 2012; Zygelman et al. 1992), to calculate n-, l-, ands-resolved charge-transfer cross sections for O- - H collision systems at low energies. In the Born-Oppenheimer (B-O) approximation, the total wave functions can be expanded in terms of adiabatic electronic wavefunctions \( \psi_{j}(R, \mathbf{r}) \),

\[
\Psi(R, \mathbf{r}) = \sum_{j} F_{j}(R) \psi_{j}(R, \mathbf{r}),
\]

where \( \mathbf{r} \) and \( \mathbf{R} \) are the electron position vector and internuclear distance vector in the body-fixed frame, respectively. The Schrödinger equation can be shown as

\[
\left[ \nabla_{R}^{2} - 2 \mu(u-E_{I}) \right] F(R) = \left( M(R) + P(R) \right) \cdot \nabla_{R} F(R),
\]

\[
M_{ij}(R) = -\int d\mathbf{r} \psi_{i}^{*}(\mathbf{R}, \mathbf{r}) \nabla_{R}^{2} \psi_{j}(\mathbf{R}, \mathbf{r}) ,
\]

\[
P_{ij}(R) = -2 \int d\mathbf{r} \psi_{i}^{*}(\mathbf{R}, \mathbf{r}) \nabla \psi_{j}(\mathbf{R}, \mathbf{r}) ,
\]

in which \( I \) and \( u \) are the unit matrix and diagonal adiabatic potential matrix. \( M \) and \( P \) are coupling matrices.

Inserting Eq. (1) into Eq. (2), we obtain

\[
\left[ \frac{d^{2}}{dR^{2}} + \frac{J(J+1)}{R^{2}} - 2 \mu(u(R)-E) \right] f^{(i)}(R) = \left( V^{R}(R) + V^{C}(R) \right) f^{(i)}(R) ,
\]

where \( V^{R} \) and \( V^{C} \) represent the radial and rotational coupling matrices. \( \langle i, \ldots, j \rangle \) represents \( \langle \psi_{i}, \ldots, \psi_{j} \rangle \), \( J \) is the total angular momentum, \( \lambda_{j} \) is the y-component of the electronic angular momentum, and \( \lambda \) is the elements of the diagonal matrix \( \lambda \).

For convenience, \( f^{i}(R) \) is usually defined as

\[
f^{(i)}(R) = C g^{(i)}(R) \frac{dC}{dR} + AC = 0 ,
\]

in which \( C \) is the orthogonal transformation matrix and satisfies the boundary condition \( C(R) \to \mathbf{I}; R \to \infty \). In this case, the coupled equations (4) are replaced by

\[
\left[ \frac{d^{2}}{dR^{2}} + \frac{J(J+1)}{R^{2}} + 2 \mu E \right] g^{(i)} - 2 \mu \sum_{\gamma} U_{\gamma\gamma}(R) g^{(\gamma)} = 0 ,
\]

\[
U_{\gamma\gamma}(R) \equiv \left[ C(u-p)C^{-1}\right]_{\gamma\gamma} ,
\]

where \( U \) and \( P \) represent the diabatic radial and rotational coupling matrices, respectively. Solving the equations by using the multichannel log-derivative method of Johnson (Johnson 1973), we can obtain the \( K \) matrix and \( S \) matrix as

\[
S = [I + IK][I - IK]^{-1} .
\]

The electron-capture cross section from state \( i \) to \( j \) can be obtained as

\[
\sigma_{(i \to j)} = \frac{\pi}{k_{i}^{2}} \left( 2J+1 \right) \left| S_{ij} \right|^{2} ,
\]

Finally, the electron translation factors (ETFs), which are important for the collision energies above 1 keV/u, are used to consider the translation effects in the collision dynamics. The radial and rotational coupling matrix elements between the states and can be transformed into

\[
< \psi_{j}(\mathbf{r}) | \partial/\partial R - (E_{K} - E_{L}) \gamma^{2} / 2R | \psi_{L} > ,
\]

\[
< \psi_{K} | L_{y} + (E_{K} - E_{L}) z \lambda | \psi_{L} > .
\]

These modifications are similar to the common ETFs approach of reference (Erroa et al. 1982). In these equations, \( E_{K} \) and \( E_{L} \) represent the electronic energies of states \( \psi_{K} \) and \( \psi_{L} \), respectively, \( z^{2} \) and \( z \lambda \) represent the components of quadrupole moment tensor.

2.2 Molecular structure calculations
We employed the MRDCI method (Buenker et al. 2014; Krebs & Buentker 1995) to calculate the adiabatic potentials and coupling matrix elements for the O- - H scattering system. For the O- ion, we used a hybrid basis set consisting of two components (Wu et al. 2012, 2011; Dunning 1989): (i) the standard Dunning neutral atom basis, and (ii) a one-electron basis of
Table 1. Asymptotic separated-atom energies of the singlet of O⁺⁺ - H⁻. Values marked with an asterisk were calculated with the Grasp method.

<table>
<thead>
<tr>
<th>Asymptotic atomic states</th>
<th>Molecular states</th>
<th>Energy (eV)</th>
<th>NIST</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>O²⁺+(1s²) + H⁺</td>
<td>1Σ⁺</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>O²⁺+(1s²) + H⁺</td>
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<td>O²⁺+(1s²) + H⁺</td>
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<td>573.8661</td>
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<td>720.9688</td>
<td>720.8379</td>
<td>0.0089</td>
</tr>
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Table 2. Asymptotic separated-atom energies of the triplet of O⁺⁺ - H⁻. Values marked with an asterisk were calculated with the Grasp method.

<table>
<thead>
<tr>
<th>Asymptotic atomic states</th>
<th>Molecular states</th>
<th>Energy (eV)</th>
<th>NIST</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>O²⁺+(1s²) + H⁺</td>
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<td>O²⁺+(1s²) + H⁺</td>
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<td>662.0119</td>
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<td>O²⁺+(1s²) + H⁺</td>
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3. Results and discussion

3.1 Potentials and couplings

Fig. 1a and Fig. 2a show the adiabatic potential energy curves of [OH]⁺⁺⁺ or the singlet and triplet states, respectively, in the range of internuclear distance from 1 a.u. to 50 a.u. The 21 1Σ⁺ and 20 3Σ⁺ represent the initial state O⁺⁺ - H(1s). The regions of the avoided crossings for the important n = 5 and 6 channels are displayed in Fig. 1b and Fig. 2b. Some avoided crossings existed between the initial channel and the final n=5,6 channels in the region of internuclear distance R=10.00 - 15.00 a.u. and R=30.00 - 35.00 a.u., respectively. The avoided crossings in the region of R=10.00 - 15.00 a.u. play a major role in the charge-transfer process. These avoided crossings of the potential energy curve were also found in previous studies for the collisions of highly charged ions with H atoms (Shipsey et al. 1981; Nolte et al. 2012; Lin et al. 2019). Therefore, the n = 5 channel will become the dominant channel for the charge-transfer process for this collision system.

Radial and rotational coupling elements were computed with the finite-difference method (Hirsch et al. 1980). In Fig. 3 and Fig. 4, radial coupling matrix elements between the adjacent channels for the dominant n = 5 manifold and some mainly rotational coupling matrix elements which considered the influence of ETMs are displayed as a function of internuclear distance R. Fig. 3 shows that for the nuclear distance R < 15.00 a.u., there are some relatively strong and sharp peaks between the initial and n=5 channels that originated from the avoided crossings of the potential energy curve in the corresponding region. Around R ~ 12.00 a.u., a strong and broad coupling exists between the 11Σ⁺ and 12Σ⁺ states and 10Σ⁺ and 11Σ⁺ states. This coupling suggests the primary gateway of electron charge-transfer flux toward the final states.

3.2 Electron-capture cross sections

In our QMOC calculations, a large expansion basis set was used that consisted of 69 13Σ⁺ and 13Π⁺ states, correlating with the n=2, 3, 4, 5, and 6 atomic manifolds of O⁺⁺ ions. The total
and $n$-, $L$-, and $S$-resolved electron-capture cross sections were calculated in the energy range $10^{-3}$ eV/u - 5.0 keV/u. Our cross section results were systematically compared with previous theoretical and experimental results. In the MOCC calculations by Nolte et al. (Nolte et al. 2011), a Gaussian basis set that contained 17s, 11p, 9d, 6f, and 5g states was used on O$^+$ and a 6s, 5p, 2d, and 1f basis contracted to 4s, 3p, 2d, and 1f was used on H in their MRDCl calculation. Their largest error for the relative asymptotic energies of [OH]$^+$ system is about 0.06629 a.u. ($\approx 1.804$ eV). This accuracy of the energies will produce certain errors in the subsequent scattering calculations. In their MOCC calculation, $3\Sigma^+$ and $1\Pi$ states were considered in the expansion basis, correlating with the n=4, 5 atomic manifolds. The contributions from n=2, 3, 6 atomic manifolds to the scattering cross sections were ignored.

We compare in Fig. 5 our total charge-transfer cross sections of the MOCC calculation with the available experimental (Panov et al. 1983; Meyer et al. 1985; Zhang et al. 2022) and other theoretical (Phaneuf et al. 1987; Janev et al. 1988; Nolte et al. 2011) results in the energy range from 0.001 to 5000 eV/u. Our QMCC results agree well with the experimental results of Zhang et al. (Zhang et al. 2022) and Meyer et al. (Meyer et al. 1985) in the overlapping energy regions, and they lie closer to the AOC results of Nolte et al. (Nolte et al. 2011) and the recommended results of Janev et al. (Janev et al. 1988) in the energy range 100-5000 eV/u. For energies below 20eV/u, our results are significantly lower than the experimental data of Zhang et al. (Zhang et al. 2022), and the MOCC results of Nolte et al. (Nolte et al. 2011) are closer to the experimental data than ours. However, in the energy region 20 eV/u -1000 eV/u, our QMCC results agree better with the experimental data of Zhang et al. (Zhang et al. 2022), mainly because more highly excited states are taken into account in our molecular structure and scattering cross-section calculation.

The singlet and triplet $n$-resolved QMCC charge-transfer cross sections for the O$^+$ - H system are shown in Fig 6a and Fig 6b, respectively. To the best of our knowledge, no other experimental or theoretical studies of $n$-resolved cross sections for electrons captured to the singlet and triplet final states for this collision system have been published so far. The n = 5 manifold clearly is the dominant path for charge transfer in the entire energy range. Fig. 6a shows that when the energy is higher than 30 eV/u, the n = 6 manifold becomes the subdominant reaction channel for the charge-transfer process. In the energy range from 3 to 30 eV/u, the n = 4 manifold is the subdominant path for the charge-transfer process. For energies lower than 3 eV/u, the n = 3 manifold is more important. Fig. 6b also shows that the n = 6 manifold is the subdominant path for the charge-transfer process in the energy range from 20 to 1500 eV/u. For energies higher than 1500 eV/u or lower than 20 eV/u, the n = 4 manifold is the subdominant charge-transfer path.
The total $n$-resolved charge-transfer cross sections for $O^{7+}$ - H system, compared with the previous MOCC and AOCC results of Nolte et al. (Nolte et al. 2011), are shown in Fig. 7. This figure shows that $n=5$ is the dominant reaction channel in the considered energy range for this collision system. Our QMOCC results agree better with the previous MOCC results of Nolte et al. (Nolte et al. 2011) than with the AOCC results (Nolte et al. 2011) in the overlapping energy region for capture to the $n=5$ shells of $O^{6+}$ ions. The AOCC cross sections (Nolte et al. 2011) have the same energy behavior as our results, but the magnitudes are slightly lower than ours. For the subdominant channels $n=4$, our results also agree well with the MOCC results of Nolte et al. (Nolte et al. 2011) in the overlapping energy region. However, the AOCC results (Nolte et al. 2011) are larger than...
our results in the energy region below about 3 keV/u. For the weakly coupled reaction channels n=3 and n=6, our QMOCC results are comparable with the AOCC results (Nolte et al. 2011) at the collision energy of 0.2 keV/u and 5 keV/u, respectively. For other energies, there are significant differences between our results and those of the AOCC (Nolte et al. 2011). This difference may arise because we neglected the contribution of the molecular states with higher angular momentum (e.g., Λ, Φ, and Γ) to the charge-transfer cross sections.

![Fig. 7. (Color online) Total n-resolved QMOCC cross sections for [OH]$^{7+}$.](image)

The total nL-resolved QMOCC charge-transfer cross sections for O$^{7+}$-H system are displayed in Fig. 8. In Fig. 9 and Fig. 10, we show our singlet and triplet nL-resolved charge-transfer cross sections for the O$^{7+}$-H system, respectively. They are compared with the previous MOCC results (Nolte et al. 2011). As observed in Fig. 8, the 5s is the dominant charge-transfer path in the energy range 3-1000 eV/u for this collision system. For energies lower than ~ 3 eV/u or higher than ~ 1000 eV/u, charge transfer to the 5p state becomes more important. Figure 9 shows that electron capture to the 5f state of O$^{7+}$ ions becomes the dominant singlet state in the energy regions below ~ 2 eV/u and 200 eV/u -1000 eV/u. However, 5s becomes the dominant singlet state in the energy regions above ~ 1000 eV/u and 2 eV/u -200 eV/u. Fig. 10 shows that for energies lower than ~ 10 eV/u and higher than ~ 800 eV/u, electron capture to the 5p state of O$^{7+}$ ions becomes the dominant triplet channel. In the energy region of 10 eV/u -800 eV/u, electron capture to the 5s state becomes the dominant triplet channel. Due to the effect of the value and statistical weight of the singlet and triplet cross sections, this difference is not reflected in the total nL-resolved cross sections. This figure also shows large differences between our results and the MOCC results of Nolte et al. (Nolte et al. 2011) for the 5d and 5g singlet states. Especially for low collision energies, our QMOCC cross sections are significantly lower than those of the MOCC method. Moreover, our results for 5p singlet states are also clearly smaller than those of the MOCC method in the energy region below about 60 eV/u. The difference between our QMOCC results and the MOCC results (Nolte et al. 2011) may arise from two facts: (1) The influence of the n=6 states of O$^{7+}$ ions are neglected in the MOCC calculations (Nolte et al. 2011), and (2) the difference in the number of radial and rotational couplings and their strengths and positions for the corresponding internuclear distance.

![Fig. 8. (Color online) Total nL-resolved QMOCC cross sections for [OH]$^{7+}$.](image)

![Fig. 9. (Color online) Singlet nL-resolved QMOCC cross sections for [OH]$^{7+}$.](image)

![Fig. 10. (Color online) Triplet nL-resolved QMOCC cross sections for [OH]$^{7+}$.](image)

Fig. 11 presents the triplet-singlet ratios for nL-resolved cross sections for O$^{7+}$-H. Previous studies (Nolte et al. 2011; Greenwood et al. 2001; Bliek et al. 1998) have shown that the triplet-to-singlet ratio for charge-transfer cross sections is related to the impact energy for the collisions between highly charged ions and the neutral particles. This ratio approaches 3:1 for col-
lision energies higher than 10 keV/u. This figure shows that only a few triplet-to-singlet ratios for n,l-resolved cross sections seem to approach 3:1. Most ratios deviate from 3 and vary widely in the considered collision energy range. This deviation may be caused by the strong dependence of the triplet-singlet ratios on the impact energy in the low collision energy region, which approaches a statistical distribution only at higher energies.

4. Summary

Highly charged solar wind ions colliding with neutral particles play an important role in the research of solar wind X-ray simulations. In the present work, the full quantum-mechanical molecular-orbital close-coupling (QMOCC) method was used to calculate the charge-transfer cross sections for the collision system O\(^{7+}\) - H. The adiabatic potentials and coupling data used in the QMOCC calculations were carried out through the ab initio multireference single- and double-excitation configuration interaction (MRDCl) approach. In our QMOCC calculations, total and n, l and S-resolved cross sections for single-electron capture to the n = 2, 3, 4, 5, 6 states of O\(^{7+}\) ions were studied in the energy range 10\(^{-3}\) eV/u - 5.0 keV/u. Throughout the entire energy range, the n = 5 manifold is the dominant charge-transfer channel for this collision system. By comparing with the existing experimental and theoretical data, we found that our results agree better with the experimental data than with the other theoretical results in the considered energy region. There are certain differences between our results and previous QMOCC results (Nolte et al. 2011) in the overlapping energy region. The discrepancy is mainly due to the following reasons: i) The differences in the sizes of the expansion bases used in the molecular structure calculations, ii) the differences in the accuracy of the energies in the respective asymptotic energies of the [OH]\(^{7+}\) system, and iii) a greater number of highly excited states are considered in our QMOCC calculation.

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