Electron capture by O\(^{3+}\) ions from He, H\(_2\)O and CO\(_2\)

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Abstract. Using the translational energy-gain spectroscopy technique, we have measured the energy-gain spectra and absolute total cross sections for single-electron capture in collisions of O\(^{3+}\) ions with He, H\(_2\)O and CO\(_2\) at impact energies between 0.3 and 1.2 keV and scattering angles between 0° and 6°. At the lowest collision energy, 300 eV, the energy-gain spectrum for O\(^{3+}\) - He collisions indicates that single-electron capture into the 2s2p\(^3\)\(^3\)P state of the product O\(^{2+}\) is the dominant reaction channel observed with smaller contributions from capture into the 2s2p\(^1\)\(^1\)D, \(^3\)S and \(^1\)P states. For O\(^{3+}\) - H\(_2\)O collisions, the dominant peak correlates with capture into the 2p3p state of O\(^{2+}\), with a significant contribution involving capture into the 2p3s state. In O\(^{3+}\) - CO\(_2\) collisions, the dominant reaction channel is due to capture into the 2p3s state of O\(^{2+}\), with contributions from capture into the 2p3p state. The measured cross sections are compared with the available measurements and theoretical results based on the multi-channel Landau-Zener (MCLZ) model.

1. Introduction

The study of electron capture processes in collisions of multiply-charged ions with molecular targets has recently received considerable theoretical and experimental attention. A number of mechanisms have been suggested for the charge balance of astrophysical plasmas and the origin of the x-ray emission from comets and planetary atmospheres. One of those is the electron capture mechanism between multiply charged ions present in the solar wind and atmospheric and cometary gases. Electron capture processes can also significantly affect the thermal and ionization structure of a wide variety of astrophysical plasmas. Data for electron capture are therefore essential to the understanding and interpretation of the O\(^+\) and O\(^{2+}\) emission lines in interstellar medium [1, 2].

Translational energy spectroscopy has been extensively used to study state-selective electron capture by multiply-charged oxygen ions from rare-gas atoms and atomic and molecular hydrogen. However in case of H\(_2\)O and CO\(_2\) targets, there have been no previous experimental measurements of cross sections, differential in translational energy-gain and projectile scattering angle, for state-selective electron capture at low energies.

In the present work, a differential energy-gain spectrometer [3], capable of measuring simultaneously the scattering angle and the energy-gain of projectile products in ion-atom collisions, has been used for the study of state-selective single-electron capture in collisions of O\(^{3+}\) recoil ions with He, H\(_2\)O and CO\(_2\) at impact energies between 0.3 and 1.2 keV and scattering angles between 0°

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and 5°. Briefly, oxygen ions were produced in a recoil ion source by using 25 MeV F⁺ ions from the Western Michigan University tandem Van de Graaff accelerator as a pump beam. An einzel lens was used to focus the ion beam extracted from the ion source into a 180° double-focusing magnet. After mass selection the ion beam was again focused by two pairs of deflectors and directed into a gas cell containing low-pressure target gas to ensure single collision conditions. Ions scattered through a nominal angle θ into a solid angle (ΔΩ) of about 3×10⁻³ sr were energy analyzed by means of a 90° double-focusing electrostatic analyzer (ESA), and then detected by a one-dimensional position sensitive channel-plate detector, which is located at the focal plane of the ESA. The scattering angle θ is selected by means of an aperture (1mm diameter) in front of ESA.

For the measurement of absolute total cross sections for single-electron capture, the target gas pressure in the collision cell was measured by a capacitance manometer (MKS Baratron), and was typically ≤ 2 mTorr, to ensure single-collision conditions. In addition, an angular acceptance of about ± 12° was used after removing the angular selector in front of the ESA. The total experimental uncertainties for absolute values of the total cross sections were obtained by quadratic sum of the statistical deviations, determination of target thickness, and counting efficiency.

Figure 1. Translational energy-gain spectra for single-electron capture by 300 eV O³⁺ ions from He at different projectile laboratory scattering angles. Also shown are reaction windows calculated on the basis of a single-crossing LZ model (dotted curve) and the ECOB model (dashed curve). Smooth lines are drawn to guide the eye.

2. Results and discussion

2.1. O³⁺ + He collisions

Figure 1 shows the translational energy-gain spectra obtained for single-electron capture by 300 eV O³⁺ ions from He at different scattering angles. At 0° scattering angle, the energy-gain spectrum indicates that the dominant reaction channel is due to transfer excitation into the 2s2p 3 3P state of the product O²⁺ from the 2s²(1S)2p 3P ground state O³⁺ ions with contributions due to capture into the 2s2p 3 1D, 3S and 1P states. In a transfer-excitation process, which results from a two-electron process, a target electron is transferred to the projectile ion with simultaneous excitation of the projectile core. Such processes are also called core-varying single-electron capture (CVSEC) [4]. This channel is observed to be the dominant reaction over the entire collision energy region studied, in agreement with the measurements of Thompson et al [5] and Bangsgaard et al [6]. Besides the dominant channel, smaller contributions from capture into the 2s2p 3 3D, 3S and 1P states can also be identified.

As the scattering angle is increased, capture into the 2s2p 3 3P state remains dominant but the relative importance of single-electron capture into the 2s2p 3 1D, 3S and 1P states is strongly decreased. Figure 1 also shows our calculated reaction windows for 300 eV O³⁺ - He collisions, using both a
single-crossing Landau-Zener (LZ) model [7] and the extended version of the classical over-the-barrier (ECOB) model [8]. Calculated peak values have been normalized to our observed peak values in the energy spectrum. The reaction based on a single-crossing LZ model favors Q values smaller than those observed and is positioned near the 2s2p $^3$D state, while the reaction window based on the ECOB model maximizes at about 11 eV and accommodates most of the dominant channel.

**Figure 2.** Translational energy-gain spectra for single-electron capture by O$^{3+}$ ions from H$_2$O and CO$_2$ at 0$^\circ$ scattering angles. Also shown are reaction windows calculated on the basis of single-crossing LZ model (dotted curve) and the ECOB model (dashed curve). Smooth lines are drawn to guide the eye.

### 2.2. O$^{3+}$ + H$_2$O and CO$_2$ collisions

Figure 2 shows the translational energy-gain spectra for single-electron capture by 300 eV O$^{3+}$ ions from H$_2$O and CO$_2$ at 0$^\circ$ scattering angles. For the He$^{2+}$ + H$_2$O collisions, the spectrum shows only one broad peak; this peak correlates with nondissociative pure single-electron capture into the 2p3p state of O$^{2+}$ ions with production of H$_2$O$^+$ in the ground state (X $^2$B$_1$). There is some contribution from an unresolved reaction at about 9 eV, involving capture into the 2p3s state of O$^{2+}$. The reaction windows coincide very well with the position of dominant channel and underestimate the contribution of the 2p3s channel.

In O$^{3+}$ - CO$_2$ collisions, the observed collision spectrum is dominated by a peak due to capture into the 2p3s state of O$^{2+}$ product ions with production of CO$_2^+$ in the ground state ($^1$A$^g$). The structure on the lower-energy side of the dominant peak corresponds to capture into 2p3p states. The reaction windows favor Q values smaller than the observed channel.

### 2.3. Total cross sections

The measured total cross sections for single-electron capture by O$^{3+}$ ions from He, H$_2$O and CO$_2$ are shown in Fig. 3 together with other available measurements and MCLZ calculations. For O$^{3+}$ - He collisions, our results are in reasonably good agreement with the experimental results of Bangsgaard *et al.* [6] and Ishii *et al.* [9] and show similar behavior. However, our data are considerably higher than the recommended cross sections of Janev *et al.* [10] and found to be 60% higher than the multi-channel Landau-Zener calculations [6], based on the Taulberg expression for the coupling matrix $H_{12}$ [11]. For O$^{3+}$ + H$_2$O and CO$_2$ collisions, the total cross sections exhibit weak energy dependence and they are almost constant with increasing impact energy, a behavior that is attributed to availability of many reaction channels that are situated nearly at the center of the reaction window. For O$^{3+}$ + H$_2$O collisions, the energy dependence of cross sections is in direct contradiction with the MCLZ calculation, which decreases with increasing energy. For O$^{3+}$ + CO$_2$ collisions, The MCLZ results are at least a factor of 2 smaller than the experimental results and show the same energy dependence.
In summary, doubly differential cross sections, in energy and angle, for single-electron capture by O\(^{3+}\) ions from He, H\(_2\)O, and CO\(_2\) have been studied by means of translational energy gain spectroscopy at collision energies between 0.3 and 1.2 keV. Translational energy gain spectra for single-electron capture by O\(^{3+}\) ions from He indicated that dominant reaction channel was correlated with transfer excitation into the 2s2p\(^{3}3P\) state, while for the H\(_2\)O, and CO\(_2\) targets the dominant channels were due to capture into 2p3p and 2p3s states respectively. The energy-gain spectra were interpreted qualitatively in terms of the reaction windows, which were calculated using the single-crossing LZ model and the ECOB model. The reaction windows provide the best description of the observed spectra for all collision systems. However, for O\(^{3+}\)-He collision system, the reaction window based on a single-crossing LZ model did not describe the position of dominant processes, probably because they involve core-varying transitions. In these collision systems, no clear evidence of molecular dissociation was observed. The energy dependence of the absolute total cross sections of the present work were compared with the available data and the theoretical calculations based on the MCLZ model. No data on single-electron capture by O\(^{3+}\) ions from H\(_2\)O, and CO\(_2\) are, however, available for comparison.

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![Figure 3. Total cross sections for single-electron capture by O\(^{3+}\) ions from He, H\(_2\)O and CO\(_2\). •, present work; □, Ishii *et al* [9]; △, Bangsgaard *et al* [6]; ▽, Janev *et al* [10]; solid line, MCLZ calculations.](image)