Differential cross sections for single-electron capture by low-energy \( \text{O}_2^{2+} \) ions from Ne and \( \text{O}_2 \)

E Y Kamber

Physics Department, Western Michigan University, Kalamazoo, MI 49008-5252, USA
E-mail: emanuel.kamber@wmich.edu

Abstract. State-selective differential cross sections for single-electron capture processes in low-energy collisions of \( \text{O}_2^{2+} \) recoil ions with Ne and \( \text{O}_2 \) at impact energy of 100 eV and scattering angles between 0° and 6° have been studied using a differential energy-gain spectrometer. In all of the collision systems studied here, contributions from processes commencing with long-lived metastable states in the incident \( \text{O}_2^{2+} \) ion beam are detected. The energy-gain spectra are interpreted qualitatively in terms of the reaction windows, which are calculated using the Landau-Zener model and the extended version of the classical over-the-barrier model.

1. Introduction

A large variety of molecular ions have been identified in cold astrophysical environments and in planetary atmospheres. Molecular oxygen ions are of particular interest due to their potential influence on the properties of the ionosphere and their involvement in many atmospheric phenomena. Furthermore, electron capture involving multiply charged molecular ions has been proposed as a mechanism for generating ions in the earth’s upper atmosphere [1,2].

Most doubly-charged molecules are not stable because the Coulomb repulsion energy between the positive holes exceeds the molecular binding energy. Only a few highly bound covalent molecules have been found, for example, \( \text{N}_2^{2+}, \text{O}_2^{2+}, \text{NO}^{2+}, \text{CO}^{2+}, \text{CO}_2^{2+} \) and \( \text{NH}_3^{2+} \), whose lifetimes may depend on the ionization method [1]. Recently we have extended our study of ion-atom collisions to include single-electron capture by \( \text{N}_2^{2+} \) and \( \text{CF}_2^{2+} \) ions from atomic and molecular targets by means of translational energy spectroscopy [3,4].

In the present work, a differential energy-gain spectrometer [5], 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 non-dissociative single-electron capture in collisions of \( \text{O}_2^{2+} \) recoil ions with Ne and \( \text{O}_2 \) at an impact energy 100 eV and scattering angles between 0° and 6°.

Unfortunately, the peak of doubly charged molecular ion \( \text{O}_2^{2+} \) coincides with the atomic ion \( \text{O}^+ \) peak in mass spectrum at \( m/q=16 \). No attempt was made to estimate the fraction of \( \text{O}_2^{2+} \) in the \( \text{O}^+ \) beam. However, we were able to easily separate the \( \text{O}_2^{2+} \) products resulting from electron capture by using an electrostatic analyzer (ESA) voltage which was double that required to transmit the elastically scattered ion beam. To identify the reaction channels involved, the energy-gain spectrum for \( \text{N}_2^{2+} \)- Ne collision system that were previously observed in the same apparatus [3], were used as a standard to calibrate the energy scale (i.e., Q scale). The energy levels for \( \text{O}_2^{2+} \) and \( \text{O}_2^{+} \) ions used in calculating the
The energy defect of the reaction were taken from photoelectron spectroscopy data [6] and other sources [7-9]. The energies were calculated assuming that the projectile, molecular target, and their product ions are at the lowest vibrational level ($\nu = 0$) and calculated on the basis of the Franck-Condon principle, i.e. the ionization energies are those for vertical processes.

Following the nomenclature described by Kamber et al. [10], the observed reaction channels are denoted in the following fashion: the designations I, II, and III represent, respectively, the ground, first, and second electronically excited states of O$_2^+$; $\alpha$, $\beta$, $\gamma$, represent the ground and subsequent electronically excited states of O$_2^+$; $X$, represents the ground state of the target product.

2. Results and discussion

2.1. O$_2^{2+}$ + Ne collisions. Figure 1 shows the translational energy-gain spectra obtained for single-electron capture by 100 eV O$_2^{2+}$ ions from Ne at different scattering angles. At 0° scattering angle, the energy-gain spectrum indicates that the dominant reaction channel is due to non-dissociative single-electron capture into the ground state (X $^2\Pi_g$) of the product O$_2^+$ from the ground state incident O$_2^{2+}$ (X $^1\Sigma_g^+$) ions with contributions due to capture from the low-lying metastable state (A $^3\Pi_u$) of the O$_2^{2+}$ into the (A $^2\Pi_u$) state of O$_2^+$. There are smaller contributions due to capture into the a $^4\Pi_u$, A $^3\Pi_u$, and b $^4\Sigma_g^-$ states from the metastable states W $^3\Delta_u$, B $^3\Pi_u$, and B$'$ $^3\Sigma_g^-$ of the O$_2^{2+}$ ions via reaction channels II$\beta$X, III$\gamma$X, III$\beta$X, VI$\delta$X, IV$\gamma$X, IV$\beta$X, and V$\beta$X. A comparison with the measurements of Pederson [11] at 100 eV, and Hamdan and Brenton [12] at 6 keV shows good agreement with the present measurements.

As the scattering angle is increased, capture into the X $^2\Pi_g$ state (the IaX channel) remains dominant but contributions from reaction channels II$\beta$X, III$\gamma$X, and VI$\delta$X, respectively, due to capture from the metastable states W $^3\Delta_u$ and B$'$ $^3\Sigma_g^-$ of the O$_2^{2+}$ ions into the a $^4\Pi_u$, A $^3\Pi_u$, and b $^4\Sigma_g^-$ states of O$_2^+$, increase with increasing the scattering angles. This indicates that the angular distribution for the IaX channel is more strongly peaked in the forward direction than for the reaction channels II$\beta$X, III$\gamma$X, and VI$\delta$X. Figure 1 also shows our calculated reaction windows for 100 eV O$_2^{2+}$ - Ne collisions, using both a single-crossing Landau-Zener (LZ) model [13] and the extended version of the classical over-the-barrier (ECOB) model [14]. Calculated peak values have been normalized to our observed peak values in the energy spectrum. The reaction based on a single-crossing LZ model does not describe the position of the dominant reaction channel, while the reaction window based on the ECOB model maximizes at about 6 eV and underestimates the contribution of the IaX channel.
2.2. \( \text{O}_2^{2+} + \text{O}_2 \) collisions.

Figure 2 shows the translational energy-gain spectra for single-electron capture by 100 eV \( \text{O}_2^{2+} \) ions from \( \text{O}_2 \) at different projectile laboratory scattering angles. The observed spectra clearly indicate that non-dissociative single-electron capture into the \( \text{O}_2^+ \) (\( ^4\Sigma_u \)) state from the low-lying metastable state (\( \text{A}^{3}\Sigma_u \)) of the \( \text{O}_2^{2+} \) is the predominant channel, although capture by the ground state (\( \text{X}^{1}\Sigma_g \)) of \( \text{O}_2^{2+} \) ions into \( ^4\Sigma_g \) and \( ^2\Sigma_g \) states are also significant. As the scattering angle is increased, a relative shift of about 0.45 eV in the energy gain of the II\( \zeta \)X channel is observed going from scattering angle of 0º to 6.71º. This is attributed to the energy given to the target and is in accordance with energy and momentum conservation rules. In addition, the shift in the energy-gain of the dominant peak could be also due to the increasing contributions from the reaction channel I\( \epsilon \)X as the scattering angle is increased. The reaction windows favor Q values smaller than those observed and are positioned near the IeX channel.

2.3. Differential cross sections

The experimental total differential cross sections (d\( \sigma \)/d\( \Omega \)) for single-electron capture by 100 eV \( \text{O}_2^{2+} \) ions from Ne and \( \text{O}_2 \) are shown in Figure 3. The differential cross sections were determined using the translational energy-gain technique, by calculating the area under the peaks in the energy-gain spectra at different projectile laboratory scattering angles using a curve fitting program. The general features of the distributions are qualitatively explained in terms of semi-classical model based on Coulomb potential curves which have been described in detail by Andersson et al. [15]. The traditional two-state model has been used to estimate the critical angle \( \theta_c \), which corresponds to capture at an impact parameter equal to the crossing radius, by assuming that capture occurs at a localized curve crossing between the potential energy curves for entrance and exit channels. For small angles, \( \theta_c = Q/2E \), where Q is the exoergicity of the collision and E is the collision energy. This angle separates the events scattered at smaller angles due to capture on the way-out of the collision and events scattered at larger angles due to capture on the way-into the collision.

For \( \text{O}_2^{2+} - \text{O}_2 \) collisions, the distribution is peaked in the forward direction inside the critical angle \( \theta_c = 1.32^\circ \), which corresponds to the II\( \zeta \)X capture channel. This distribution represents contributions from electron capture that takes place on the way-out of the collisions. For \( \text{O}_2^{2+} - \text{Ne} \) collisions, the measurements show that the projectile products which correlate with capture into the (X \( ^5\Pi_g \)) state are distributed forward inside the critical angle \( \theta_c = 0.8^\circ \), indicating that capture takes place on the way-out of the collision.
In summary, doubly differential cross sections, in energy and angle, for single-electron capture by 100 eV O$_2^{2+}$ ions from Ne and O$_2$ have been studied by means of translational energy gain spectroscopy. Translational energy gain spectra for single-electron capture by O$_2^{2+}$ ions from Ne indicated that dominant reaction channel was correlated with capture into the (X $^2\Pi_g$) state, while for the O$_2$ the dominant channel was due to capture into the O$_2^+$ (c $^4\Sigma_u$) state from the low-lying metastable state (A $^3\Sigma_u$) of the O$_2^{2+}$. 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 did not describe the position of dominant processes. We have also studied differential cross sections for single-electron capture processes, the angular distribution spectra contain a mean peak lying just inside a critical angle $\theta_c$, corresponding to capture at an impact parameter equal to the crossing radius of the dominant reaction channels. The peaks are qualitatively explained by a two-state model and are attributed to a capture process on the way-out from the collision. No data on single-electron capture by O$_2^{2+}$ ions from O$_2$ are, however, available for comparison.

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