Volume 3, Number 1, 2010. pp. 9-15

Jordan Journal of Physics

ARTICLE

Non-Dissociative Single-Electron Capture Studied for O_2^{2+} Ions on Ar, N_2 and He at 100 eV

Osama A. Abu-Haija

Applied Physics Department, Tafila Technical University, P. O. Box 179, Zip Code 66110, Tafila-Jordan.

Received on: 15/2/2010; Accepted on: 13/5/2010

Abstract: Energy-gain spectra for single-electron capture by O_2^{2+} ions colliding with Ar, He and N_2 have been measured at an impact energy of 100 eV and 0º scattering angle by means of translational energy-gain spectroscopy. In O_2^{2+} - Ar and N_2 collisions, only one peak is observed at the energy-gain around 3.5 eV, which is correlated with non-dissociative single-electron capture from ground state ($X\ ^1\Sigma_g^+$) of O_2^{2+} ions into the $A\ ^2\Pi_u$ state of O_2^+. However, for the O_2^{2+} - He collision system, the dominant channels are due to capture into the ground state $X\ ^2\Pi_g$ of O_2^+ from $W\ ^3\Delta_u$, $B\ ^3\Pi_g$ and $B/\ ^3\Sigma_u^-$ metastable states of the O_2^{2+}, respectively. A reasonable description of the dominant final states is obtained qualitatively in terms of the reaction windows, which are calculated using the Landau-Zener (LZ) model and the extended version of the classical over-the-barrier (ECOB) model. Differential cross sections for single-electron capture by 100 eV O_2^{2+} ions from Ar have also been measured. The results are quantitatively explained by semi-classical model based on Coulomb potential energy curves.

Keywords: Single-electron capture; Non-dissociative electron capture; Reaction window.

Introduction

Experimental and theoretical investigations of electron capture processes occurring in collisions between doubly charged molecular ions and atomic/molecular targets have recently received considerable attention. The need to understand ion-atom/molecule collision processes is important in a number of applications, such as: material science, plasma science -where low temperature plasmas play a key role in determining characteristics of target materials and of plasma behavior- and astrophysics. Also, atmospheric molecular ions (O_2^+, N_2^+, CO^+ and CO_2^+) are important constituents of the earth's upper atmosphere. Information on mechanisms responsible for their excitation is crucial to a complete understanding of atmospheric phenomena [1-4]. Single-electron capture by doubly charged molecular ion O_2^{2+} from atomic targets has been studied previously in the keV region [5]. However, in the case of molecular targets, the only experimental measurement at low-energy collisions has been recently made by Kamber [6]. In his work, the translational energy-gain spectroscopy technique has been used to measure the energy gain spectra of 100 eV O_2^{2+} ions with O_2 and Ne at different scattering angles.

Presented herein are energy-gain spectra for state-selective non-dissociative single-electron capture in collisions of O_2^{2+} recoil ions with N_2, Ar and He targets at a laboratory impact energy of 100 eV and 0^o scattering angle.

The present measurements were performed on a differential energy

Corresponding Author: O. Abu-Haija. **Email**: oabuhaija@ttu.edu.jo

spectrometer, which has been fully described previously [7]. Briefly, doubly molecular oxygen ions were produced in a recoil ion source from oxygen molecules by using 25 MeV F^{4+} ions from the Western Michigan University tandem Van de Graaff accelerator as a pump beam. After being mass analyzed by a 180^o double-focusing magnet, the ions were guided with the aid of horizontal and vertical parallel deflection plates into the entrance of a gas cell containing a low-pressure target gas. The projectile ions that had undergone capture were energy analyzed by means of a 90^o double-focusing electrostatic analyzer (ESA). These ions were scattered through a nominal angle θ into a solid angle ($\Delta\Omega$) of about 3 x 10^{-3} sr. The scattering angle θ is selected by means of an aperture located in front of the ESA. The analyzed ions were then detected by a one-dimensional position sensitive channel-plate detector located at the focal plane of the ESA.

Results and Discussion

When doubly charged molecular oxygen ions collide with atomic/molecular targets, a variety of reaction channels is possible through which electron capture may take place. Non-dissociative single-electron capture has been found the most probable event as a result of low-energy ion-atom/molecule collisions. This process of charge transfer, by which an electron from a neutral target is captured to a doubly charged ion, can be presented by the expression:

$$O_2^{2+} + X \rightarrow O_2^{+} + X^{+} + Q, \quad (1)$$

where Q is the energy gained by the projectile ion during the collision. In classical two-body dynamics, the energy gained by the projectile ion during a collision can be expressed as the difference between the final kinetic energy E_f of the scattered projectile ion and the initial kinetic energy E_0 of the incident projectile ion, $Q = E_f - E_0$. However, the relationship of the energy gain Q to the energy defect ΔE, which is defined as the difference in the binding energies of the collision products, is found to be [8]:

$$Q = \Delta E - \Delta K \quad (2)$$

where ΔK, defined below, is the translational energy given to the target and ΔE is calculated from spectroscopic data according to the following formula:

$$\Delta E = I_p(O_2^{+}) - I_p(X) - E_x, \quad (3)$$

where $I_p(O_2^{+})$ and $I_p(X)$ are, respectively, the ionization energies of the projectile product ion (O_2^{+}) and the target atom/molecule X, with the target atom/molecule being assumed to be in its ground electronic state and the captured electron being in the most loosely bound orbital and E_x is the excitation energy of the x^{th} level of the projectile product ion (O_2^{+}) or the target product ion X^{+}. The general expression of the translational energy ΔK given to the target is given by [9]:

$$\Delta K = \left.\begin{aligned} &\frac{M}{M+m}\left(1-\cos\theta\right)\left[\frac{2mE_0}{M+m} - \Delta E\right] \\ &+ \frac{M\left(\Delta E\right)^2}{4mE_0}\cos\theta \end{aligned}\right\}, \quad (4)$$

where M and m are, respectively, the projectile and target masses, E_0 is the laboratory translational energy of the projectile and θ is the laboratory scattering angle of the projectile. It should be pointed out that for these collision systems, the calculated values of ΔK are very small and can be neglected, giving $Q = \Delta E$. Therefore, the energy spectra are expressed in terms of the Q values. The energy levels for O_2^{2+} and O_2^{+} ions used in calculating the energy defect of the reaction were taken from published tables [10-14].

The reaction channels observed in the measured energy gain spectra have been labeled according to the notation previously described by Kamber et al. [15]. The designations I, II and III represent, respectively, the ground, first and second electronically excited states of O_2^{2+}; α, β and γ represent the ground and subsequent electronically excited states of O_2^{+} ion; X represents the ground state of the target product (see Table 1). In the following sections, the results for single-electron capture processes in collisions of O_2^{2+} ions with Ar, N_2 and He are presented and discussed.

TABLE 1. Description and nomenclature of O_2 ionic states and ionized target states.

Projectile O_2^{2+}		O_2^+ Products		Target Products	
State	Symbol	State	Symbol	State	Symbol
$X\ ^1\Sigma_g^+$	I	$X\ ^2\Pi_g$	α	$Ar^+ (3p^5\ ^2P^o_{3/2})$	X
$A\ ^3\Sigma_u^+$	II	$a\ ^4\Pi_u$	β	$Ar^+ (3p^6\ ^2S_{1/2})$	A
$W\ ^3\Delta_u$	III	$A\ ^2\Pi_u$	γ	$N_2^+ (^2\Sigma_g^+)$	X
$B\ ^3\Pi_g$	IV	$b\ ^4\Sigma_g^-$	δ	$N_2^+ (^2\Pi_u)$	A
$B/\ ^3\Sigma_u^-$	V	$B\ ^2\Sigma_g^-$	ε	$He^+ (1s\ ^2S_{1/2})$	X
$1\ ^3\Delta_g$	VI	$C\ ^4\Sigma_u^-$	ζ	$He^+ (2p)$	A

Sources: [10-14].

I. O_2^{2+} + Ar Collisions

Fig. 1 shows the translational energy-gain spectra obtained for single-electron capture by 100 eV O_2^{2+} ions from Ar at different scattering angles. At 0^o scattering angle, only one peak is clearly seen at energy-gain around 3.5 eV. This peak is correlated with non-dissociative single-electron capture reaction channel from the ground state of ($X\ ^1\Sigma_g^+$) of O_2^{2+} ions into the $A\ ^2\Pi_u$ state of O_2^+. There are smaller contributions due to capture into the $B\ ^2\Sigma_g^-$ and $b\ ^4\Sigma_g^-$ states of O_2^+ from the low-lying metastable state $A\ ^3\Sigma_u^-$ of the O_2^{2+} ions via reaction channels IIεX and IIδX. It is of interest to compare our data with the earlier spectrum of Hamdan and Brenton [5]. The spectrum was measured at O_2^{2+} incident energy of 6 keV. Their measurements disagree with the present results for which the dominant peak was observed to be due to electron capture by O_2^{2+} ($A\ ^3\Sigma_u^+$) excited state. This is attributed to the high collision energy they used in their measurements, since the reaction window depends modestly on the collision energy.

As the scattering angle is increased, the IγX channel remains dominant and contributions from reaction channel IIεX and IIδX remain the same with increasing the scattering angle. At a scattering angle of 1.87º, peak IγX is observed to be shifted toward a larger Q-value due to the populations of different vibrational states of the $A\ ^2\Pi_u$ state of O_2^+. The amount of the energy given to the target in this collision system is very small (less than 0.1 eV, see equation (4)). Also shown are our calculated reaction windows, the range of Q values where the probability for single-electron capture is large, using both a single-crossing Landau-Zener (LZ) model [16-18] and the extended version of the classical over-the-barrier (ECOB) model [19]. Calculated peak values have been normalized to our observed peak values in the energy spectrum. The reaction window based on a single-crossing LZ model predicts the IγX channel to be the dominant process, since its Q value lies very close to the maximum of the reaction window. The reaction window based on a single-crossing ECOB model accommodates the IγX channel and favors larger Q values compared to the dominant channel.

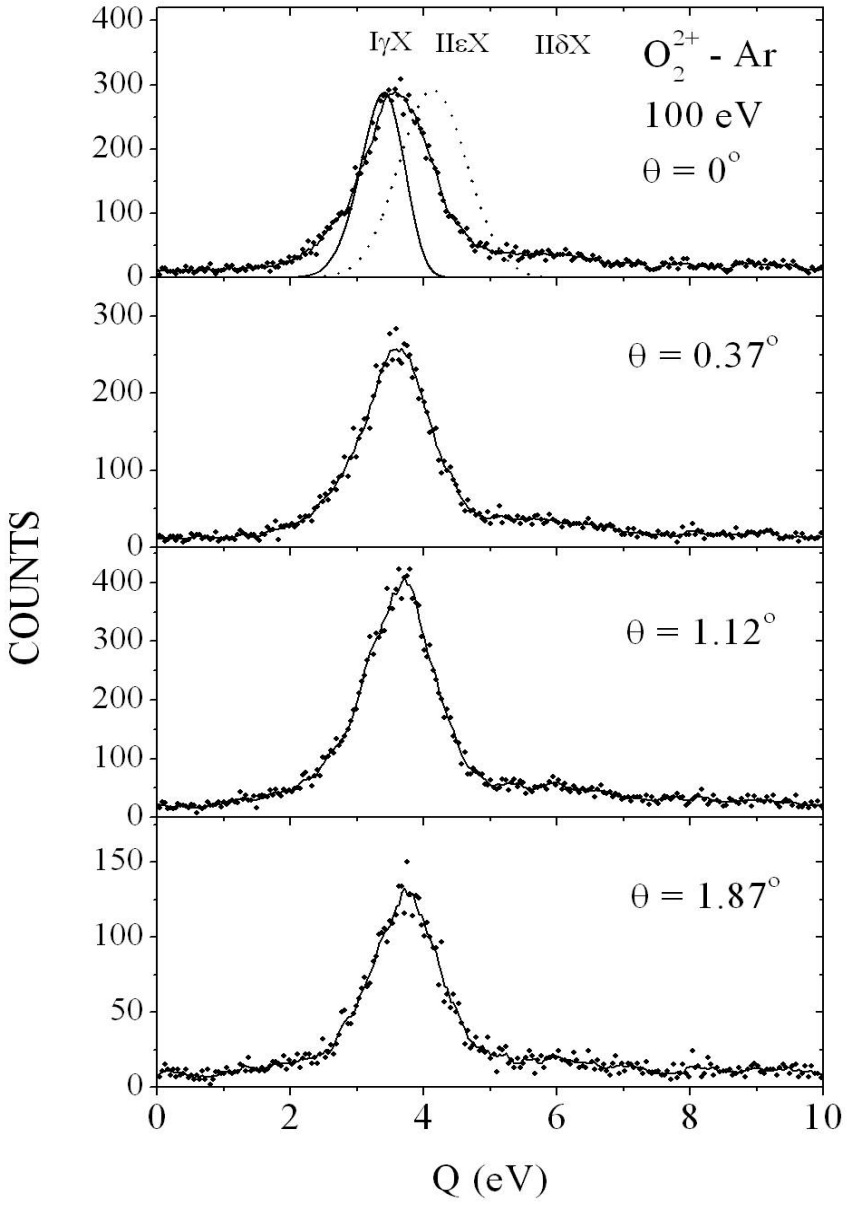

FIG. 1. Translational energy-gain spectra for single-electron capture by 100 eV O_2^{2+} ions from Ar at different projectile laboratory scattering angles. Also shown are reaction windows calculated on the basis of a single-crossing LZ model (full curve) and the ECOB model (dashed curve). Smooth lines are drawn to guide the eye.

The experimental differential cross sections ($d\sigma/d\Omega$) for single-electron capture by 100 eV O_2^{2+} ions from Ar were found using the translational energy-gain technique, by calculating the area under the peaks (total intensity) in the energy-gain spectra at different projectile laboratory scattering angles using curve fitting program. The general features of the distributions are qualitatively explained in terms of a semi-classical model based on Coulomb potential curves [20]. The traditional two-state model has been used to estimate the critical angle θ_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 laboratory scattering angles, $\theta_c = Q/2E_0$, where Q is the exoergicity of the collision and E_0 is the laboratory impact energy. This angle separates the events scattered at smaller angles due to capture on the way-out and events scattered at larger angles due to capture on the way-into the collision. The experimental differential cross sections and the theoretical calculations folded with the

experimental resolution are shown in Fig. 2. The value of the largest calculated cross section has been normalized to the experimental value of the peak observed in the spectrum. The calculation is performed assuming that capture through IγX channel is the only dominant reaction channel with the IIεX channel strongly promoting the entrance channel. The experimental data show a forward peak inside the critical angle θ_c = 1.01°, which corresponds to the IγX capture channel. The forward peak clearly represents contributions from electron capture that takes place on the way-out of the collision. The calculated distribution shows a peak lying near θ_c and underestimates the contribution from capture on the way-out of the collision.

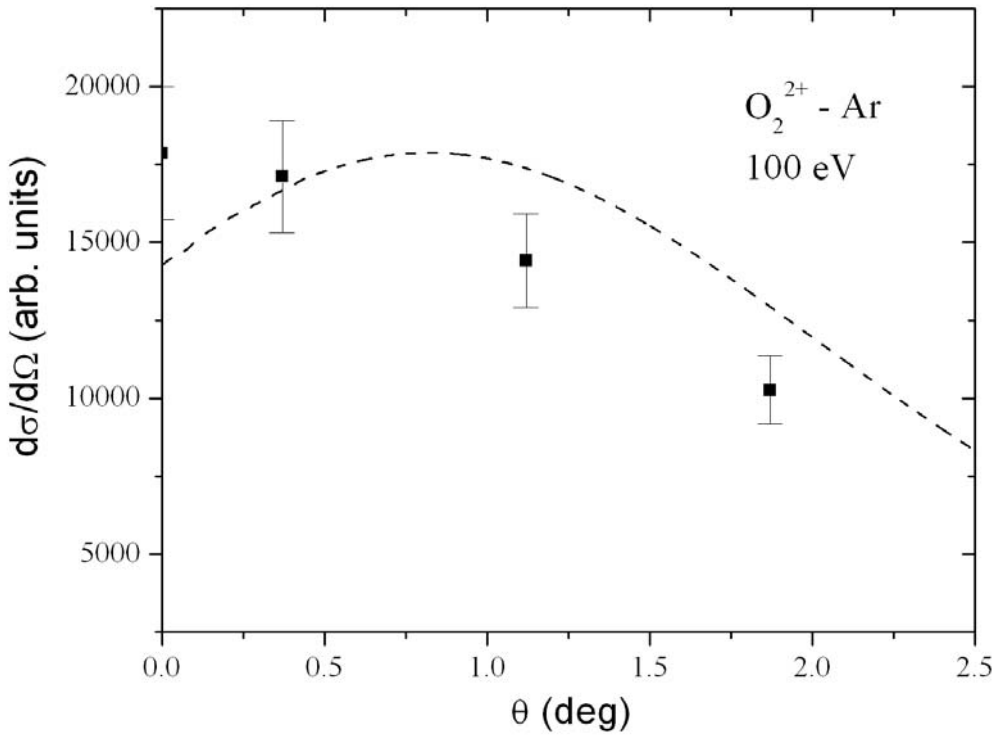

FIG. 2. Experimental and calculated differential cross sections (dσ/dΩ) for single-electron capture by 100 eV O_2^{2+} ions from Ar. ■, present results; the broken curve is the theoretical calculation folded with experimental resolution.

II. O_2^{2+} + N_2 Collisions

Fig. 3 shows the translational energy-gain spectrum obtained for single-electron capture by O_2^{2+} ions from N_2 at zero-degree scattering angle. The shape and the peak position are almost the same as those for the Ar target. The peak in the spectrum is due to the non-dissociative single-electron capture from the ground state of ($X\ ^1\Sigma_g^+$) of incident ions into the $A\ ^2\Pi_u$ state of O_2^+. The reaction channel IγX is positioned near the center of the reaction windows based on the ECOB model and LZ model. Both reaction windows accommodate most of the observed features in the spectrum.

III. O_2^{2+} + He Collisions

Fig. 4 shows the translational energy-gain spectrum for the formation of O_2^+ ions from the reaction of 100 eV O_2^{2+} ions with He at zero-degree projectile scattering angle. The spectrum shows only one peak centered at about 5.8 eV. This peak correlates with non-dissociative single-electron capture into the ground state $X\ ^2\Pi_g$ of O_2^+ from $W\ ^3\Delta_u$, $B\ ^3\Pi_g$ and $B'\ ^3\Sigma_u^-$ metastable states of the O_2^{2+}, respectively. Again, the comparison with the results of Hamdan and Brenton [5] at 6 keV impact energy shows good agreement with the present measurements. The reaction window based on a single-crossing LZ model favors Q values smaller than those observed and is positioned near the dominant reaction channel IIαX, while the reaction window based on the ECOB model provides the best description of the observed spectrum.

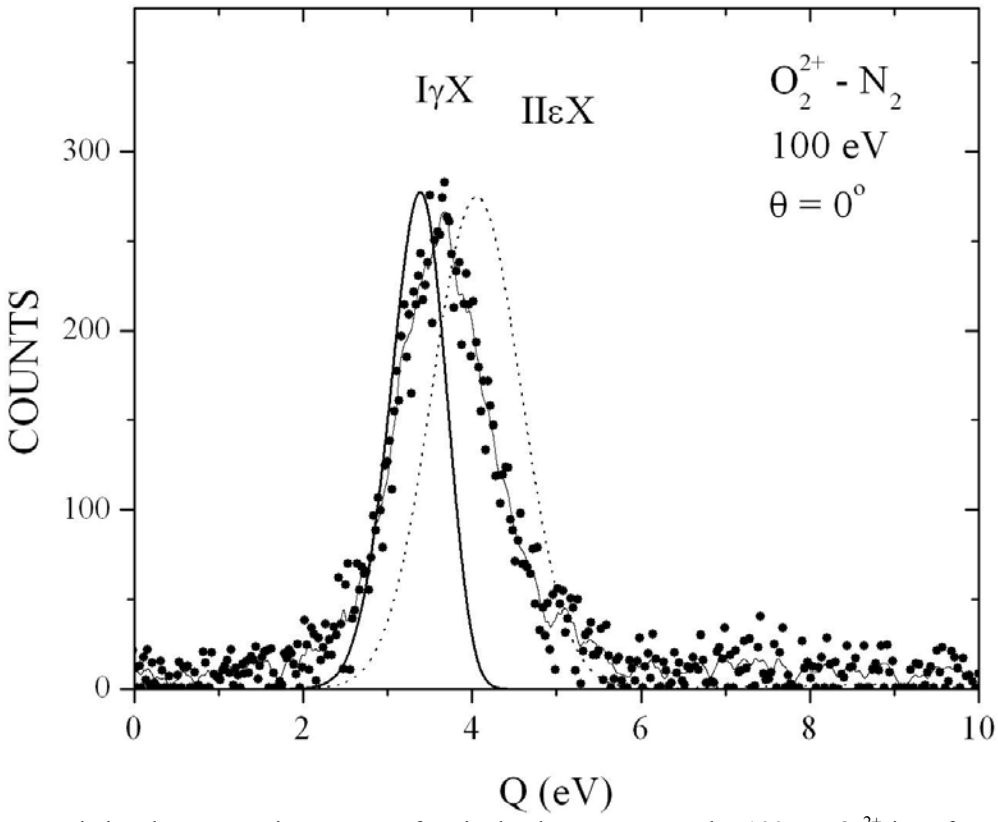

FIG. 3. Translational energy-gain spectrum for single-electron capture by 100 eV O_2^{2+} ions from N_2 at zero-degree projectile laboratory scattering angle. Also shown are reaction windows calculated on the basis of LZ model (full curve) and the ECOB model (dashed curve). Smooth line is drawn to guide the eye.

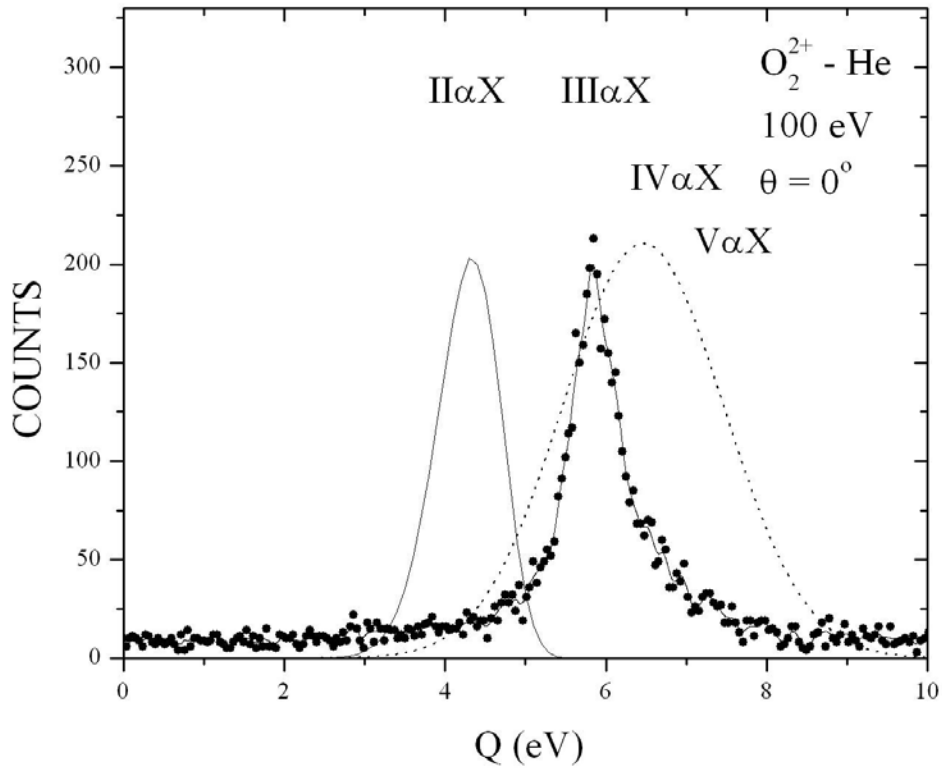

FIG. 4. Translational energy-gain spectrum for single-electron capture by 100 eV O_2^{2+} ions from He at zero-degree projectile laboratory scattering angle. Also shown are reaction windows calculated on the basis of LZ model (full curve) and the ECOB model (dashed curve). Smooth line is drawn to guide the eye.

It is interesting to note that the Q-scale distribution of translational energy gain for single-electron capture by 100 eV O_2^{2+} ions from Ar and N_2 appear Gaussian whereas the distribution from He is Pearson or Lorentzian in shape. This is probably due to the fact that for Ar or N_2, only one reaction channel contributes to the capture process, while for the He target, more than one channel contribute to the capture process.

Conclusion

The main objective of the present investigation has been to study single-electron capture in low-energy collisions of O_2^{2+} ions with Ar, N_2 and He by means of translational energy-gain spectroscopy. Translational energy-gain spectra for single-electron capture by O_2^{2+} ions from Ar and N_2 indicated that the dominant reaction channels were correlated with non-dissociative single-electron capture from the ground state ($X\ ^1\Sigma_g^+$) of O_2^{2+} ions into the $A\ ^2\Pi_u$ state of O_2^+, while for He target the dominant channel is due to capture into the ground state $X\ ^2\Pi_g$ of O_2^+ from $W\ ^3\Delta_u$, $B\ ^3\Pi_g$ and $B'\ ^3\Sigma_u^-$ metastable states of the O_2^{2+}, respectively. The energy-gain spectra were interpreted qualitatively in terms of the reaction windows, which are calculated using the single-crossing LZ model and the ECOB model. The reaction windows based on the ECOB model provide the best description of the observed spectra.

Acknowledgements

The author wishes to express his gratitude for the kind hospitality extended to him during his stay (summer 2009) at Western Michigan University, where this work was performed. I am indebted to Prof. E.Y. Kamber (Western Michigan University) for many fruitful discussions and friendly assistance. This work was supported in part by a research grant Tafila Technical University.

References

[1]Mathur, D., Phys. Rep. 225 (1993) 193.

[2]Cravens, T.E., Geophys. Res. Lett. 24 (1997) 105.

[3]Wargelin, J.B. and Dark, J.J., Astrophys. J. 546 (2001) L57.

[4]Pequignot, D., Astronomy and Astrophysics, 81 (1980) 356.

[5]Hamdan, M. and Brenton, A.G., Chem. Phys. Lett. 164 (1989) 413.

[6]Kamber, E.Y., Journal of Physics: Conference Series 163 (2009) 012066.

[7]Yaltkaya, S., Kamber, E.Y. and Ferguson, S.M., Phys. Rev. A, 48 (1993) 382.

[8]Kamber, E.Y. and Cocke, C.L., Springer Series in Chemical Physics, 54 (1991) 91.

[9]Cooks, R.G., "Collision Spectroscopy", (Plenum Press, New York, 1978).

[10]Turner, D.W., Baker, A.D., Baker, C. and Brundle, C.R., "Molecular Photoelectron Spectroscopy", (Wiley, London, 1970).

[11]WWW homepage of the NIST Atomic Spectra Database (http://physics.nist.gov/).

[12]Leputsch, P., Dumitriu, F., Aumayr, F. and Winter, H.P., J. Phys. B, 30 (1997) 5009.

[13]Wetmore, R.W. and Boyd, R.K., J. Chem. Phys. 90 (1986) 5540.

[14]Koslowski, H.R., Lebius, H., Staemmier, V., Wiesemann, K. and Huber, B.A., J. Phys. B, 24 (1991) 5023.

[15]Kamber, E.Y., Mathur, D. and Hasted, J.B., J. Phys. B, 16 (1982) 3025.

[16]Landau, L.D., Phys. Z. Sowjetunion, 2 (1932) 46.

[17]Zener, C., Proc. R. Soc. London Ser. A, 137 (1932) 696.

[18]Oslon, R.E. and Salop, A., Phys. Rev. A, 14 (1976) 579.

[19]Niehaus, A., J. Phys. B, 19 (1986) 2925.

[20]Anderson, L.R., Danared, H. and Barany, A., Nucl. Instrum. Meth. Phys. B, 23 (1987) 54.