

Available online at www.sciencedirect.com





International Journal of Mass Spectrometry 248 (2006) 25–28

www.elsevier.com/locate/ijms

Short communication

# Formation of  $O^{2+}$  in collisions between  $O^+$  ions and  $N_2$  molecules

H. Martinez a, F.B. Yousif <sup>b</sup>*,*<sup>∗</sup>

<sup>a</sup> Centro de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, Morelos, *P.O. Box 48-3, 62251, Cuernavaca, Morelos, Mexico*

<sup>b</sup> *Facultad de Ciencias, Universidad Aut ´onoma del Estado de Morelos, Avenida. Universidad 1001, 62210, Cuernavaca, Morelos, Mexico*

Received 29 September 2005; received in revised form 25 October 2005; accepted 25 October 2005

Available online 28 November 2005

# **Abstract**

We report measurements of the total and absolute differential electron loss cross sections of 2.0–5.0 keV O<sup>+</sup> ions in collisions by N<sub>2</sub> target at scattering angles between  $-3.2° \le \theta \le 3.2°$  in the laboratory frame. The behavior of the absolute differential cross sections display an expected decreasing behavior with increasing angle. The measured total electron loss cross section show a monotonically increasing behavior as a function of the incident kinetic energy and found to be within the order of magnitude between 10−<sup>19</sup> and 10−<sup>21</sup> cm2. © 2005 Elsevier B.V. All rights reserved.

*PACS:* 34.70.+e

*Keywords:* Electron loss; Ion–molecule collisions; Total cross section; Angular distribution

# **1. Introduction**

The importance of charge changing processes in keV atomic collisions is well established, and these reactions have been studied very extensively both experimentally and theoretically. The bulk of the prior work has, however, focused on the simplest processes and the most accessible collisions systems, while more technically formidable reactions, such as considered here, have received scant attention for the molecular target investigated in this work. The only measurements of electron loss cross sections of  $O^+$  with N<sub>2</sub> are those of Lo and Fite [\[1\]](#page-3-0) at collisional energies above 60 keV. Fogel' et al. [\[2\]](#page-3-0) considered the possibility of electron loss in reactions between  $O^+$  and  $N_2$  target, although their work was concerned in obtaining the equilibrium fractions for the neutral and charged products. Collisions between atomic ions and neutral atoms and molecules are of considerable importance and interest from a fundamental atomic physics point of view, equally,  $O^+$ –N<sub>2</sub> collisional processes are of importance to the field of aeronomy [\[3,5\]](#page-3-0) where  $O^+$  is the dominant ion in the *F* region of the atmosphere.

1387-3806/\$ – see front matter © 2005 Elsevier B.V. All rights reserved. doi:10.1016/j.ijms.2005.10.012

The lack of data at low-keV energies for electron loss processes limits our ability to determine the chemical processes in astrophysical plasmas and planetary objects.  $O^+$  ions are possibly present as one of the major magnetospheric ions (beside  $H^+$ , and  $N^+$ ) near the orbit of Titan [\[4\]](#page-3-0) and as  $N_2$  is the major species in Titan's atmosphere up to an altitude of 1700 km, therefore, in describing Titan's interaction with magnetospheric or solar wind ions, cross sections of  $O^+$  with N<sub>2</sub> as the target are important. The scattered  $O^{2+}$  ion, which is also of particular importance in ionosphere physics [\[6\], h](#page-3-0)as been studied with a large variety of spectroscopic methods, such as Auger electron spectroscopy [\[7\], d](#page-3-0)ouble charge transfer spectroscopy [\[8\],](#page-3-0) translational energy loss spectroscopy [\[9\],](#page-3-0) photoion–photoion coincidence spectroscopy [\[10\]](#page-3-0) [a](#page-3-0)nd photoelectron–photoelectron coincidence spectroscopy [\[11\].](#page-3-0) Although our experimental apparatus is incapable of resolving the different components of the  $O^+$  ions produced by electron bombardment (electron energy well above the threshold for excited ion production), and in light of the fact that in almost all the studies on state-selected  $O^+$ ions, in which metastable cross sections have been determined, at some level, most of these studies, involved attenuation curve technique, which it must be emphasized that it is not as precise as one would like. The use of such technique to derive total cross section is a matter of dispute [\[12\]](#page-3-0) due to elastic scattering issues as well as due neglect of second-order effects. All

<sup>∗</sup> Corresponding author. Tel.: +52 7773297020; fax: +52 7773297040. *E-mail address:* fbyousif@servm.fc.uaem.mx (F.B. Yousif).

that, plus the fact there is a complete lack of measured or calculated differential cross sections within the energies considered in this investigation, motivated the measurements reported in this work. Here, we report the measurements of the absolute differential and total electron loss cross section of the reaction  $O^+ + N_2 \rightarrow O^{2+} + \cdots$  in the energy range 2.0–5.0 keV.

## **2. Experimental apparatus**

The experimental apparatus and technique needed to generate the fast ion beam were recently reported [\[13\].](#page-3-0) Briefly, the  $O^+$  ions formed in an arc discharge source containing  $O_2$  gas (99.99% purity) at ion source pressures of 0.04–0.07 mTorr were accelerated to the desired energy and selected by a Wien velocity filter. The  $O^+$  ions were then allowed to pass through a series of collimators before entering the gas target cell, which was a cylinder of 2.5 cm in length and diameter, with a 1 mm entrance aperture, and a 2 mm wide, 6 mm long exit aperture. The target cell was located at the center of a rotatable, computer controlled vacuum chamber that moved the whole detector assembly, which was located 47 cm away from the target cell. A precision stepping motor ensured a high repeatability in the positioning of the chamber over a large series of measurements. The detector assembly consisted of a Harrower-type parallel-plate analyzer and two channel-electron multipliers (CEMs) attached to its exit ends. The O atoms passed straight through the analyzer. Separation of charged particles occurred inside the analyzer, which was set to detect the  $O^{2+}$  ions ( $I_f(\theta)$  particles per unit solid angle per second detected at a laboratory angle *θ* with respect to the incident beam direction with the lateral CEM. A retractable Faraday Cup was located 33 cm away from the target cell, allowing the measurement of the incoming  $O^+$  ion-beam current ( $I_0$  is the number of  $O<sup>+</sup>$  ions incident per second on the target). Under the thin target conditions used in this experiment, the differential cross sections for the  $O^{2+}$  formation were evaluated from the measured quantities by the expression:

$$
\frac{d\sigma(\theta)}{d(\Omega)} = \frac{I_f(\theta)}{I_0 n l} \tag{1}
$$

where *n* is the number of target atoms per unit volume (typically  $1.2 \times 10^{13}$  atoms/cm<sup>3</sup>) and *l* is the length of the scattering chamber ( $l = 2.5$  cm). The total cross section  $\sigma_{12}$  for the production of the  $O^{2+}$  particles was obtained by the numerical integration of d*σ/*d*<sup>Ω</sup>* over all angles measured. For *<sup>θ</sup>* <sup>≥</sup> *θm*, the differential cross sections vanish. Care was taken when the absolute differential cross section was measured. The reported value of the angular distribution was obtained by measuring it with and without gas in the target cell with the same steady beam in order to eliminate the counting rate due to ionization of the  $O^+$  beam on the slits and those arising from background distributions. The estimated rms error is 15%, while the total cross sections were reproducible to within 15% from day to day. Several sources of systematic errors are present and have been discussed in a previous paper [\[13\]. T](#page-3-0)he absolute error of the reported cross sections is believed to be less than 15%. This estimate accounts for both random and systematic errors.

#### **3. Results and discussion**

Various reaction channels may be involved in collisions of  $O^+$  ions with N<sub>2</sub>, some of which are

$$
O^{+} + N_{2} \rightarrow O^{2+} + \cdots
$$
  
\n
$$
O^{+} + N_{2} \rightarrow O + N_{2}^{+}
$$
  
\n
$$
O^{+} + N_{2} \rightarrow O^{+} + N_{2}^{+} + e, \text{ and } O^{+} + N_{2} \rightarrow O^{+} + N_{2}
$$

corresponding to projectile single electron loss (SEL), projectile electron capture, target ionization and elastic process respectively. Our present investigation is concerned with the first reaction channel (SEL).

Absolute differential cross sections (DCS's) data for SEL of  $O^+$  ions impinging on N<sub>2</sub> target have been obtained at laboratory angles  $-3.2° \le \theta \le 3.2°$  and collision energies  $2.0 \le E \le$ 5.0 keV. Our DCS's for SEL of  $O^+$  in N<sub>2</sub> at laboratory energies of 2.0, 3.0, 4.0 and 5.0 keV are shown in Fig. 1, with the error bars representing the reproducibility of the data. All the DCS's for all the energies show a decrease with increasing angle. The SEL data show slight structures in the DCS's, which tend to disappear as the incident energy decreases. The limitation of the present experimental apparatus do not permit the evaluation of the  $O^+$ composition ions as to the  ${}^{2}D$  and the  ${}^{2}P$  low lying excited states and the ratio of the metastable states to that of the ground state. The  ${}^{2}D$  and the  ${}^{2}P$  metastable states has been verified by numerous groups [\[14–18\]](#page-3-0) to compose the  $O^+$  ions with the <sup>4</sup>*S* ground state ions in most of the ion sources employed. Stebbings et al. [\[14\]](#page-3-0) employed an ion source similar to that used in this work. Their interpretation of the  $O^+$  attenuation curve led them to suggest that the ion beam was composed mainly of ground state  ${}^{4}S$  and metastable component  ${}^{2}D$ , subsequent researchers have often agreed with this interpretation. Nevertheless it should be noted that if both expected metastable components <sup>2</sup>*D* and  $^{2}P$  are present and have similar cross sections then they are indistinguishable. I index et al. [12] confirmed the results of indistinguishable. Lindsay et al. [\[12\]](#page-3-0) confirmed the results of



Fig. 1. Differential cross sections for single electron loss of  $O^+$  ions in N<sub>2</sub> molecular target.

Stebbings et al. [\[14\]](#page-3-0) and agreed also with the composition of the ion beam to be about 65% ground state and about 35% that of metastable species  ${}^2D$ . Since we are employing an electron bombardment ion source similar to that used by Lindsay et al., therefore, it is assumed here that the  $O^+$  ions produced in our ion source are expected to be a mix of ground state and metastables at some unknown ratio. Our DCS's at 2.0 keV show a monotonic decrease with a constant slope up to 1*.*5◦ that is followed by slower decrease within the flatter region of  $1.5 - -2.66°$ . Similar trends are observed for impact energies 3–5 keV with the limit of the constant slope moving toward smaller angular limit. This limit is at about 0*.*5◦ for the higher impact energy of 5 keV.

It is known that charge exchange cross section depend markedly on the initial electronic state of the oxygen ion. The  $O^+(^2D)$  metastable excited state is essentially in energy reso-<br>nance with the  $N^+(A^2H)$  and the charge exchange cross section nance with the  $N_2^+(A^2\Pi)$  and the charge exchange cross section<br>is expected to be large, while there is approximately 2 eV beis expected to be large, while there is approximately 2 eV between the  $O^+(4S)$  ground state energy and that of the nearest<br>N<sup>+</sup> state  $(X^2 \Sigma^+)$  resulting in smaller cross section. However  $N_2^+$  state  $(X^2 \Sigma_g^+)$ , resulting in smaller cross section. However,<br>it is rather difficult to speculate over the above mentioned beit is rather difficult to speculate over the above mentioned behavior of the DCS's and to relate the two different regions of the DCS's to two different cross sections resulting from ground and metastable states, since in fact for electron loss cross section measurements reported here, the  $2 \text{ eV}$  available to the  $2D$  state is relatively small in comparison to the second ionization energy (35.11 eV) that is required to remove the second electron in electron loss process. Therefore, unlike the electron capture process, the influence of the initial state of the ions (ground or metastable state) on the measured DCS's is expected to be negligible and both ground and excited states cross sections in collisions with  $N_2$  are expected to be the same. No other experimental or theoretical data exist with which to compare these differential cross sections.

The differential cross sections were integrated to yield total electron loss cross section. Scattered particles for 2 keV ions at 2*.*66◦ correspond to about 3% of those at near zero degrees. Smaller cross section and background effect prevented any meaningfully measurements at scattering angle higher than <sup>2</sup>*.*66◦ for this energy. Therefore, an extrapolation of the data at 2 keV to angles higher than 2*.*66◦ was performed in order to evaluate possible contributions to the total cross section at this energy. The slope of the DCS's at 2 keV between 1.8 and 2*.*66◦ was considered in the extrapolation up to 5◦. Integration of extrapolated data up to 5◦ yielded a total cross section that was 23% higher than that resulting from the integration of the DCS's up to 2*.*66◦. At higher collisional energies the signal at 3*.*2◦ is of three orders of magnitude lower than that at zero degrees. Scans above 3*.*2◦ and up to 5◦ yielded no measurable signals and any possible contribution to the total cross section at these energies is expected to be negligible.

The total cross section are shown in Fig. 2 with that for 2 keV being corrected for possible loss of signal. Measurements of Lo and Fite [\[1\]](#page-3-0) [in](#page-3-0) the high energy region are also displayed in Fig. 2. The error bars are given to indicate the maximum reproducibility of the data in the present energy range (15%). Fig. 2, manifest the overall general shape of the curve of SEL cross sections for the

Fig. 2. Total cross sections for single electron loss of  $O^+$  ions in N<sub>2</sub> molecular target. Solid circles for present measurements, solid squares from Lo and Fite.

 $O<sup>+</sup>-N<sub>2</sub>$  system over a wide range of energies (2.0–3000 keV). Our total cross sections for SEL of  $O^+$ –N<sub>2</sub> system are found to be of the order of magnitude between  $10^{-\overline{19}}$  and  $10^{-21}$  cm<sup>2</sup> and show a monotonic increase with energy. An extrapolation of the high energy experimental data of Lo and Fite [\[1\]](#page-3-0) to low energies seem to overlap with the present measurements. Although no quantitative data were measured by Fogel' et al. [\[2\]](#page-3-0) for the electron loss in  $O^+$ –N<sub>2</sub> reactions, yet their finding within the energy region of 12.3–46.2 keV showed that the relative amount of the resulting doubly charged oxygen ions increased with the beam energy in accordance with the monotonic increase in the cross section observed in this work The expected monotonically increasing behavior (Massey Criteria [\[19\]\)](#page-3-0) of the non-resonant  $O^+$ –N<sub>2</sub> system total cross section as a function of the incident energy would reach a maximum at  $E_{\text{max}} = 2.93 \text{ MeV}$ , to be followed by an expected decrease (not shown in Fig. 2) in the cross section as predicted by Massey [\[19\].](#page-3-0) This can be understood in term of momentum transfer and projectile–target interaction time, for energies smaller than  $E_{\text{max}}$  since smaller momentum can be transferred to the projectile electrons as the energy of the projectile decreases.

#### **4. Conclusion**

The results of the present work can be summarized as follows:

- (a) Absolute differential and total cross sections for SEL in  $O^+$ - $N_2$  collisions were obtained at scattering angles between  $-3.2° \le \Theta \le 3.2°$  in the laboratory frame and at laboratory energies between 2.0 and 5.0 keV.
- (b) The SEL cross sections are found to be of the order of magnitude between  $10^{-19}$  and  $10^{-21}$  cm<sup>2</sup>, and show a monotonically increasing behavior as a function of the incident energy.
- (c) The measured total SEL cross sections are expected to be independent of the initial state of the  $O^+$  ions.



### <span id="page-3-0"></span>**Acknowledgments**

We are in debt to Dr. B.G. Lindsay for valuable comments and suggestions. We are grateful to F. Castillo, B.E. Fuentes for helpful suggestions and comments, also we are grateful to Jose Rangel, A. Bustos and A. Gonzalez for their technical assistance. This research was supported by DGAPA IN-109103 and CONACYT 41072-F.

#### **References**

- [1] H.H. Lo, W.L. Fite, Atomic Data 1 (1970) 305.
- [2] M. Fogel', L.I. Krupnik, A.G. Koval', R.P. Slabospitskii, Sov. Phys. Tech Phys. 2 (1957) 902.
- [3] M. Ishimoto, M.R. Torr, P.G. Richards, D.G. Torr, J. Geophys. Res. 91 (1986) 5793.
- [4] H. Luna, M. Michael, M.B. Shah, R.E. Johnson, C.J. Latimer, J.W. Mc-Conkey, J. Geophys. Res. 108 (E4) (2003) 5033.
- [5] D. Smith, N.G. Adams, in: S. Veprek, M. Venugopalan (Eds.), Topics in Current Chemistry, vol. 89, Springer-Verlag, Berlin, 1980, p. 1.
- [6] S.S. Prasad, D.R. Furman, J. Geophys. Res. 80 (1975) 1360.
- [7] N. Larson, P. Balzer, S. Svensson, B. Wannberg, N. Martensson, A.N. de Brito, N. Correia, M.P. Keane, M. Carlsson-Gothe, L. Karlsson, J. Phys. B 23 (1990) 1175.
- [8] O. Furuhashi, T. Kinugawa, T. Hirayama, T. Koizumi, Phys. Rev. A 70 (2004) 052501.
- [9] M. Hamdan, A.G. Brenton, Chem. Phys. Lett. 164 (1989) 413.
- [10] D.M. Curtis, J.H.D. Eland, Int. J. Mass Spectrom. Ion Processes 63 (1985) 241.
- [11] S.D. Price, J.H.D. Eland, J. Phys. B 24 (1991) 4379.
- [12] B.G. Lindsay, R.L. Merrill, H.C. Straub, K.A. Smith, R.F. Stebbings, Phys. Rev. A 57 (1997) 331.
- [13] H. Martinez, F.B. Yousif, Phys. Rev. A 69 (2004) 062701.
- [14] R.F. Stebbings, B.R. Turner, J.A. Rutherford, J. Geo. Phys. Res. 71 (1966) 771.
- [15] T.F. Moran, B.P. Mathur, Phys. Rev. A 21 (1980) 1051.
- [16] A. Rutherford, D.A. Vroom, J. Chem. Phys. 55 (1971) 5622.
- [17] X. Li, Y.-L. Huang, G.D. Flesch, C.Y. Ng, J. Chem. Phys. 106 (1997) 1373.
- [18] E.E. Ferguson, F.C. Fehsenfeld, D.L. Albritton, in: T. Michael, Bowers (Eds.), Gas Phase Ion Chemistry, Academic, New York, 1979.
- [19] H.S.W. Massey, E.H.S. Burhop, Electronic and Atomic Impact Phenomena, Oxford U.P., New York, 1952, p. 450.