Int. J. Mol. Sci. **2007**, *8*, 1158-1164

International Journal of
Molecular Sciences
ISSN 1422-0067

http://www.mdpi.org/ijms

Full Research Paper

Electron-Capture Cross Sections of Ground-State O_2^+ Recoil Ions in Slow Collisions with H_2 and O_2

Asad T. Hasan [1,*] and Tom J. Gray [2]

1 Department of Physics, American University of Sharjah, Sharjah, UAE
2 Department of Physics, Kansas State University, Manhattan, KS 66506, USA; E-mail: tgray@phys.ksu.edu

[*] Author to whom correspondence should be addressed; Tel.: 97165152507; Fax: 97165585066; Email: ahasan@aus.edu

Received: 19 October 2007; in revised form: 9 November 2007 / Accepted: 13 November 2007 / Published: 22 November 2007

Abstract: We report the measured total charge-transfer (electron-capture) cross sections for the ground state $O_2^+(X^2\Pi_g)$ ions with H_2 and O_2 molecular gases in the collision energy range between 0.50 and 2 keV. The time-of-flight technique has been used to measure the fast neutral products from O_2^+ charge transfer reactions. The analyzed process has cross sections that continue to increase slowly, as a function of incident energy. Measured cross sections for $O_2^+ + H_2, O_2$ systems are compared with previously available experimental and theoretical results in the literature.

Keywords: Single electron-capture; total cross-sections

---

1. Introduction

A detailed understanding of charge-transfer processes of the type

$$A^{q+} + B \rightarrow A^{(q-1)+}(n,l) + B^{+}(n,l`)$$

has been the goal of many experimental studies [1-4]. These processes have become extremely important in many research areas such as plasma fusion [5], astrophysics and atmospheric science [6,7], atomic physics [8] and the design of controlled thermonuclear fusion devices [9]. At low

collision energies, where charge-transfer is the dominant process in collisions between multicharged ions and neutral particles, there are fundamental physics issues that have yet to be resolved. At such low energies, the collision process possesses strong molecular features, which yield stringent tests for theoretical calculations. For these reasons, the study of charge-transfer processes has recently received considerable attention toward accurately determining the cross sections, both experimentally and theoretically. Such processes have proven difficult to treat theoretically, because multi-electron systems cannot be described classically to a good approximation. The quantum-mechanical study of these multi-electron systems in the time-dependent field is very complicated. Various empirical scaling-laws are well known in the intermediate- and high-energy regimes [10]. Scaling-laws do not exist for low-energy collisions (i.e. <2 keV/amu). Theoretical description of the charge-transfer from molecular gas is very complex. For these complex systems, Moran *et al.* [11] based their work on semi-empirical approaches to calculate the charge-transfer cross sections for vibrationally diatomic molecular particles. Yevseyev *et al.* [12] utilized the asymptotic theory of resonance charge-transfer between a ground-state diatomic molecular ion and its neutral parents. They assumed that the transition of the valence electron occurs at large distances between the colliding particles as compared to their sizes.

In the present investigation, measurements have been made of charge-transfer cross sections by O_2^+ ions colliding on molecular H_2 and O_2 gases with both reactants are initially in their ground states.

$O_2^+ + H_2$:

In case of ground-state O_2^+ incident ions:

$$O_2^+(\mathrm{X}^2\Pi_g;v=0) + H_2(\mathrm{X}^1\Sigma_g^+) \rightarrow O_2(\mathrm{X}^3\Sigma_g^-) + H_2^+(\mathrm{X}^1\Sigma_g^+) + \Delta\mathrm{E}\ (\sim 11.8\ \mathrm{eV})$$

For electronically-excited state O_2^+ incident ions:

$$O_2^+(\mathrm{a}^4\Pi_u;v=0) + H_2(\mathrm{X}^1\Sigma_g^+) \rightarrow O_2(\mathrm{X}^3\Sigma_g^-) + H_2^+(\mathrm{X}^1\Sigma_g^+) + \Delta\mathrm{E}\ (\sim 15.8\ \mathrm{eV})$$

$O_2^+ + O_2$:

In case of ground-state O_2^+ incident ions:

$$O_2^+(\mathrm{X}^2\Pi_g;v=0) + O_2(\mathrm{X}^3\Sigma_g^-) \rightarrow O_2(\mathrm{X}^3\Sigma_g^-) + O_2^+(\mathrm{X}^2\Sigma_g^-) + \Delta\mathrm{E}\ (\sim 12.1\ \mathrm{eV})$$

For electronically-excited state O_2^+ incident ions:

$$O_2^+(\mathrm{a}^4\Pi_u;v=0) + O_2(\mathrm{X}^3\Sigma_g^-) \rightarrow O_2(\mathrm{X}^3\Sigma_g^-) + O_2^+(\mathrm{X}^2\Sigma_g^-) + \Delta\mathrm{E}\ (\sim 16\ \mathrm{eV})$$

The energy defect ΔE is determined by the difference between the recombination energy, which is released after the capture of an electron by the projectile, and the energy needed to ionize the target. At low impact energy, the reaction window of single electron moderately favors exothermic reactions over endothermic or strongly exothermic reactions.

The aim of the paper is to present an experimental study of the total charge-transfer cross sections for the ground state $O_2^+(\mathrm{X}^2\Pi_g)$ ions with H_2 and O_2 molecular gases in the collision energy range between 500 and 2000 eV. We have extended this work to cover a wider energy range and emphasis is given to the importance of charge-transfer processes in ion-molecule collisions in this range.

2. Experimental Approach

The experimental apparatus and measuring procedure have previously been described in detail [1] and only the main features need to be mentioned here. A beam of O_2^+ ions with typical spread (FWHM) of 1 eV was extracted directly from a recoil ion source identical to that used previously [1]. These slow ions were formed by passing a collimated pulsed F^{4+} beam of energy 1 MeV/amu through the recoil ion source (RIS) containing O_2, the molecular gas. The collisions that take place in the RIS between the fast F^{4+} pulsed beam and the gas molecules generate recoil ions that are extracted by the voltage gradient across the RIS electrodes. Upon exiting the RIS, these ions travel through the first acceleration unit, a seven-plate apparatus, of which only the fifth plate is not grounded. This plate (the Einzel lens) focuses and drifts the primary ions toward the secondary pressurized gas-target cell containing the H_2 or O_2 molecular gases. After exiting the gas-target cell, the slow ions were extracted using a 90^o double-plate electrostatic analyzer and detected using a microchannel plate detector. The O_2^0 molecules passed straight through the analyzer onto the detector. To measure the charge-transfer cross sections of O_2^+, the detector was moved as close as possible to the target cell which has a larger exit aperture. Therefore, the angular acceptance of the apparatus was set such that essentially all fast O_2^0 were detected. The recoil ions scattered through an angle θ into a solid angle ΔΩ of 3×10^{-3} sr were analyzed after their passage through H_2 or O_2 molecular gases using the electrostatic analyzer. In the present experiment, the yield of O_2^0 molecules produced through single-charge-transfer by the O_2^+ ions and the total yield of parent ions was used to determine the total cross sections. Separation between the O_2^+ ions and O_2^0 molecules could only be achieved when the fifth plate of the second acceleration unit was not grounded.

The use of the electrostatic analyzer in conjunction with the time-of-flight (TOF) technique enables one to identify the various events associated with the charged ions. One must keep in mind, here, that only the reaction energy window favoring single charge-transfer by ground state O_2^+ ions has been studied. This reaction window corresponds to moderately exothermic reactions, with about 9 eV $\leq \Delta E \leq$ 13 eV and 10 eV $\leq \Delta E \leq$ 14 eV for $O_2^+ + H_2$ and O_2 systems, respectively. The basic TOF procedure used in these measurements was identical to that described in our previous papers [1].

3. Determination of the Cross Sections

When making cross-section measurements, the pressure in the target cell is chosen to ensure a single collision and the total cross section for the charge-transfer is then evaluated from the formula [1]:

$$\sigma\ (\mathrm{cm}^2) = \frac{N_t^o}{N_t\, n\varepsilon\, l}$$

where N_t^0 is the total number of the neutral events, N_t is the measured number of incident ions, n is the number of gas particles per cm^3 per mTorr in the collision target-cell and is related the measured pressure p in Pa according to $n = 2.45 \times 10^{14}\ p$ (at 22 °C), ε is the detection efficiency of detector and l is the effective thickness of the target cell. The gas target cell was 2 cm long, in which the gas target pressure was typically 0.8mTorr. Calculations by Toburen *et al.* [13] indicate that the effective length of the target cell may be obtained by adding the sum of the diameters of its two apertures to the

geometric length. This would represent a correction of 10% to the cross section. The efficiency of the channel-plate detector has been determined by multiplying the active area ratio of the first channel-plate from the manufacturer's manual with the transmission of the grids at the entrance of the detector (ε=34%) [14]. The total number of the neutral events N_t^0 is determined by applying a transverse field on the analyzer to deflect ions away after they pass through the second acceleration unit, allowing only the neutral products to impact the detector.

4. Results and Discussion

$O_2^+ + H_2$

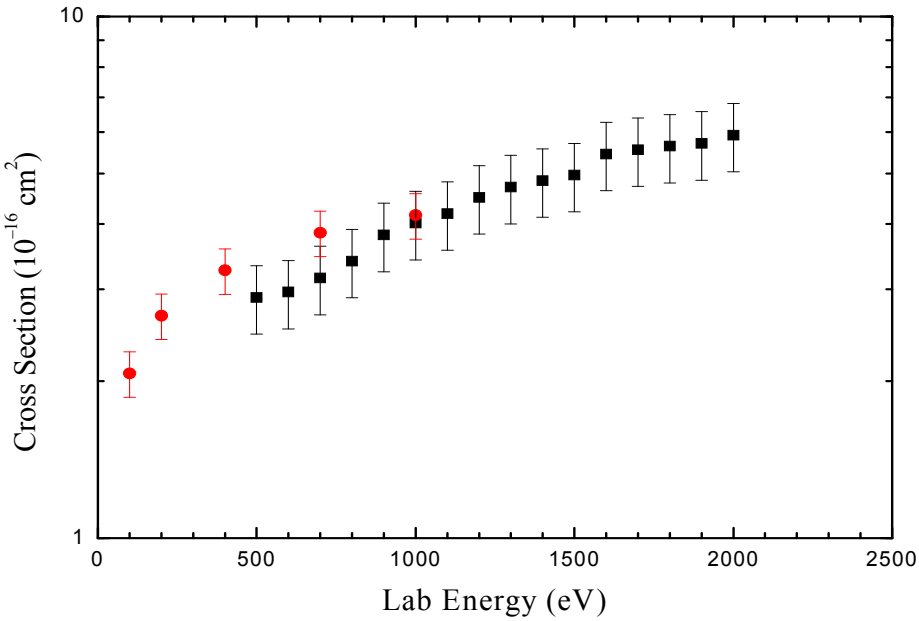
The total cross sections for single charge exchange by O_2^+ ions from H_2 at collision energies between 0.5 and 2 keV are measured as a function of the ion kinetic energy. The total uncertainty is estimated to be 15%. This uncertainty corresponds to a quadrature sum of statistical and systematic errors.

Figure 1 depicts the values of these cross sections measured in this investigation with the results of those of Irvine *et al.* [2]. The present measurements of the total cross sections slowly increase with increasing collision energies and are in accordance with Irvine results. Irvine also reported that there is no significant dependence of the ground-state cross-section on the vibrational energy at these energies.

$O_2^+ + O_2$

A comparison of the experimental total charge transfer cross sections and theoretical calculations for the system $O_2^+ + O_2 \rightarrow O_2 + O_2^+$ as a function of the ion kinetic energy is displayed in Figure 2.

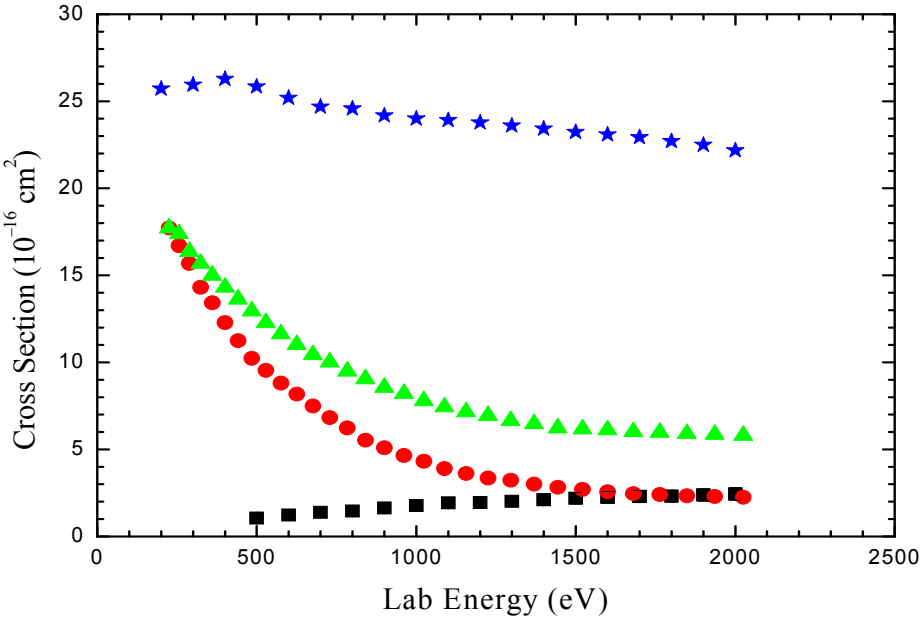
Figure 1. Comparison of the experimental total charge transfer cross sections for the system $O_2^+ + H_2 \rightarrow O_2 + H_2^+$ as a function of the ion laboratory energy. The squares are the present results; and the circles are from Irvine [2].



The total charge-exchange cross sections measured in this investigation exhibit slowly increasing behavior as a function of incident energy. The present data are in reasonable agreement with the theoretical calculations of Moran [11] using the low-velocity approximation at energies above 1.2 keV. Below this energy, there is an increasing disparity between the two results, quantitatively and qualitatively. It is also apparent that there is a real discrepancy between the multistate treatment and the experiment. It should be noted that in the energy 1-100 eV, the multistate treatment overestimated the $O_2^+ + O_2$ and $NO^+ + NO$ total charge exchange cross sections by a factor of 2 [11]. This discrepancy may be related to the various approximations introduced into these theoretical computations. The theory also neglects the effect of ion-induced dipole forces, which would be expected to dominate the interaction at low energies. This may be considered another source of discrepancy.

A disagreement between the two theoretical computations caused by the use of two fundamentally different theoretical models can also be seen in Figure 2. Moran utilized the multistate impact parameter treatment and the low velocity limit in calculating the total charge-transfer cross sections. In another study, Yevseyev [12] used the asymptotic theory of resonance charge-exchange between a ground-state diatomic molecular ion and its neutral parent. The principal difference between these two models lies in the method of calculating the exchange interaction potential $\Delta_{el}(R)$ for colliding molecular gases. $\Delta_{el}(R)$ is determined by Yevseyev using the asymptotic parameters of the valence electron in the molecule and the quantum numbers of the quasimolecular compound. Moran computed $\Delta_{el}(R)$ using the semi-empirical method.

Figure 2. Comparison of the present experimental total charge transfer cross sections [squares] and theoretical calculations of Moran [11] and Yevseyev [12] for the system $O_2^+ + O_2 \rightarrow O_2 + O_2^+$ as a function of the ion kinetic energy. The squares are the present experimental data. The statistical errors are smaller than the data points. The circles and triangles are the computations of Moran using the low velocity approximation and multistate treatments, respectively, and the stars are the computations of Yevseyev using the asymptotic approach for the initial vibrational characteristics $v_1 = v_2 = 0$.



Conclusions

The present study of one-electron capture in slow $O_2^+ + H_2$, O_2 systems has provided new measurements on these collision mechanisms at low impact energy. Our $O_2^+ + H_2$ measurements in the energy range of 0.50 and 2 keV confirm the findings of Irvine's studies. The satisfactory agreement between the present data and the findings of Irvine is a meaningful indicator of the overall reliability of the present measurements of total cross sections for charge-transfer.

The present measurements of $O_2^+ + O_2$ systems are only in reasonable agreement with the low-velocity approximation of Moran at energy above 1.2 keV. The multistate model overestimated the total charge transfer cross sections. The electronically excited and dissociative channels are neglected in the theoretical model calculations. A disagreement between the two theoretical computations is also observed.

We conclude that further measurements along these lines are needed for resolving this discrepancy and for better understanding of the charge transfer processes.

Acknowledgements

The authors are grateful to A. Alnasser for his helpful suggestions and assistance and gratefully acknowledge the experimental support of the accelerator crew of the J.R. McDonald laboratory at Kansas State University for providing a high quality beam during the course of the experiment.

References

1. (a) Hasan, A.T. Experimental study of single- and double-electron-capture by Ne ions from He gas. *Eur. Phys. J.* **2005**, *D35*, 461-466; (b) Hasan, A.T. Single electron capture in slow collisions of H_2^+ ions with H_2, O_2 and N_2 diatomic molecules. *Int. J. Mass Spect.* **2005**, *247*, 81-84; (c) Hasan, A.T. Low-energy electron capture by N_2^+ ions from O_2 and H_2 molecular gases. *J. Elect. Spec. Rel. Phen.* **2004**, *135*, 159-162; (d) Hasan, A.T.; Gray, T.J. Absolute Total Single–Electron–Capture Cross Sections of O_2^+ with N_2 Gas. *Int. J. Mol. Sci*. **2003**, *4***,** 284-290; (e) Hasan, A.T.; Gray, T.J. Experimental Study of Single-Electron-Captue Cross Section by Low-Energy N_2^+ and N^+ Ions in N_2 Molecular Gas. *Int. J. Mod. Phys.* **2002**, *E11***,** 567-562; (f) Hasan, A.T.; Gray, T.J. Formation of *N* and N_2 recoil ions from the bombardment of N_2 gas by a 19 MeV F^{4+} beam. *Nucl. Instr. Methods B* **2002**, *49*, 1-4.
2. Irvine, A.D.; Latimer, C.J. Charge-exchange processes involving ground- and excited-state O_2^+ and H_2^+ ions with H_2 and O_2. *Int. J. Mass Spec. Ion. Proc.* **1997**, *164***,** 115-120.
3. Baer, T.; Murray, P.T.; Squires, L. Total cross sections for symmetric charge transfer reactions of O_2^+ in selected translational and internal energy states. *J .Chem. Phys.* **1978**, *68*, 4901-4906.
4. Lindsay, B.G.; Merrill, R.L.; Straub, H.C.; Smith, K.A.; Stebbings, R.F.; Absolute differential and integral cross sections for charge transfer of keV O^+ with N_2**.** *Phys. Rev. A* **1998**, *57*, 331-337.
5. Janev, R.K. *Atomic and Molecular Data for Plasma Edge Studies; Summary Report of Second Research Coordination Meeting on Atomic and Molecular Data for Plasma Edge Studies*; International Energy Report: Vienna, **1993**, *276*.

6. Cravens, T.E. Comet Hyakutake X-ray source: Charge transfer of solar wind heavy ions. *Geophys. Res. Lett.* **1997**, *24*, 105-108.
7. Pequignot, D. Charge transfer reactions in some astrophysical situations. *Astron. Astrophys.* **1980**, *81*, 356-358.
8. Datz, S.; Drake, G.W.F.; Gallagher, T.F.; Kleinpopen, H.; Putlitz, G.Zu. Atomic physics**.** *Rev. Mod. Phys.* **1999**, *71*, S223-S241.
9. Maggi, C.F.; Horton, L.D.; Summers, H.P. The effect of charge exchange with neutral deuterium on carbon emission in JET divertor plasmas. *J. Phys. B* **2000**, *42*, 669-700.
10. Olson; R.E.; Salop, A. Electron transfer between multicharged ions and neutral species. *Phys. Rev. A*. **1976,** *14*, 579 -585.
11. Moran, T.F.; Flannery, M.R.; Cosby, P.C. Molecular charge transfer. II. Experimental and theoretical investigation of the role of incident-ion vibrational states in O_2^+-O_2 and NO-NO collisions. *J. Chem. Phys.* **1974**, *61*, 1261-1273.
12. Yevseyev, A.V.; Radtsing, A.A.; Smirnov, B.M. The asymptotic theory of resonance charge exchange between diatomics. *J. Phys. B* **1982**, *15*, 4437-4452.
13. Toburen, L.H; Nakai, L.H.; Langley, R. A. 1967 Oak Ridge National Laboratory Report ORNL-TM-**1988**, pp. 1-231 Thesis.
14. Gray, T.J.; Ben-Itzhak, I.; Malhi, N.B.; Needham, V.; Cranes, K.; Legg, J.C. Low divergence low energy recoil ion source. *Nucl. Instr. Methods B* **1989**, *40*, 1049-1052.