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Measurements and Theoretical Predictions of Charge Exchange Cross Sections and Emission Spectra for O⁶⁺ with H₂O, CO, CO₂, CH₄, N₂, NO, N₂O and Ar

J. R. Machacek¹, D. P. Mahapatra^{2, 3}, D. R. Schultz^{4*}, Yu. Ralchenko⁵, A. Moradmand², M. O. A. El Ghazaly², and A. Chutjian²[†]

¹Positron Physics Group, The Australian National University, ACT 2601, Australia ²Astrophysics and Space Sciences Section, Jet Propulsion Laboratory/Caltech, Pasadena CA 91109 ³ Department of Physics, Utkal University, Bhubaneswar-751004, India

⁴ Department of Physics, Univ. of North Texas, Denton, TX 76203

⁵ Atomic Spectroscopy Group, National Institute of Standards and Technology, Gaithersburg, MD 20899-8422 Synopsis Relevant to modeling and understanding X-ray emission from cometary and planetary atmospheres, total charge-exchange cross sections for 1.17 and 2.33 keV/u O⁶⁺ ions colliding with H₂O, CO, CO₂, CH₄, N₂, NO, N₂O, and Ar have been measured and calculated for the processes of single, double, and triple exchanges. Synthetic emission spectra spanning the X-ray, UV, and visible ranges have also been calculated, based on theoretical treatment of the transfer of between one and six electrons from the target neutral to the projectile ion, followed by radiative and nonradiative decay of the resulting highly-excited projectile states.

The phenomenon of charge exchange (CE) between highly-charged ions (HCIs) and neutral molecules is observed throughout our Solar System, and is very likely occurring in moredistant stellar atmospheres. In such exchanges an HCI in (for example) the solar wind (SW) captures an electron from the neutral gas into a state with high principal quantum number *n* that subsequently de-excites by emitting one or more photons at visible-to-X-ray wavelengths [1]. The gaseous targets can be comet or planetary atmospheres, circumstellar clouds, and the interplanetary medium; while the HCIs arise from the SW, the Jovian magnetosphere and cosmic rays [2]. Since O^{6+} is the most abundant heavy ion in the SW, its interactions can be used to probe objects as distant as Pluto.

Reported herein are absolute CE cross sections for up to three exchanges of the O^{6+} ion with electrons from the comet/planetary gases H₂O, CO, CO₂, CH₄, N₂, NO, N₂O and Ar. The measurements are compared with results in calculations using the classical trajectory Monte Carlo (CTMC) method. With the measurements as benchmarks, synthetic emission spectra spanning the X-ray, UV, and visible range have been calculated based on theoretical treatment of the transfer of between one and six electrons from the target neutrals to O^{6+} , followed by radiative and non-radiative decay of the highlyexcited ion states.

Experimental measurements were carried out using the HCI source at JPL. Details are given in [3] for results with He and H₂ targets; as well as details of the CTMC calculational approach.

Extension of the theory for calculating cross sections and spectra for 1-6 captures using an ab initio formulation of the atomic structure and decay parameters will be described in [4, 5].

Shown in Table 1 are results of measurements and calculations for CO and H₂O, for three exchanges, at the lower energy of 1.17 keV/u [4]. Results will be presented for three exchanges in all the target gases at 1.17 and 2.33 keV/u, and simulated emission spectra for relaxation of the $O^{(5-3)+}$ ions to their lower electronic states.

Target	CE	CE Cross	CE Cross
	Channel	Section (Exp.)	Section
			(Theory)
CO	σ ₆₋₅	5.41±0.35	4.51
	σ_{6-4}	1.10 ± 0.08	0.58
	σ ₆₋₃	0.37±0.03	0.05
H ₂ O	σ ₆₋₅	4.73±0.31	5.50
	σ ₆₋₄	0.83±0.06	0.63
	σ ₆₋₃	0.37±0.03	0.06

Table 1. Experimental and CTMC results for CE of O^{6+} with CO and H₂O at an energy of 1.17 keV/u. Units are 10^{-15} cm², and errors are at the 2σ level.

References

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*E-mail: <u>david.schultz@unt.edu</u> †E-mail: <u>ara.chutjian@jpl.nasa.gov</u>

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