FINAL REPORT FOR GRANT NAG5-11990

TITLE: Laboratory Studies of Thermal Energy Charge Transfer of Multiply Charged Ions in Astrophysical Plasmas

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A:  INTRODUCTION:

The laser ablation/ion storage facility at the UNLV Physics Department has been dedicated to the study of atomic and molecular processes in low temperature plasmas. Our program focuses on the charge transfer (electron capture) of multiply charged ions and neutrals important in astrophysics. The electron transfer reactions with atoms and molecules is crucial to the ionization condition of neutral rich photoionized plasmas.

With the successful deployment of the Far Ultraviolet Spectroscopic Explorer (FUSE) and the Chandra X-ray Observatory by NASA, high resolution VUV and X-ray emission spectra from various astrophysical objects have been collected. These spectra will be analyzed to determine the source of the emission and the chemical and physical environment of the source. The proper interpretation of these spectra will require complete knowledge of all the atomic processes in these plasmas. In a neutral rich environment, charge transfer can be the dominant process. The rate coefficients need to be known accurately.

We have also extended our charge transfer measurements to KeV region with a pulsed ion beam (Wong and Kwong, 1997, Gao, Fang, and Kwong, 2001). The inclusion of this facility into our current program provides flexibility in extending the measurement to higher energies (KeV) if needed. This flexibility enables us to address issues of immediate interest to the astrophysical community as new observations are made by high resolution space based observatories.

B.  RESEARCH SUMMARY

During the grant year, we pursue our investigation to include association reactions involving molecular ions and neutral molecules and substitution reactions between hydrogen and deuterium. Specifically, we study the following reactions:

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\begin{align*}
\text{H}_2\text{O}^+ + \text{D}_2 & \rightarrow \text{H}_2\text{DO}^+ + \text{D} & (1) \\
\text{H}_2\text{DO}^+ + \text{H}_2\text{O} & \rightarrow \text{HDO} + \text{H}_3\text{O}^+ & (2) \\
\text{H}_2\text{DO}^+ + \text{D}_2 & \rightarrow \text{HD}_2\text{O}^+ + \text{D} + \text{H} & (3) \\
\text{HD}_2\text{O}^+ + \text{D}_2 & \rightarrow \text{D}_3\text{O}^+ + \text{D} + \text{H} & (4) \\
\text{CO}^+ + \text{D}_2 & \rightarrow \text{DCO}^+ + \text{D} & (5) \\
\text{CH}_3^+ + \text{D}_2 & \rightarrow \text{CH}_2\text{D}^+ + \text{D} & (6)
\end{align*}
\]

Our preliminary investigation suggests that the rate coefficients for the association reactions, i.e. (1) and (5), are of the order of $10^{-10} \text{cm}^3\text{s}^{-1}$ while that for the H/D substitution reactions, i.e. (2), (3) and (4), are of the order of $10^{-12} \text{cm}^3\text{s}^{-1}$ and (6) is about $10^{-11} \text{cm}^3\text{s}^{-1}$. These results may explain the hydrogen/deuterium fractionation discrepancies in planetary atmospheres (Krasnopolsky et al., 1998, Yung and Kass 1998) and set a limit on the cosmic deuterium-
hydrogen abundance in dense interstellar cloud (Dalgaro and Lepp, 1984, Robert, Herbst, and Millar, 2002). For example, Yung et al. (1988) proposed a one-dimension photochemical model involving several physical and chemical processes that lead to the preferential escape of hydrogen over deuterium in Martian atmosphere. However, the amount of the water they estimated on Mars is too low. To reconcile the measurement (Krasnopolsky et al. 1998) with the photochemical model, Yung and Kass (1998) revise their model that the D/H ratio of the hydrogen that escapes from Mars may be determined by thermodynamic equilibrium between HD and H2O in the reaction:

$$\text{HD} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{HDO} \quad (7)$$

with the partitioning of D between HD and HDO in the atmosphere defined by

$$R = \frac{\text{D/H}_2}{\text{HD/O/H}_2\text{O}}$$

This revised model on H/D fractionation gives a $R = 0.14$, a value closer to measured value of 0.09. However, this will require the rate coefficient of reaction (7) to be greater than $10^{-23} \text{cm}^3\text{s}^{-1}$, 10 orders of magnitude larger than the laboratory value of $10^{-33} \text{cm}^3\text{s}^{-1}$ (Lecluse & Robert, 1994). Yung and Kass (1998) suggest two possible solutions to this paradox. First, he suggests that there is an unknown reaction that can reduce the value of R in the thermodynamic equilibrium model of his. Second, there is an unknown catalyst on Mars that can raise the rate coefficient of reaction (7) by 10 orders of magnitude.

The basic assumption in Yung’s model is: H2O exists in neutral form. However, the Martian atmosphere is constantly bombarded by solar wind ions as well as x-ray, VUV, and UV from the sun. It is not unreasonable to assume that a small fraction of H2O is in the form of H2O+. The presence of the H2O+ can significantly reduce HD concentration in the Martian atmosphere by ion-molecule reactions:

$$\text{H}_2\text{O}^+ + \text{HD} \rightarrow \text{H}_2\text{DO}^+ + \text{H} \quad (8a)$$

$$\rightarrow \text{H}_3\text{O}^+ + \text{D} \quad (8b)$$

Our preliminary measurement on the reaction (1) i.e. H2O+ + D2 $\rightarrow$ H2DO+ + D, indicates a rate coefficient of the order $10^{-10} \text{cm}^3\text{s}^{-1}$. Even though this measurement is for H2O+ and D2, the D2 reaction is a good pointer to how HD will react with H2O+. This suggests that the rate coefficients for reaction (8a) and (8b) are of the order of $10^{-10} \text{cm}^3\text{s}^{-1}$, 23 orders of magnitude larger than the neutral reaction (7). Even if we were to assume that the ionization fraction of H2O is small, the vast difference in their rate coefficients provides a significant alternate channel to remove HD from the atmosphere. This can make reaction (8a) and (8b) appear to have a significantly higher rate coefficient. Furthermore, the fast reaction (2) also suggests a rapid production of HDO thus making the R value much smaller.

We are in the process of refining these measurements. These results will form the basis for the next proposed research to NASA.
C. PAPERS PUBLISHED AND PAPERS SUBMITTED

"Charge transfer between C$_2^+$ and H$_2$, N$_2$, He, and CO at eV energies", H. Gao and Victor H.S. Kwong, Accepted for publication in Physical Review A, 2003.


D. CONFERENCE PRESENTATIONS


"Charge transfer between S$_2^+$ ions and H$_2$ at electron volt energies," Victor H.S. Kwong, De Chen, and Hui Gao, NASA Laboratory Astrophysics Workshop, Ames Research Center, Moffett Field, California, May -1 -03, 2002.
E. REFERENCES: