A.4.3. Slow Ion-Molecule Collisions--*E. Wells, K.D. Carnes, R. Ali,* M. Stöckli and I. Ben-Itzhak*

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Fragmentation of molecules caused by slow highly charged ions has been attracting increasing interest in recent years. Measurements of the fragmenting molecule, which have been mostly qualitative in nature, are evolving to be more detailed. Vancura and Kostroun [1], for example, have studied the qualitative behavior of the fragmentation of CO caused by 2.3 keV/q highly charged Ar^{q+} ions (q=8-14). Such studies were followed by quantitative studies of electron capture and dissociation of the transient N_2^{q+} molecular ions produced by 8-16 keV Ar^{8+} ion impact on N_2. Folkerts *et al*. [3-5] studied the breakup of the heteronuclear CO molecule over a similar energy range. The quantitative measurements provide electron capture cross-sections, breakup branching ratios, and kinetic energy release distributions. From the detailed information gathered one hopes to learn about the molecular states involved and the dissociation pathways (see for example, Folkerts *et al*. [5]), though detailed understanding of the complex breakup process is still desired. Recently, momentum imaging techniques have been applied to such fragmentation studies, thus providing the momentum vector of both dissociating fragments, from which the molecular alignment and orientation can be determined [6].** This technique was used in our laboratory by Cocke *et al*. to study the effect of the field produced by the highly charged ion on the dissociation process [Abstract #99].

Our measurements were performed (some during the previous grant period) using the coincidence time-of-flight method for the recoil ions while preserving the correlation of each event to the projectile final charge state [Publication #5]. Specifically we studied the molecular fragmentation of molecular hydrogen and carbon monoxide following charge transfer to a slow highly charged ion, C^{6+} (at 15.8 keV/amu) and Ar^{11+} (at 0.8, 3.3, 10, and 14.3 keV/amu).

For the C^{6+} + D_2 (at v=0.8 a.u.) and Ar^{11+} + HD or D_2 (at 0.63 a.u.) single electron capture with no target excitation is the dominant process. Double capture and transfer excitation are about 30% relative to single capture. Most projectiles (~95%) auto-ionize rapidly following the double electron capture. Model calculations using classical trajectory Monte Carlo (CTMC) to provide active electron probabilities for capture, ionization and excitation within the independent electron approximation are only partially successful. The prediction of the model

that direct ionization is negligible compared to electron capture is consistent with our data. Transfer excitation, however, is predicted to be much smaller (about a factor of 7.5) than double capture, a prediction not consistent with their similar experimental yields. The ratio of double capture to single capture (with and without target excitation) predicted using the model is the same as that predicted by extended over barrier (EOBM) calculations. Both overestimate the measured ratio by about a factor of 2 [7]. Though one might argue that these simple models can serve as a rough estimate of the relative reaction rates, there is clearly room for improvement.

Some of the information about the CO target was reported in Publication #5 while the rest of the information which contains details about electron capture cross sections, breakup branching ratios, and kinetic energy release distributions is being organized for presentation in a forthcoming publication.

For the C^{6+} + CO collisions, for example, *n*-electron capture cross sections fall off approximately as $\sigma_n \sim \sigma_1 e^{-(n-1)/\alpha}$ ($\alpha \sim 1.1$) and they are in disagreement with the predictions of EOBM calculations for a model molecular potential, as shown in Fig. 1. The fragmentation pattern and kinetic energy release upon dissociation were also determined.

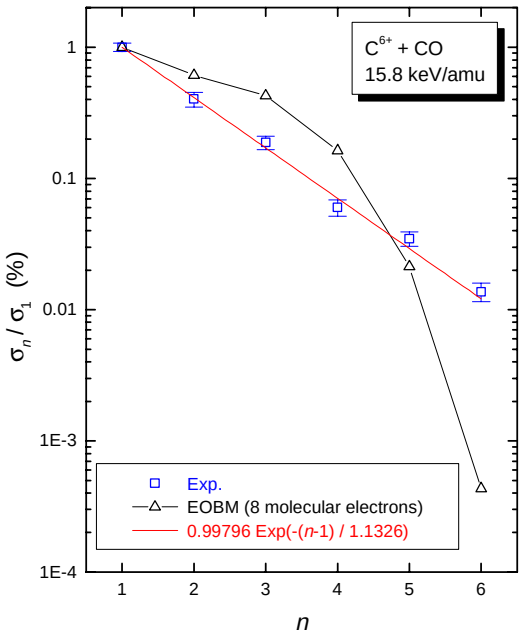

Figure 1. The measured relative cross sections for multiple-electron capture from CO by 15.8 keV/amu C^{6+} (squares). EOBM calculations (triangles) and a simple exponential scaling (dashed line) which fits the data much better than the EOBM calculations.

References

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**Note that this is a fast ion-molecule collision, but the method is similar for slow and fast collisions.

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