

Fragmentation of multiply-charged small hydrocarbon molecules in C_nH^{q+} ($n=1-3$, $q=2-6$) produced in high velocity collisions: Branching Ratios and associated Kinetic Energy Releases of the H^+ fragment

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Synopsis: Dissociation Branching Ratios of C_nH^{q+} molecules formed by multi-ionization of incident C_nH^+ projectiles colliding in high velocity collisions with a Helium atom have been measured. In addition, the KER of the H^+ fragment for each channel was extracted. A striking feature that we obtained is the fact that the KER (Kinetic Energy Release) is always far below predictions of the point charge coulomb model (PCCM) even at large q values. For CH^{q+} , we could explain this result on the basis of electronic state calculations and taking into account the fact that 1s ionization of the carbon atom occurs and has its own dynamics.

In a recent work, we showed how fragmentation of multi-charged carbon clusters strongly evolves with the strength of the coulomb interaction [1]. In order to pursue in this topics, we performed measurements on C_nH^{q+} species and added a new experimental observable through the measurement of the kinetic energy release (KER) of the H^+ fragment. Experiments were performed at the Tandem accelerator in Orsay with beams of C_nH^+ molecules of high velocity (3.6 a.u and 4.5 a.u) colliding with a helium target atom. The experimental set-up has been described elsewhere [2], the only change in the present work being the replacement of the solid-state detector of the H^+ fragment by a position sensitive detector made of three MCP's and a resistive anode.

Multi-ionization cross sections, branching ratios of C_nH^{q+} molecules and KER of H^+ for each channel were extracted. A striking feature that we obtained is the fact that the KER is always far below predictions of the point charge coulomb model (PCCM) even at large q values. For CH^{2+} and CH^{3+} , we could explain this result on the basis of electronic state calculations (see figure 1 for CH^{2+}). Excited-state Calculations were performed using the MOLPRO package in the framework of the MRCI (Multi-Reference Configuration Interaction) method and using a cc-pVQZ basis set. Intensity of the peaks were computed using the monopole approximation implemented in the Gaussian package.

For the case of CH^{4+} and C_nH^{q+} with large q/n ratios, one must take into account ionization in the inner shell, whose cross section is larger than mul-

tiply valence ionization. The dynamics of relaxation is then modified, driven by two competing processes important in the same time domain, fragmentation and relaxation by Auger effect. This will be discussed at the conference.

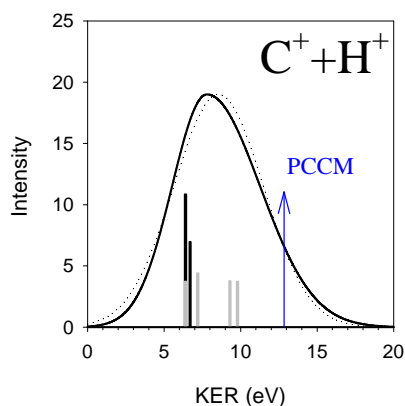


Figure 1: Comparison, for CH^{2+} , between the measured total KER distribution (solid et dotted line) and theoretical predictions extracted from MRCI excited state calculations (vertical bars in black and gray); in blue, predictions of the point charge coulomb model.

References

- [1] Chabot et al 2010 PRL **104**, 043401
- [2] T.Tuna et al, 2008 J.Chem.Phys. **128**, 124312

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