

## Study of fragmentation dynamics of benzene and halogenized benzenes following inner-core excitation.

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### Introduction

Highly charged molecular ions are quite unstable and are quickly destroyed due to the Coulomb repulsion. Analysis of three dimensional momenta of fragment ions often enables us to retrieve the structure of parent ions. This technique is referred to as Coulomb explosion imaging (CEI) [1]. CEI has been successful for the study of doubly and triply charged small molecules in which the sudden dissociation is expected and the dissociation processes are well described by simple Coulomb explosion scheme. In the case of polyatomic molecules such as benzene, complicated dissociation process is expected and the relation between structure of molecules and momentum correlation of fragment ions is not clear.

In the present study, benzene and halogenized benzene molecules are multiply ionized through inner-core ionization and the momenta of fragment ions are measured by using velocity-map imaging spectrometer. Momentum correlations are discussed in relation with the structure of parent molecules.

### Experiment

The photoionization experiment has been performed using the coincidence velocity-map imaging spectrometer [2] at the undulator beamline BL-2C and 28B. In the present study, the photon energy was tuned at 20 eV above the absorption edge energy of target element. Photo-electrons and ions were extracted by a uniform electrostatic field and directed through a drift tube to position sensitive micro-channel plate (MCP) detectors equipped with a delay-line anode (RoentDek, DLD80 for electrons and HEX80 for ions). The time of flight (TOF) measurement was triggered by the first electron detection and signals of fragment ions which were coincidentally detected with photo-electrons were analyzed to obtain their momentum vectors.

### Results and discussions

The momenta of ( $H^+-F^+$ ) and ( $H^+-C^+$ ) following the C 1s photoionization of  $FC_6H_5$  are shown in fig. 1. Figure 1(a) and 1(b) are density plots of momentum correlations in which the momentum of fragment  $A^+$  is represented by an arrow of fixed length and direction, and the relative momentum of  $B^+$  is mapped in the upper half of the polar plot. While three clear peaks at around  $\theta = 60^\circ, 120^\circ, 180^\circ$  are found in the correlation of ( $H^+-F^+$ ), which may reflect the angles between C-H bonds and C-F bond of parent molecules, no such peaks are found in the

correlation of ( $C^+-F^+$ ). Our results show that the momentum of  $H^+$  and  $F^+$  strongly reflects the hexagonal structure of the parent molecules while the momentum of  $C^+$  do not. This would originate from the difference in the stability of each fragment atom in the parent molecule. Carbon atoms in  $C_6H_5F$ , which consist of a benzene ring, have relatively large binding energy. This stable structure would lead to slow dissociation in which the benzene ring structure deforms along potential energy surface.

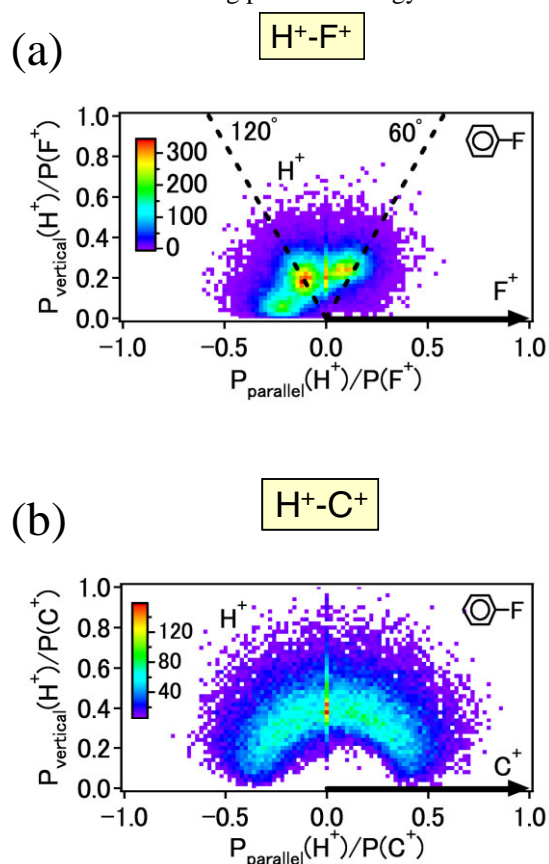


Figure 1; Density plots of the relative momentum relations (see text) of (a) ( $H^+-F^+$ ) and (b) ( $H^+-C^+$ ) following C 1s photoionization.

### References

- [1] Z. Vager, R. Naaman and E.P.Kanter, Science, 244 (1989) 426.
- [2] K. Hosaka, J. Adachi and A. Yagishita. Jpn. J. Appl. Phys., 45 (2006) 2006.

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