Site-specific production of H_3^+ by core ionization of CH_3Cl

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Synopsis Fragmentation reactions following the core ionization of CH_3Cl was investigated by Auger-electron–ion coincidence measurements. A clear difference in fragmentation patterns of the production of H_3^+ was observed after Cl 2p and C 1s photoionization. The enhanced production of H_3^+ following Cl 2p photoionization is related to the formation of specific Auger final states.

The trihydrogen cation, H_3^+, is an interesting molecule which plays a key role in reactions that lead to complex molecules characterizing interstellar clouds. H_3^+ can be produced from fragmentation reactions of several hydrocarbon molecules using intense laser fields, soft x-rays, and electron impact [1–3]. In this study, we investigate efficient H_3^+ production mechanisms of fragmentation reactions of CH_3Cl, after site specific core ionization with soft x-rays, by Auger-electron–ion coincidence measurements.

Experiments were performed on the soft x-ray beamline BL6U at UVSOR in Japan. Radiation from an undulator was monochromatized and introduced into an Auger-electron–ion coincidence spectrometer; electrons ejected at 54.7° from the polarization vector were detected by a position sensitive detector (PSD) of the double toroidal analyzer (DTA), while the ions were extracted by an applied pulsed electric field, also to a PSD, according to each electron detection. From the recorded position of each electron, the energy distribution was obtained. The arrival time and position for each ion was recorded to calculate its momentum. We also measured ions detected in coincidence with core level photoelectrons, in order to obtain the time-of-flight (TOF) spectra. The electron pass energy of the DTA was set to 200 eV, and the corresponding energy resolution was ~1.9 eV. The photon energies used were 220 eV and 302 eV for the C 2p and C1 1s photoionization, respectively.

Figure 1 shows the TOF spectra of fragment ions detected in coincidence with (a) Cl 2p and (b) C 1s photoelectrons. The major ions are labeled within the figure. The most notable difference between the two spectra, is the significantly larger relative abundance of H_3^+ and CH_3Cl^{2+} produced after the Cl 2p photoionization. Figure 2 shows the total Auger-electron and Auger-electron–ion coincidence spectra after the Cl 2p core ionization. The formation of H_3^+ is related to the Auger final states around the binding energy at 32 eV. Theoretical calculations are planned, in order to elucidate the site-specific mechanism of production of H_3^+ and will be discussed.

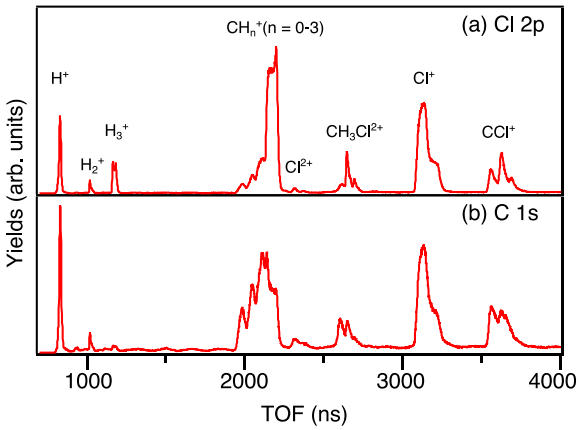

Figure 1. TOF spectra of ions in coincidence with (a) Cl 2p and (b) C 1s photoelectrons

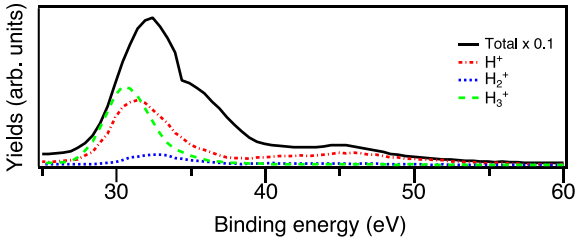

Figure 2. Normal Auger and coincidence Auger spectra with H_n^+ (n = 1-3) following Cl 2p photoionization

References

[1] S. Pilling *et al.* 2007 *Mon. Not. R. Astron. Soc.* **375** 1488
[2] K. Hoshina *et al.* 2008 *J. Chem. Phys.* **129** 104302
[3] J. H. D. Eland. 1996 *Rapid Commun. Mass Spectrom.* **10** 1560

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