

## Reaction Mechanism on Site-Specific Bond Dissociation of a Potent Greenhouse Gas $\text{CF}_3\text{SF}_5$ using Soft X-Rays

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In the previous beamtime (2003A0528-NS1-np) we measured total photoabsorption cross sections of  $\text{CF}_3\text{SF}_5$  in the C, F and S K-shell regions [1], and site-dependent photo-fragmentation was clearly observed. In the present study PIPICO mass spectra were measured in order to detect the pairs of ions released after cascade Auger processes. Fig. 1 shows PIPICO spectra at the C1s and F1s ionization and the  $\text{Si1s} \rightarrow \sigma^*_{\text{SF}}$  excitation. The observed ion pairs are: (1)  $\text{C}^+ - \text{S}^{2+}$ , (2)  $\text{CF}_3^{2+} - \text{SF}_2^{2+}$ , (3)  $\text{C}^+ - \text{S}^+$ , (4)  $\text{CF}_3^+ - \text{SF}_3^+$ , (5)  $\text{CF}_3^{2+} - \text{SF}^+$ , (6)  $\text{CF}_3^{2+} - \text{S}^{2+}$ , (7)  $\text{CF}_2^+ - \text{SF}_2^{2+}$ , (8)  $\text{F}^+ - \text{CS}^+$ , (9)  $\text{CF}_2^+ - \text{SF}_3^+$ , (10)  $\text{CF}_3^+ - \text{SF}_2^{2+}$ , (11)  $\text{CF}_3^{2+} - \text{SF}_3^+$  and (12)  $\text{C}^+ - \text{SF}^+$ . The peak with the highest probability is the  $\text{C}^+ - \text{F}^+$  ion pair. The observed highest charged ion is  $\text{CF}_3\text{SF}_5^{4+}$ , which decomposes into  $\text{CF}_3^{2+} + \text{SF}_2^{2+}$  and  $\text{CF}_3^{2+} + \text{S}^{2+}$ . The PIPICO mass patterns for the direct ionization of C1s and F1s electrons are similar in forming  $\text{CF}_3\text{SF}_5^{n+}$  ( $n=2-4$ ) ions. On the contrary, the PIPICO pattern for the  $\text{Si1s} \rightarrow \sigma^*_{\text{SF}}$  transition shows the dominant formation of  $\text{C}^+ - \text{F}^+$  ion pair, and the highly charged  $\text{CF}_3\text{SF}_5^{n+}$  ( $n=3, 4$ ) ions are minor in spite of

high energy. This finding is consistent with the observation that the PEPICO mass patterns are similar between the C1s and F1s excitation in forming  $\text{CF}_n^+$  and  $\text{SF}_n^+$  ions, which are negligibly small in the S1s excitation.

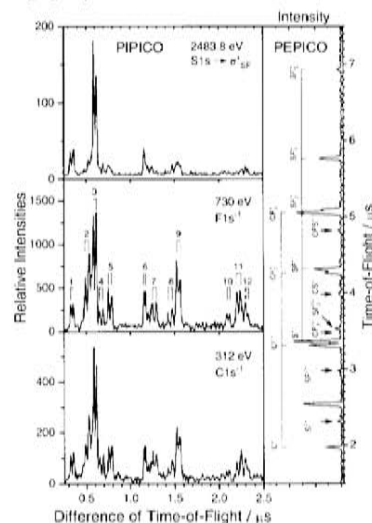


Fig. 1 PIPICO spectra of  $\text{CF}_3\text{SF}_5$ .

### Reference

[1] T. Ibuki et al., Chem. Phys. Lett. 392 (2004) 303.

## A Study on Photo-Manipulation for Molecules by Using Si:KVV-Resonant-Auger-Electron Photoion Coincidence Spectroscopy: Site-Specific Fragmentation Revealed in Energy-Selected Si:1s-Photoelectron Photoion Coincidence Spectra

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In the present study, we have studied the ionic fragmentation caused by Si:1s core-level photoionization of  $\text{F}_3\text{SiCH}_2\text{CH}_2\text{Si}(\text{CH}_3)_3$  (FSMSE) by using energy-selected Si:1s-photoelectron photoion coincidence (Si:1s-PEPICO) spectroscopy. Since FSMSE has two Si atoms in fairly different chemical environments (Si[F] and Si[Me]), it has the potential of showing site-specific fragmentation, which may be used as a tool of manipulation of atoms and molecules.

The figure shown below represents the Si:1s-photoelectron spectrum (a) and the corresponding Si:1s-PEPICO spectra (b)-(g). In the figure (a), an electric-field gradient applied across the ionization region smears the energy distribution of the photoelectrons. The positions of the Si:1s binding energies obtained from a high-resolution photoelectron spectrum (data not shown) are indicated by arrows in the figure (a).

In the Si[Me]:1s photoionization,

productions of heavy ions ( $m/e > 10$ ) are enhanced [figures (b)-(g)]. Especially, enhancement of  $\text{SiF}_3^+$  is characteristic. Moreover,  $\text{H}^+$  ions with high kinetic energy are abundant in the Si[Me]:1s photoionization (data not shown). Thus, site-specific fragmentation is clearly revealed in the Si:1s photoionization of FSMSE.

