Fragmentation of multiply ionized CF₃–CH₂F induced by charge-changing collisions with fast carbon ions

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We have investigated multiple ionization and fragmentation of 1,1,1,2-tetrafluoroethane (CF₃–CH₂F) in charge-changing collisions with 580-keV C⁺. By measuring the number of emitted electrons in each collision, we obtained the charge state (r) distribution of multiply ionized CF₃–CH₂F^{r+*} ions transiently formed as intermediate states prior to fragmentation. The mean charge states of CF₃–CH₂F^{r+*} in single-electron (1e)-capture, 1e-loss, and double-electron-loss collisions were determined to be 1.9, 3.2, and 4.0, respectively. Time-of-flight mass spectra of the product ions from CF₃–CH₂F^{r+*} were obtained as a function of r from coincidence measurements with the number of emitted electrons. Production of specific fragment ions and variation of the

fragmentation patterns were systematically revealed up to r = 4. For example, it was found that proton emission becomes the dominant decay process from multiply ionized CF₃–CH₂F^{*r*+}. The results also show that coincidence measurements can distinguish ion species with the same mass-to-charge ratio but different charge states. The characteristic features of the fragmentation processes of CF₃–CH₂F^{*r*+*} were investigated by the correlation among the product ions for $r \ge 2$. C⁺ and C₂⁺ fragment ions are emitted to the same side as H⁺ even at r = 2, reflecting the structural feature of the asymmetric location of the heavier atoms (F) in the molecule.

Keywords: Multiple ionization; Coulomb explosion; Fast ion collision; Time of flight; Hydrofluorocarbon

1. Introduction

Multiple ionization of molecules is a fundamental process induced by fast heavy ion or highly charged ion collisions. It is an important process in radiation physics, astrophysics, and the atmospheric sciences for initiating a series of physicochemical reactions [1,2]. Understanding the fragmentation processes of multiply ionized molecules is important because these processes may generate characteristic product ions with high kinetic energy by specific unimolecular reaction processes that depend on the charge state.

The recent development and increased usage of intense short laser pulses have made it easier to access highly charged molecular ions. One of unique applications of highly ionized molecules is Coulomb explosion imaging [3], which can be used to determine the geometrical structures of molecules for some special purposes, such as determination of the chirality of enantiomers [4–7] or transient structures existing for only a limited period of time [8,9]. In this regard, careful consideration is required because the explosion images do not always simply represent the original geometrical configurations. For example, when a molecule includes a heavy atom, the heavy atom can strongly affect the emission directions of other lighter fragments, such as in fragmentation of multiply ionized hexa-fluorobenzene (C_6F_6) [10] and diiodoacetylenes (C_2I_2 and C_4I_2) [11,12]. To take full advantage of the techniques, further investigation of the mechanisms of Coulomb explosion for various types of molecules is required.

A large number of detailed studies of the fragmentation processes of multiply ionized molecules have focused on relatively small molecules using coincidence measurements of the fragment ions [2,13]. For small molecules, the distribution of multiple ionization is obtained from the sum of the charges of the fragment ions [14–16].

However, it is not straightforward to extend the techniques to larger polyatomic molecules because a large number of fragment ions and neutrals can be produced. Martin *et al.* overcame this difficulty by using a technique to measure the number of electrons emitted in each collision with a semiconductor detector [17]. Measurement of the number of electrons directly provide the degree of multiple ionization. Thus, coincidence measurements of the number of emitted electrons with product ions enable systematic investigation of the fragmentation processes of multiply ionized molecular ions as a function of the charge state. In our previous works, we applied this technique to study fragmentation of multiply ionized C_{60} [18,19] and ethane (C_2H_6) [20] in fast heavy ion collisions.

In this study, we investigated multiple ionization and fragmentation of 1,1,1,2-tetrafluoroethane (CF₃–CH₂F) induced by charge-changing collisions with 580-keV C⁺. This hydrofluorocarbon molecule has an analogous structure to C₂H₆, but four of the hydrogen atoms of C₂H₆ are substituted by fluorine atoms, as shown in Fig. 1. The number of fragmentation pathways is thus higher than for C₂H₆ because of the presence of C–F bonds in addition to C–C and C–H bonds. Furthermore, this molecule is a good example to study the Coulomb explosion dynamics because of the structural feature that the heavier atoms (F) are asymmetrically located outside the lighter atoms (C). Fragmentation of singly charged CF₃–CH₂F⁺ ions has previously been investigated by vacuum-ultraviolet (VUV) irradiation in the context of atmospheric science, because CF₃–CH₂F is known to have a high global warming potential even though it is used as an alternative refrigerant to chlorofluorocarbons to protect the ozone layer [21–23]. Two independent groups have reported consistent results of the product ion species from combined studies of photoelectron–photoion coincidence spectroscopy and quantum

chemical calculations [21–23]. Here, we report the product ion distributions from the multiply ionized states of CF_3 – CH_2F^{r+*} for r = 1–4. We also show the potential of this measurement to distinguish ion species with the same mass-to-charge ratio but different charge states. The influence of a different amount of internal excitation is also qualitatively investigated by separately measuring the distributions under different charge-changing conditions of single-electron (1*e*)-capture, 1*e*-loss, and double-electron (2*e*)-loss collisions. In addition, the fragmentation processes and dynamics are discussed by considering the correlation between the fragment ions produced in each event.

2. Experimental

The experiments were performed at the 1.7-MV tandem accelerator facility of the Quantum Science and Engineering Center, Kyoto University. The experimental procedures used in this study have been described in detail elsewhere [20]. In brief, a well-collimated 580-keV C⁺ beam was incident on a gaseous CF₃–CH₂F target after being charge purified by a magnetic charge selector just before entering the collision chamber. The target gas pressure was about 5×10^{-4} Pa. The product ions were detected by a microchannel plate (MCP) detector. The detection efficiency is limited by the transmission of the grid meshes of the electrodes and the efficiency of the detector. The detection probability of each product ion was estimated to be about 0.2 [20]. Thus, the probability of the detection of three or more fragment ions produced in a single event becomes extremely low. The ion signals were recorded with a digital storage oscilloscope (WavePro7000, LeCroy, Chestnut Ridge, NY) at every event. The mass-to-charge ratios of the detected ions were analyzed by time-of-flight (TOF)

measurements. The outgoing projectile ions with different charge states were separated by an electrostatic deflector and selectively detected by a movable semiconductor detector. Detection of the charge-selected outgoing ions was used as a timing trigger for the TOF measurements. The measurements were performed under three different charge-changing conditions: 1*e*-capture, 1*e*-loss, and 2*e*-loss collisions, corresponding to the detection of C^0 , C^{2+} and C^{3+} , respectively.

The electrons emitted in the collisions were detected by another semiconductor detector (SSD_e) at a potential biased at +25 kV to measure the number of electrons n_e . When n_e electrons are detected in a certain collision event, the pulse height of the SSD_e signal corresponds to $25n_e$ keV. The pulse heights of the SSD_e signals were recorded by a multichannel analyzer in coincidence with the product ions of each collision event. Hereafter, the pulse height distribution will be referred to as the " n_e spectrum". The distribution of n_e can be derived by analyzing the n_e spectrum with a fitting procedure [18–20]. In the fitting analysis, we corrected for the effects of the collection efficiency of the electrons and backscattered electrons on the surface of the SSD_e [24].

The TOF spectra of the product ions were separately determined for the different charge states of the intermediate states (referred to as "partial TOF spectra") from the coincidence measurements as follows. First, we extracted the data of the collision events in which the SSD_e signals have pulse heights within a suitable range corresponding to a specific n_e . In the extracted data, some contributions from collision events with higher n_e are mixed owing to the effects of missed and backscattered electrons. The fraction of the mixed component can be readily estimated in the fitting analysis of the n_e spectrum. The extracted data were thus corrected by subtracting the mixed contributions of higher n_e .

3. Results and discussion

Figure 1 shows an example of a two-dimensional (2D) coincidence map between the TOF of the product ions on the horizontal axis and the pulse height of the SSD_e signal on the vertical axis. The latter represent the number of emitted electrons n_e . Projection of the 2D data onto the horizontal axis provides the total TOF spectrum. A variety of fragment ions are observed, as denoted above the TOF peaks. Projection onto the vertical axis provides the total n_e spectrum. It has successive peaks up to $n_e \approx 6$ or 7 in this example. Note that data points in the region of $n_e = 0$ and 1 appear owing to the effects of the missed and backscattered electrons. The 2D map shows a correlation between the product ion species and n_e (or the charge state of the intermediate ion). For example, higher degrees of multiple ionization tend to be correlated with smaller fragment ions. Variation of the fragmentation pattern as a function of n_e will be discussed in detail in Section 3.2. Another feature of the 2D map is that the shape of the F⁺ spots becomes broader with increasing n_e . This clearly shows an increase of the kinetic energy (KE) of F⁺ as a function of n_e .

3.1. Multiple ionization

Figure 2(a) shows the distributions of the charge state r of the intermediate CF₃-CH₂F^{r+*} ions under the three different charge-changing conditions obtained by analyzing the total n_e spectra with the fitting procedure. r is related to n_e by $r = n_e + 1$, $n_e - 1$, and $n_e - 2$ for 1*e*-capture, 1*e*-loss, and 2*e*-loss collisions, respectively. This is because in 1*e*-capture collisions, one electron is transferred to the projectile ion in addition to ejection of n_e electrons into the vacuum, while in electron-loss collisions,

electrons emitted from the projectile ions are also included in the n_e electrons. In 1*e*-capture collisions, about half of the events are pure electron capture processes, which involve no direct ionization, and the other half accompany emission of a few electrons. In contrast, electron-loss collisions induce higher degrees of multiple ionization up to $r \approx 10$. The mean charge states of the intermediate ions are 1.9, 3.2 and 4.0 for 1*e*-capture, 1*e*-loss, and 2*e*-loss collisions, respectively. This means that electron-loss collisions preferentially occur with smaller impact parameters in this collision system.

In Fig. 2(a), the r distributions are compared with those obtained with a C_2H_6 target in 1e-capture and 1e-loss collisions with the same projectile conditions [20]. The appearance energies of CF₃-CH₂F⁺ and C₂H₆⁺ were reported to be 12.64 ± 0.05 [23] and 11 ± 1 eV [25], respectively. The distribution for the 1*e*-loss condition is normalized at r = 1 to compare the relative probabilities of multiple ionization with single ionization. The distribution for the 1*e*-capture condition is normalized at r = 2 to compare the multiple ionization probabilities in addition to the 1*e*-capture process. Compared with CF_3 - CH_2F , the relative probabilities of multiple ionization of C_2H_6 are considerably lower for r > 3. Figure 2(b) shows a plot of the ratios of the relative probabilities of multiple ionization of C₂H₆ to those of CF₃-CH₂F. The ratios rapidly decrease at r = 4 and monotonically decrease for both 1*e*-capture and 1*e*-loss collisions. The results indicate that the total ionization energies required to produce multiply ionized CF₃–CH₂F^{r+} are lower than those required to produce C₂H₆^{r+} for r > 3, although the appearance energy of singly ionized CF_3 - CH_2F^+ ions is slightly higher than that of $C_2H_6^+$, as mentioned above. This is probably because of the larger number of valence electrons in CF₃–CH₂F.

3.2. Distributions of the product ions in charge-changing collisions

The TOF spectra obtained under the different charge-changing conditions are shown in Fig. 3. The distribution of the product ions shifts to smaller fragment ions from 1*e*-capture to 1*e*- and 2*e*-loss conditions. This again indicates that electron-loss collisions occur with smaller impact parameters involving higher amounts of energy deposition, as shown in the distributions of multiple ionization.

The partial TOF spectra for r = 1-4 are shown in Fig. 4. For the same r, the partial spectra have similar distributions regardless of the charge-changing conditions. This is in contrast to the different total TOF spectra. This means that the fragmentation behavior is mainly governed by the intermediate r. The different total spectra can be mainly explained by the different distribution of r achieved under the different charge-changing conditions.

Careful inspection of Fig. 4 shows that the degrees of fragmentation are slightly enhanced in electron-loss collisions compared with those in 1*e*-capture collisions at the same *r*. This is attributed to the higher amounts of internal excitation energy in the electron-loss collisions when the same *r* is achieved. This feature is the same as that observed for C_{60} [18,19] and C_2H_6 targets [20]. As discussed in previous studies [18–20], from a statistical viewpoint, the amount of internal excitation is considered to be correlated with the number of "pure ionizations", which does not include the number of electrons captured in the projectile. In other words, electron-capture collisions can shift the relationship between the degree of multiple ionization and the internal excitation.

3.3. Product ions from singly charged states (r = 1)

As shown in Fig. 4, in 1e-capture collisions, singly charged intermediate ions

 $C_2H_2F_4^{+*}$ (r = 1) mainly produce $C_2H_2F_3^+$, CF_3^+ , and CH_2F^+ ions. This is consistent with the fragmentation pattern observed after VUV photoabsorption [21,23]. In 1*e*- and 2*e*-loss collisions, smaller fragment ions, including atomic fragment ions (H⁺, F⁺ and C⁺), are enhanced by higher internal excitation. The intensity of the intact CF_3 – CH_2F^+ ion is negligible. It has been reported that the threshold for C–C bond breaking (CH_2F^+ + CF_3 , 12.99±0.05 eV) is only 0.35 eV above the appearance energy of the intact CF_3 – CH_2F^+ ion (12.64±0.05 eV) [23]. Thus, in fast ion collisions, singly ionized intermediate CF_3 – CH_2F^{+*} ions are unstable against fragmentation owing to internal excitation together with ionization.

The mean KEs of CF_3^+ and CH_2F^+ are 0.10 and 0.20 eV from the full widths at half maximum (FWHMs) of the TOF peaks, which are fitted well by Gaussian functions. They provide kinetic energy release (KER) values of 0.30 eV for both the $CF_3^+ + CH_2F$ and $CF_3 + CH_2F^+$ processes based on the assumption of two-body fragmentation. The mean KER values associated with these two processes as a function of the photon energy have been reported in a VUV photoabsorption study [23]. The KER of 0.30 eV corresponds to the results at photon energies around 17–20 eV. This means that the fragmentation pathways of $CF_3^+ + CH_2F$ and $CF_3 + CH_2F^+$ are associated with an average energy transfer of about 17–20 eV (including the ionization energy of 12.64 eV [23]) in the present collision system.

The $C_2H_2F_3^+$ ion is produced by C–F bond breaking ($C_2H_2F_3^+ + F$). The mean KE of $C_2H_2F_3^+$ is estimated to be 0.26 eV from the FWHMs of the fitted Gaussian functions. This gives a KER of 1.4 eV for the fragmentation process $C_2H_2F_3^+ + F$. This KER is in good agreement with the KER of 1.44 eV obtained in a photodissociation experiment at the photon energy of 18.02 eV [23]. This indicates that this fragmentation pathway is associated with an average energy transfer of about 18 eV. It has been reported that $C_2H_2F_3^+$ is selectively observed through the first and second excited states of the singly charged CF_3 - CH_2F^{+*} ion after electron removal from the F $2p \pi$ lone-pair orbitals [21,23]. This process proceeds as "direct impulsive fission", in which removal of a localized electron in a F atom leads to rapid fission of the C-F bond before energy dispersion into other vibrational modes. The same order of the KER obtained in the present experiment indicates that this is also valid for fragmentation induced by fast ion collisions.

The high probability of C-C bond breaking of the singly charged intermediate $CF_3-CH_2F^{+*}$ ion is in contrast to the case of $C_2H_6^{+*}$. The sums of the branching ratios producing fragment ions containing only one carbon atom, i.e., $CH_nF_m^+$ (n = 0-2, m =0-3), are 66%, 60%, and 52% at r = 1 in 1*e*-capture, 1*e*-loss, and 2*e*-loss collisions, respectively. In contrast, for C₂H₆, the branching ratios producing C₂H_n⁺ ions (n = 0-6) are 92% and 71% under the 1e-capture and 1e-loss conditions of 580-keV C⁺, respectively [20], indicating that the branching ratios of C-C bond breaking are less than 8% and 29%. Low branching ratios of C–C bond breaking for $C_2H_6^{+*}$ were also obtained in VUV photodissociation [25] and electron-impact experiments [26]. The fragmentation pathways of $CH_2F^+ + CF_3$ and $CH_2F + CF_3^+$ have lower appearance energies of 12.99 and 13.12 eV compared with that of 15.07 eV for $C_2H_2F_3^+ + F$ [23]. According to a quantum chemical calculation, production of $CF_{3^{+}}$ or $CH_{2}F^{+}$ by C–C bond breaking can be induced by ionization or excitation of the highest occupied molecular orbital electron, which has C–C σ -bonding character [23]. On the other hand, the lowest fragmentation pathway from $C_2H_6^+$ has been reported to be $C_2H_4^+ + H_2$, where the appearance energy is in the range 11.0–12.7 eV [25,26]. The lowest threshold

for breaking of the C–C bond of $C_2H_6^{+*}$ is $CH_3^+ + CH_3$, which has a slightly higher appearance energy of 14.0 eV [25,26]. Therefore, the different probabilities of C–C bond breaking seem to be explained by the different lowest pathways of CF_3 – CH_2F^{+*} and $C_2H_6^{+*}$. Nevertheless, we consider that this selectivity is nontrivial because, energetically, higher fragmentation pathways are also readily accessible in fast ion collisions. To elucidate the large difference of the branching ratios between these two molecules, further theoretical studies of the potential energy curves and fragmentation dynamics are required.

Production of CHF_{2}^{+} is the fourth strongest peak in the 1*e*-capture condition, as observed in previous studies with VUV irradiation [21–23]. Observation of CHF₂⁺ ions provides clear evidence of migration of H or F atoms before fragmentation because this ion cannot be constructed from either side of the CF₃ or CH₂F groups. Although F atoms are unlikely to migrate compared to H atoms, we cannot exclude the possibility of migration of an F atom because it might be possible if the singly ionized CF_3 - CH_2F^{+*} ions have a sufficiently long lifetime against dissociation. This assignment demonstrates an advantage of the present measurement of the number of emitted electrons. The CHF₂⁺ ion has the same mass-to-charge ratio as the doubly charged intact CF₃–CH₂F²⁺ ion. Thus, in principle, they cannot be definitely assigned only from the TOF. If they have greatly different KE distributions, such as the case of N^+ and N_2^{2+} produced from nitrogen molecules, they could be readily distinguished because of different broadening of the peaks in the TOF spectra [27-30]. However, this is not the case in the present measurements because CHF_2^+ ions are mainly produced from singly charged intermediate ions with low KE. Thus, the peak of CHF₂⁺ has only a single narrow structure. In the present study, production of the CHF_2^+ ion was confirmed with the aid of measurements of the number of electrons. This example demonstrates another advantage of counting the number of electrons to separate product ions with equal mass-to-charge ratio.

3.4. Product ions from multiply charged states ($r \ge 2$)

When doubly charged intermediate $C_2H_2F_4^{2+*}$ (r = 2) ions are produced, H⁺ emission becomes the dominant process. Production of CF_n^+ (n = 0-3) and CH_n^+ (n = 0-2) ions increases by enhancement of C–C bond breaking and emission of neutral H and F atoms. The TOF peaks of the CF_n^+ and CH_n^+ ions are broader than those for r = 1 because of the higher KEs caused by Coulomb repulsion. F⁺ ions are also emitted, although the intensity of the F⁺ peak is lower than that of the H⁺ peak. Product ions retaining the C–C bond are observed in the form of $C_2HF_n^+$ (n = 0-3) and C_2^+ . Note that the $C_2HF_3^+$ ion is only formed from doubly charged intermediate ions (r = 2), and it has not been observed in photofragmentation experiments with VUV irradiation [21,23]. Atomic fragment and CF^+ ions are the major fragment ions produced from triply charged intermediate ions (r= 3). For r = 4, doubly charged fragment ions (i.e., C^{2+} and F^{2+}) start to be observed.

 $C_2F_n^+$ ions (with no hydrogen atoms) are nearly absent, except for C_2^+ . This means that after one H atom or ion is emitted, the second H atom seems to be strongly bound and is only released when all of the F atoms are released together. To investigate the fragmentation processes of multiply charged $CF_3-CFH_2^{r+*}$ ions, a correlation map of the TOFs between two ions detected in coincidence is plotted in Fig. 5. Here, we show integrated data including the contributions from all of the charge states because the main features of the islands in the correlation map discussed below are common for different *r* in the present experiment. $C_2HF_n^+$ (*n* = 1–3) ions are preferentially produced together with H^+ rather than F^+ . In addition, production of H_2^+ ions is mainly correlated with the CF⁺ fragment ion, although the production mechanism is unclear. To understand the behavior of emission of two H atoms, further theoretical evidence is required.

The slope of an island in the correlation map represents the relationship between the momenta of the two product ions [31]. As a typical example, various combinations of $CH_nF_m^+-CH_n'F_{m'}^+$ pairs have distributions with a slope of nearly -1. A slope of -1 indicates that the two ions are emitted in opposite directions with the same momentum. Thus, pairs of $CH_nF_m^+$ and $CH_n'F_{m'}^+$ ions are essentially generated by two-body fragmentation, although the shapes of the islands becomes broader with decreasing *n*, *m*, *n'*, and *m'* owing to the influence of the momentum carried away by other fragments.

In Fig. 5, the slopes of the islands associated with the H⁺ ion have long vertical shapes. The vertical shapes indicate that H⁺ ions have smaller momentum than the momentum of the counterions. Momentum conservation requires that undetected other fragments carry away the corresponding momentum. A similar tendency has been reported for fragmentation of gas-phase nucleobase molecules [32,33] and C₂H₂ [34]. It has been suggested that H⁺ is rapidly emitted prior to fragmentation of the residual part consisting of heavier atoms [33,35]. The heavier fragments gain high momentum owing to the relatively large KER in a subsequent fragmentation step. Similar sequential fragmentation processes followed by prompt proton emission are expected to occur in fragmentation of multiply charged CF_3 - CFH_2^{r+*} .

The island for the correlation between H^+ and C^+ ions has a positive slope, meaning that these two fragment ions are mostly emitted in the same direction. The correlation between H^+ and C_2^+ also has a slightly positive slope. This clearly show the "mass effect", as reported in studies of fragmentation of diiodoacetylenes [11,12] where C fragment ions are emitted in the vertical direction of the molecular axis because of the existence of heavy I atoms. Interference of C atoms by F atoms was also reported in the Coulomb explosion of multiply ionized C_6F_6 [10]. In the present experiment, C⁺ and C₂⁺ ions are blocked and repelled by the three F atoms existing on one side of the molecule. As a result, C⁺ and C₂⁺ are emitted in the direction of H⁺. This tendency is observed for $r \ge 2$. For r = 2, the momentum of the C⁺ or C₂⁺ ions balances that of the neutral F atoms rather than that of the H⁺ ions, regardless of the Coulomb repulsion. This shows the characteristic fragmentation dynamics of a molecule with asymmetric location of heavy atoms in the molecule.

4. Summary

We have investigated multiple ionization and fragmentation of CF_3 – CH_2F molecules induced by 580-keV C⁺ under 1*e*-capture, 1*e*-loss, and 2*e*-loss conditions. By measuring the number of emitted electrons, the relative probabilities of multiple ionization of CF_3 – CH_2F were obtained. The distribution of *r* of intermediate CF_3 – CH_2F^{r+*} ions drastically changes depending on the charge-changing conditions. The mean charge states of the intermediate ions are 1.9, 3.2, and 4.0 in 1*e*-capture, 1*e*-loss and 2*e*-loss collisions, respectively. Coincidence measurements between the number of electrons and TOFs of the product ions gave the product-ion distributions as a function of *r* of the intermediate CF_3 – CH_2F^{r+*} ion. The results show that the degree of fragmentation increases with increasing *r*. The partial TOF spectra for a certain *r* exhibit comparable fragmentation patterns regardless of the charge-changing condition. The markedly different fragmentation patterns in the total TOF spectra can be ascribed to the different degree of multiple ionization achieved in the different charge-changing conditions. We also found that the degree of fragmentation in the partial TOF spectra is slightly enhanced in electron-loss collisions, reflecting higher internal energies. The product ion species from singly charged intermediate ions (r = 1) are in good agreement with those obtained by VUV irradiation. Prompt H⁺ emission seems to be the dominant decay process from multiply ionized CF₃–CH₂F^{r+}. As a characteristic feature of fragmentation of CF₃–CH₂F^{r+*}, we found that C⁺ and C₂⁺ fragment ions are emitted to the same side as H⁺ even at r = 2. The directions of the C⁺ and C₂⁺ ions are governed by the imbalance of the geometrical distribution of F atoms rather than repulsion from the H⁺ ion. We also shown that coincidence measurements with the number of emitted electrons can identify product ion species with the same mass-to-charge ratio but different charge states.

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Figure captions

Figure 1. 2D coincidence map between the TOF and n_e obtained in 1*e*-loss collisions of 580-keV C⁺ with CF₃–CH₂F molecules.

Figure 2. (a) Distribution of the charge state r of the intermediate CF₃-CH₂F^{r+*} ions produced by 580-keV C⁺ collisions under different charge-changing conditions. The distributions for C₂H₆ are also shown under the 1*e*-capture and 1*e*-loss conditions [20]. (b) Ratios of the relative probabilities of multiple ionization of C₂H₆ to those of CF₃-CH₂F for different r. The values are normalized at r = 2 and 1 for the 1*e*-capture and 1*e*-loss conditions, respectively.

Figure 3. Total TOF spectra of the product ions from CF_3 – CH_2F molecules in 1*e*-capture, 1*e*-loss, and 2*e*-loss collisions of 580 keV C⁺.

Figure 4. Partial TOF spectra of the product ions from multiply ionized $CF_3-CH_2F^{r+*}$ in 1*e*-capture, 1*e*-loss, and 2*e*-loss collisions with 580-keV C⁺ for r = 1-4.

Figure 5. Correlation map between TOF of the first detected ion (TOF 1) and TOF of the second detected ion (TOF 2) in 1*e*-capture collisions between 580-keV C⁺ and CF₃-CH₂F.



Fig. 1







Fig. 3



Fig. 4



580 keV $C^+ \rightarrow CF_{3-}CH_2F$ (1e cap.)

Fig. 5