Coulomb explosion dynamics of 1-chloropropane induced by few-cycle intense laser fields

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It has been revealed in a series of our recent studies on hydrocarbon molecules in an intense laser field [1,2] that hydrogen atoms migrate within hydrocarbon cations promptly in the course of the ionization processes in an intense laser field as well as after the ionization. Associated with the hydrogen migration, a large-scale deformation of the skeletal structure of hydrocarbon molecules is expected to proceed. In the present study, we investigate ultrafast nuclear dynamics of 1-chloropropane ($CH_3CH_2CH_2Cl$) having two rotational isomers, i.e., the *gauche* conformer and the *trans* conformer [3], induced by a few-cycle intense laser field by the coincidence momentum imaging (CMI) [4] of the fragment ions produced after the three-body Coulomb explosion of triply-charged parent ions.

Few-cycle near-IR laser pulses (7.2 fs, 800 nm, 5 kHz) are generated by spectral broadening of a Ti:Sapphire laser output using a hollow-core fiber filled with Ar gas and pulse compression using chirped mirrors. The laser beam crosses a sample molecular beam at right angles and it is focused by a concave mirror at the crossing so that the laser field intensity becomes 3.9×10^{14} W/cm^2. The fragment ions generated at the crossing are recorded by a position sensitive detector equipped with delay-line anodes under the velocity map imaging conditions. The momentum vectors of the respective fragment ions are determined by the position of the ions detected on the detector plane and their arrival time at the detector.

In the CMI data, the following two kinds of three-body Coulomb explosion pathways are identified:

$$CH_3CH_2CH_2Cl^{3+} \rightarrow CH_3^+ + C_2H_4^+ + Cl^+ \text{ (\textit{Non-hydrogen-migration pathway})} \quad (1)$$

$$CH_3CH_2CH_2Cl^{3+} \rightarrow CH_3^+ + C_2H_3^+ + HCl^+ \text{ (\textit{Hydrogen-migration pathway}).} \quad (2)$$

Based on the correlation among the momentum vectors of the three fragment ions in the respective pathways, we have revealed that the non-hydrogen-migration pathway is composed of two types of distributions representing the sequential three-body dissociation represented as

$$CH_3CH_2CH_2Cl^{3+} \rightarrow [CH_3CH_2CH_2^{2+} + Cl^+] \rightarrow CH_3^+ + C_2H_4^+ + Cl^+ \quad (3)$$

and the concerted three-body dissociation, in which all the three fragment ions are produced simultaneously from $CH_3CH_2CH_2Cl^{3+}$.

On the other hand, for the hydrogen-migration pathway, we have identified only a distribution assigned to the sequential three-body dissociation represented as

$$CH_3CH_2CH_2Cl^{3+} \rightarrow [CH_3^+ + C_2H_4Cl^+] \rightarrow CH_3^+ + C_2H_3^+ + HCl^+, \quad (4)$$

which indicates that only the sequential process can be realized associated with the finite time duration necessary for the hydrogen migration to proceed.

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