Proton migration in hydrocarbons induced by highly charged ion impact

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Synopsis  After impact by highly charged ion, the trihydrogen ion (H3+) formation channel is observed in CH₄, C₂H₄, and so does the isomerization channel (CH⁺ +CH₂⁺) in C₂H₄. In particular, for the channel H₃⁺ +C₂H⁺, the multi-dimensional potential energy surface of the C₂H₄²⁺ dication has been calculated to find the responsible transition states, in order to figure out the H₃⁺ ion formation mechanism.

Proton migration of hydrocarbon molecules plays a vital role in the chemical reactions concerning, e.g., combustion and interstellar media, which can significantly change the molecules’ properties and thus result in bond rearrangement and/or isomerization processes. Different from the most of previous studies using the light to generate and steer the proton migration channels, the present study reports the dynamics of corresponding channels in three typical hydrocarbon molecules, i.e. CH₄, C₂H₂ and C₂H₄, observed on the 150 kV highly charged ion collision platform at Fudan University in Shanghai [1]. As shown in Fig. 1, kinetic energy releases (KERs) of all two-body breakup channels of CH₄, C₂H₂ and C₂H₄ dications produced by 3 keV/u Ar⁸⁺ ion impact are determined.

Compared to previous photoinduced proton migration studies [2, 3], in the present work the trihydrogen ion (H₃⁺) formation channel is observed with much lower abundance in CH₄, and so does the isomerization channel (C⁺ +CH₂⁺) in C₂H₂. As for C₂H₄ not containing the methyl group, both of the above two kinds of breakup channels are intriguingly present, namely the H₃⁺ +C₂H⁺ and CH⁺ +CH₂⁺ channels. In particular, for the channel H₃⁺ +C₂H⁺, we have explored the multi-dimensional potential energy surface of the C₂H₄²⁺ dication by density functional theory calculations to find the responsible transition states, in order to figure out the H₃⁺ ion formation mechanism. Furthermore, to some extent to control the proton migration processes of e.g. C⁺ +CH₂⁺ employing the highly charged ion beam of different parameters (projectile species, charge state and velocity), as the light have done successfully [4-6].

Figure 1. KER distributions for the (a) H⁺ + C₂H₃⁺, (b) H₂⁺ + C₂H₂⁺, and (c) H₃⁺ + C₂H⁺ channels, respectively.

References

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