Proton migration in hydrocarbons induced by highly charged ion impact

Y. Zhang[1,2], T. Jiang[1,2], L. Wei[3], W. Yu[1,2], R. Hutton[1,2], Y. Zou[1,2], L. Chen[1,2], and B. Wei[1,2] *

[1]Institute of Modern Physics, Fudan University, Shanghai 200433, China
[2]Key Laboratory of Nuclear Physics and Ion-Beam Application (MOE), Fudan University, Shanghai 200433, China
[3]School of Nuclear Science and Technology, Lanzhou University, Lanzhou 730000, China

Synopsis After impact by highly charged ion, the trihydrogen ion (H_3^+) formation channel is observed in CH_4, C_2H_4, and so does the isomerization channel ($CH^+ + CH_3^+$) in C_2H_4. In particular, for the channel $H_3^+ + C_2H^+$, the multi-dimensional potential energy surface of the $C_2H_4^{2+}$ dication has been calculated to find the responsible transition states, in order to figure out the H_3^+ 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. CH_4, C_2H_2 and C_2H_4, 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 CH_4, C_2H_2 and C_2H_4 dications produced by 3 keV/u Ar^{8+} ion impact are determined.

Compared to previous photoinduced proton migration studies [2, 3], in the present work the trihydrogen ion (H_3^+) formation channel is observed with much lower abundance in CH_4, and so does the isomerization channel ($C^+ + CH_2^+$) in C_2H_2. As for C_2H_4 not containing the methyl group, both of the above two kinds of breakup channels are intriguingly present, namely the $H_3^+ + C_2H^+$ and $CH^+ + CH_3^+$ channels. In particular, for the channel $H_3^+ + C_2H^+$, we have explored the multi-dimensional potential energy surface of the $C_2H_4^{2+}$ dication by density functional theory calculations to find the responsible transition states, in order to figure out the H_3^+ ion formation mechanism. Furthermore, to some extent to control the proton migration processes of e.g. $C^+ + CH_2^+$ employing the highly charged ion beam of different parameters (projectile species, charge state and velocity), as the light have done successfully [4-6].

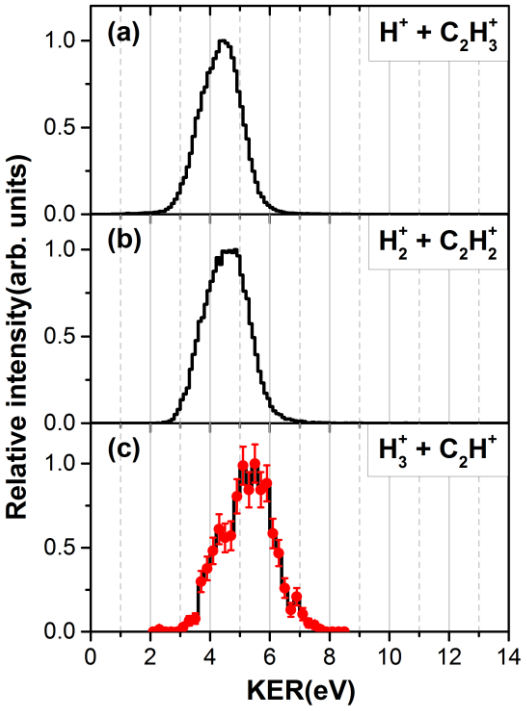

Figure 1. KER distributions for the (a) $H^+ + C_2H_3^+$, (b) $H_2^+ + C_2H_2^+$, and (c) $H_3^+ + C_2H^+$ channels, respectively.

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* E-mail: brwei@fudan.edu.cn