

Isotopic effects on the dynamics of the $\text{CH}_3^+ + \text{H}_2 \rightarrow \text{CH}_5^+ \rightarrow \text{CH}_3^+ + \text{H}_2$ reaction

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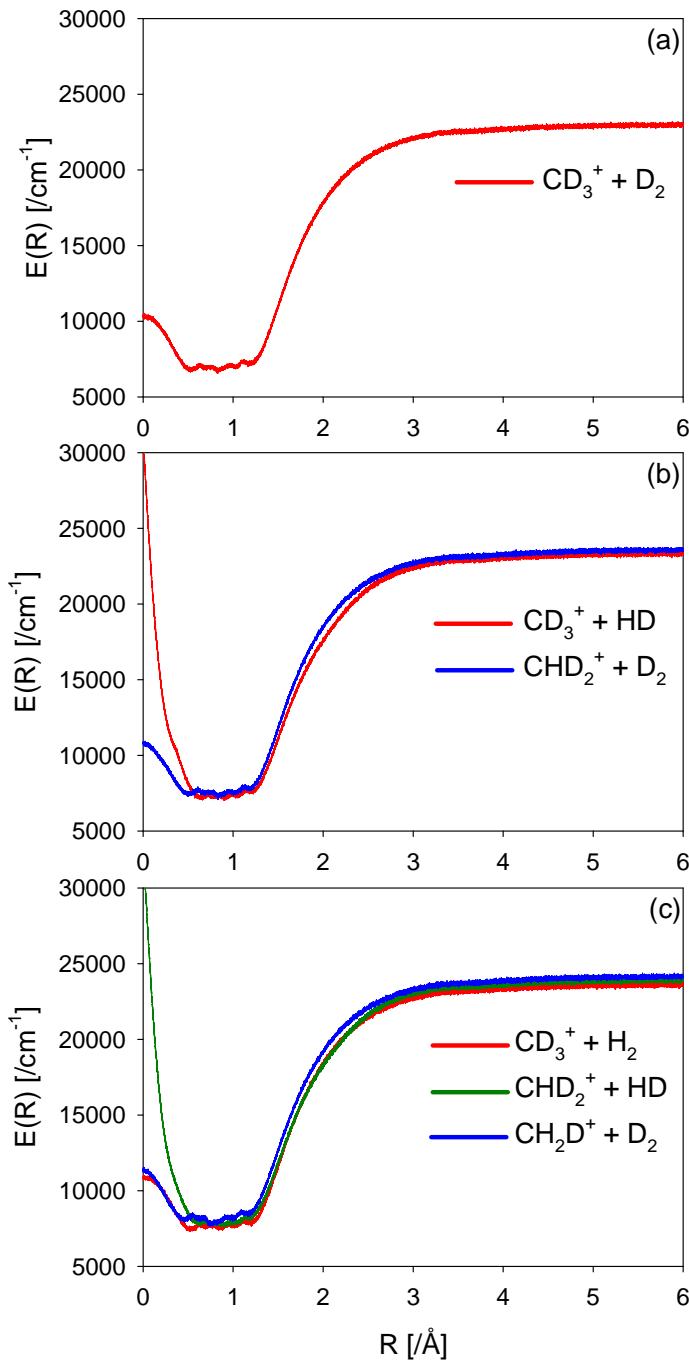


Figure S1: Anharmonic zero-point energy corrected energies as a function of fragment separation for the (a) CD_5^+ , (b) CHD_4^+ , and (c) CH_2D_3^+ systems. The zero in energy is the minimum of the potential surface.

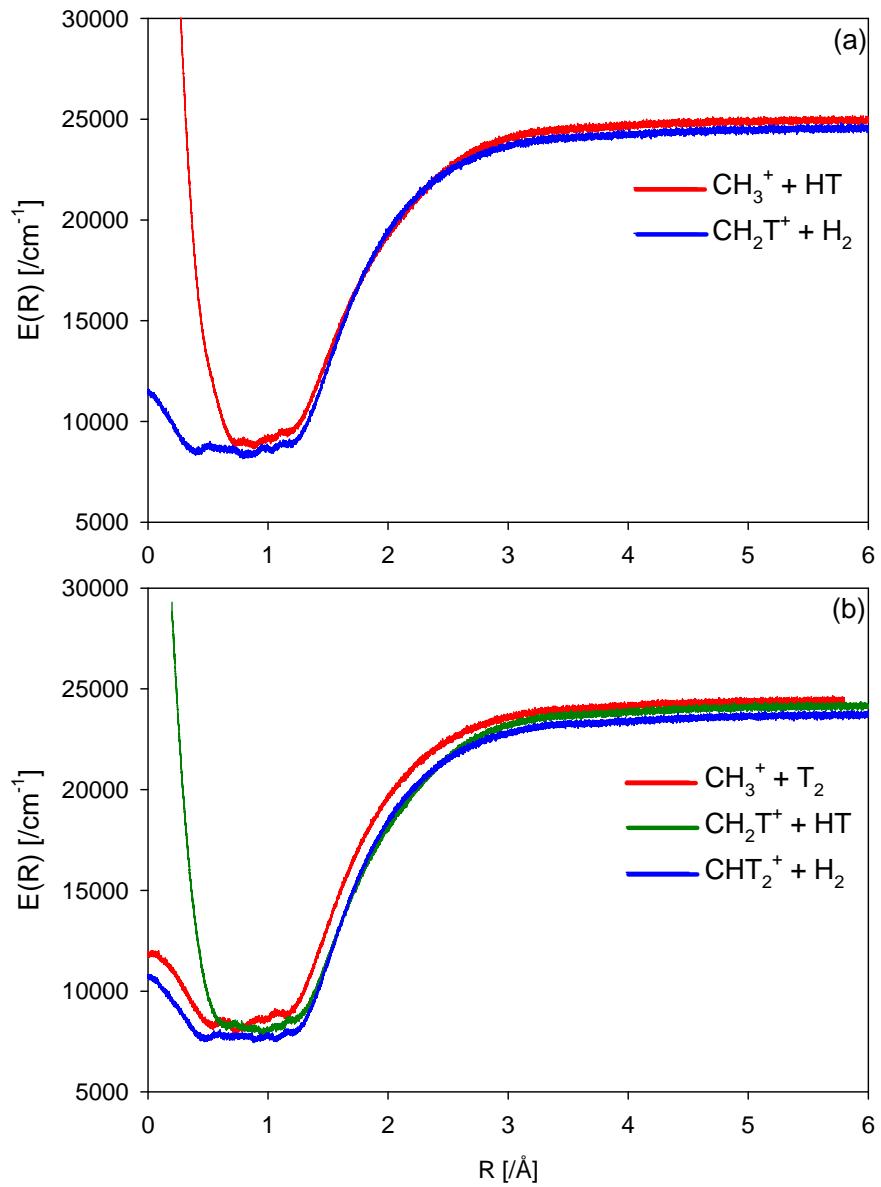


Figure S2: Anharmonic zero-point energy corrected energies as a function of fragment separation for the (a) CH_4T^+ and (b) CH_3T_2^+ systems. The zero in energy is the minimum of the potential surface.

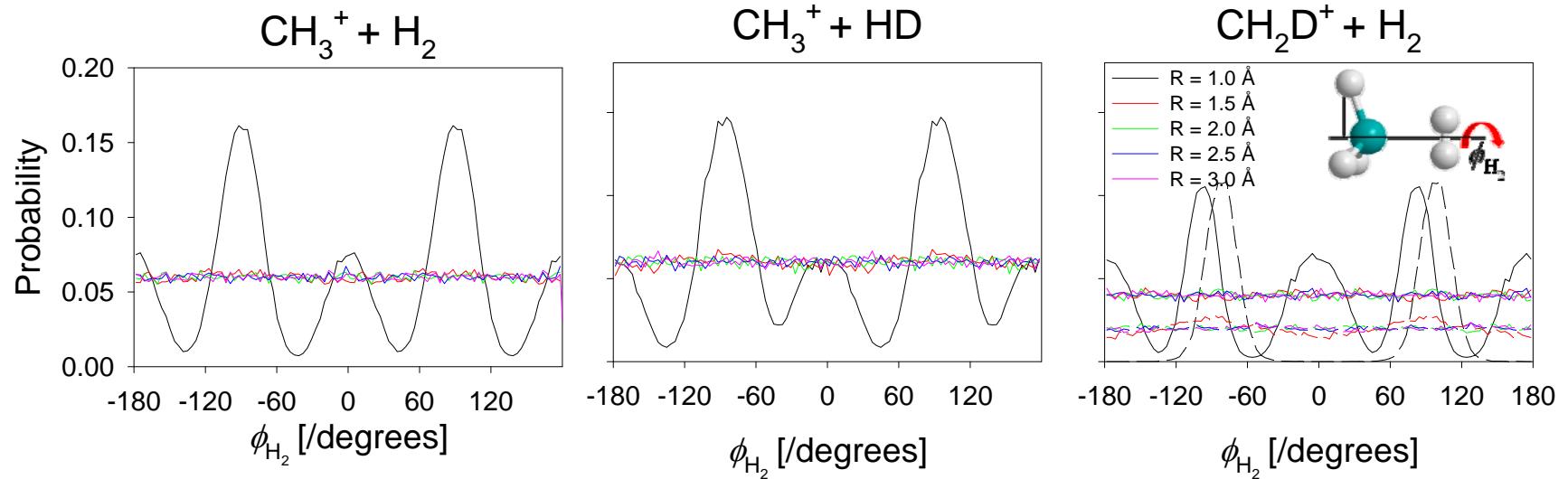


Figure S3: Probability distributions projected onto ϕ_{H_2} (shown in the inset) for $CH_3^+ + H_2$ [left], $CH_3^+ + HD$ [center], and $CH_2D^+ + H_2$ [right] for R ranging from 1.0 to 3.0 Å. Here ϕ_{H_2} is defined as the dihedral angle between the HH bond vector and the vector that connects one of the hydrogen atoms in the CH_3^+ subunit to the center of mass of the carbon atom and the other two hydrogen atoms in that fragment. In the case of $CH_2D^+ + H_2$, there are two unique definitions for ϕ_{H_2} , and the dashed lines represent the case where ϕ_{H_2} is defined using the deuterium atom in the CH_3^+ fragment, while the solid lines provide the results when the hydrogen atom is used to define ϕ_{H_2} .

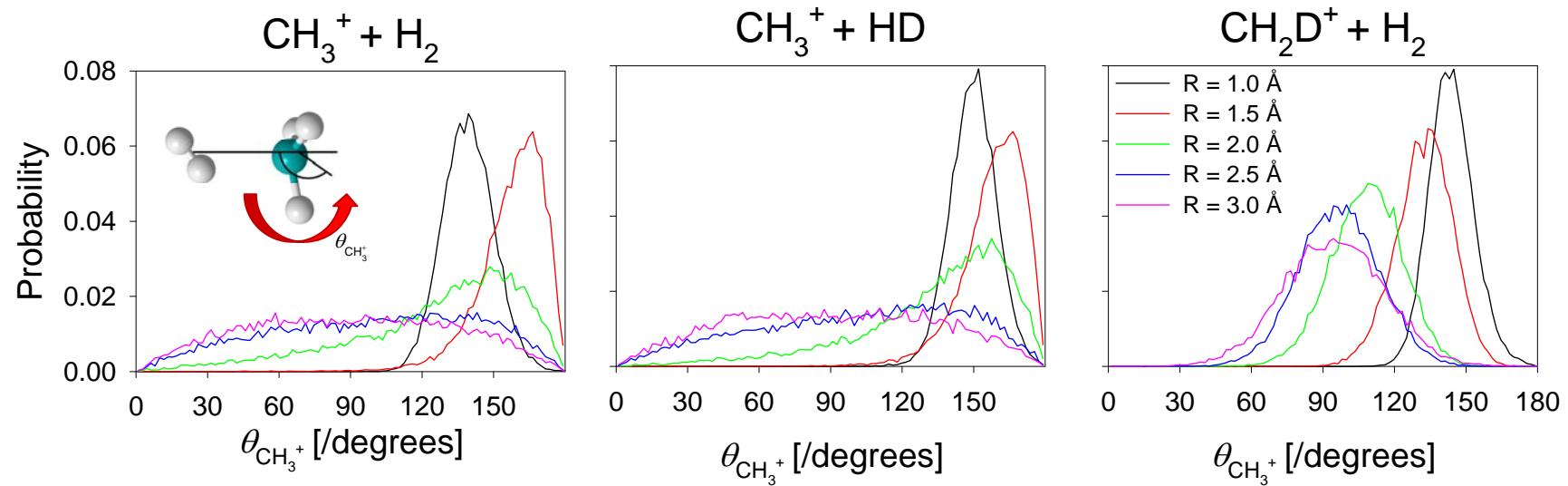


Figure S4: Probability distributions projected onto $\theta_{\text{CH}_3^+}$ (shown in the inset) for $\text{CH}_3^+ + \text{H}_2$ [left], $\text{CH}_3^+ + \text{HD}$ [center], and $\text{CH}_2\text{D}^+ + \text{H}_2$ [right] when $R = 1.0$ to 3.0 Å. The $\theta_{\text{CH}_3^+}$ angle is defined as the angle between R and the vector that connects the center of mass of CH_3^+ to the center of mass of the three hydrogen atoms in the CH_3^+ fragment.

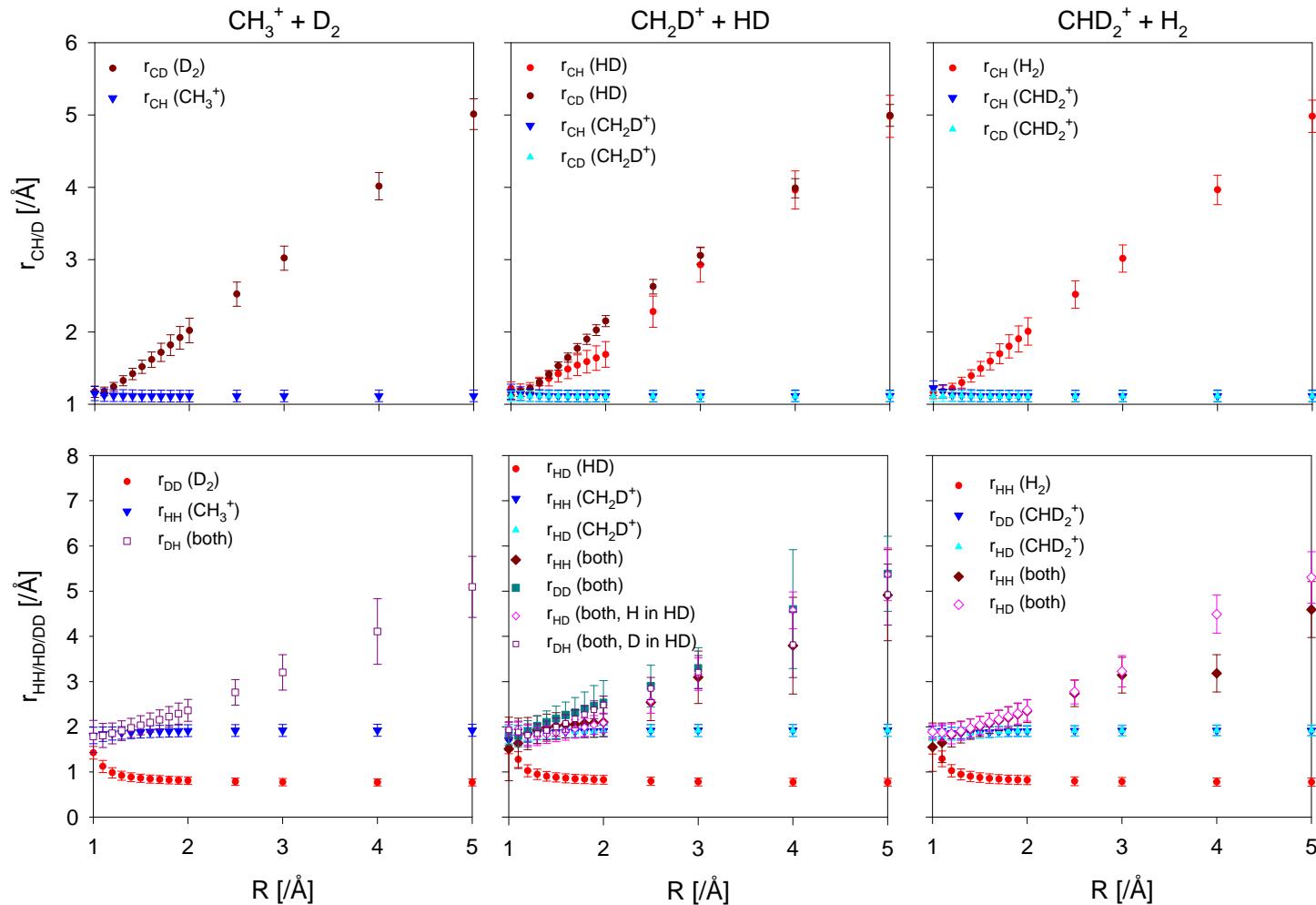


Figure S5: Projections of the probability amplitude for $\text{CH}_3^+ + \text{D}_2$ [left], $\text{CH}_2\text{D}^+ + \text{HD}$ [center], $\text{CHD}_2^+ + \text{H}_2$ [right] onto r_{CH} or r_{CD} [top] and r_{HH} , r_{HD} , or r_{DD} [bottom] are plotted as functions of R . The symbols represent the average values of the quantities of interest, while the error bars provide the widths of the distributions.

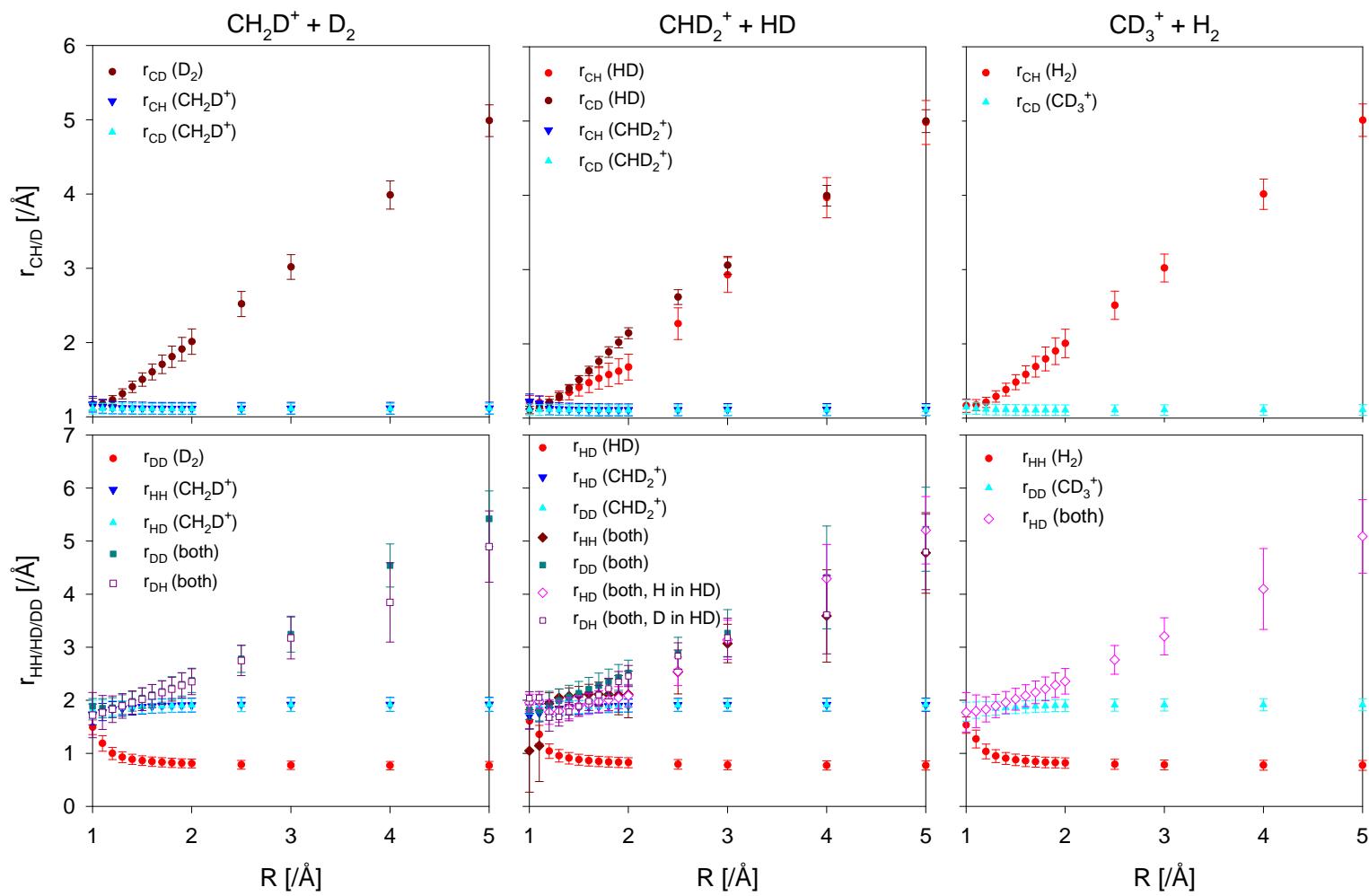


Figure S6: Projections of the probability amplitude for $\text{CH}_2\text{D}^+ + \text{D}_2$ [left], $\text{CHD}_2^+ + \text{HD}$ [center], $\text{CD}_3^+ + \text{H}_2$ [right] onto r_{CH} or r_{CD} [top] and r_{HH} , r_{HD} , or r_{DD} [bottom] are plotted as functions of R . The symbols represent the average values of the quantities of interest, while the error bars provide the widths of the distributions.

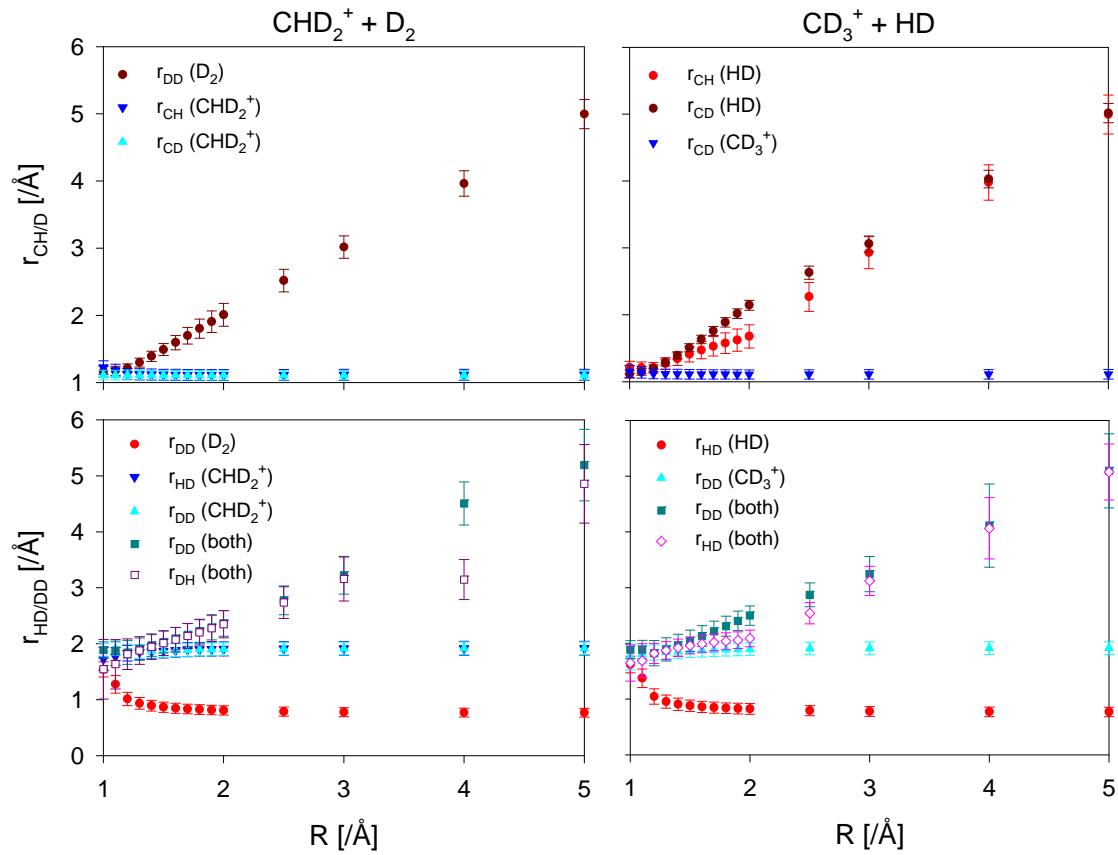


Figure S7: Projections of the probability amplitude for $\text{CHD}_2^+ + \text{D}_2$ [left], $\text{CD}_3^+ + \text{HD}$ [right] onto r_{CH} or r_{CD} [top] and r_{HD} or r_{DD} [bottom] are plotted as functions of R . The symbols represent the average values of the quantities of interest, while the error bars provide the widths of the distributions.

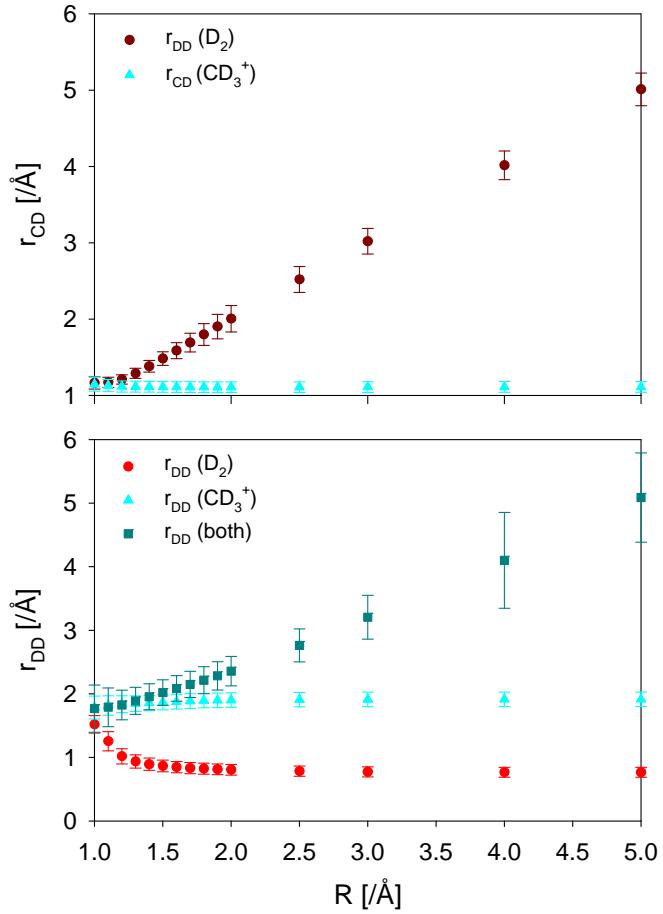


Figure S8: Projections of the probability amplitude for $CD_3^+ + D_2$ onto r_{CD} [top] and r_{DD} [bottom] are plotted as functions of R . The symbols represent the average values of the quantities of interest, while the error bars provide the widths of the distributions.

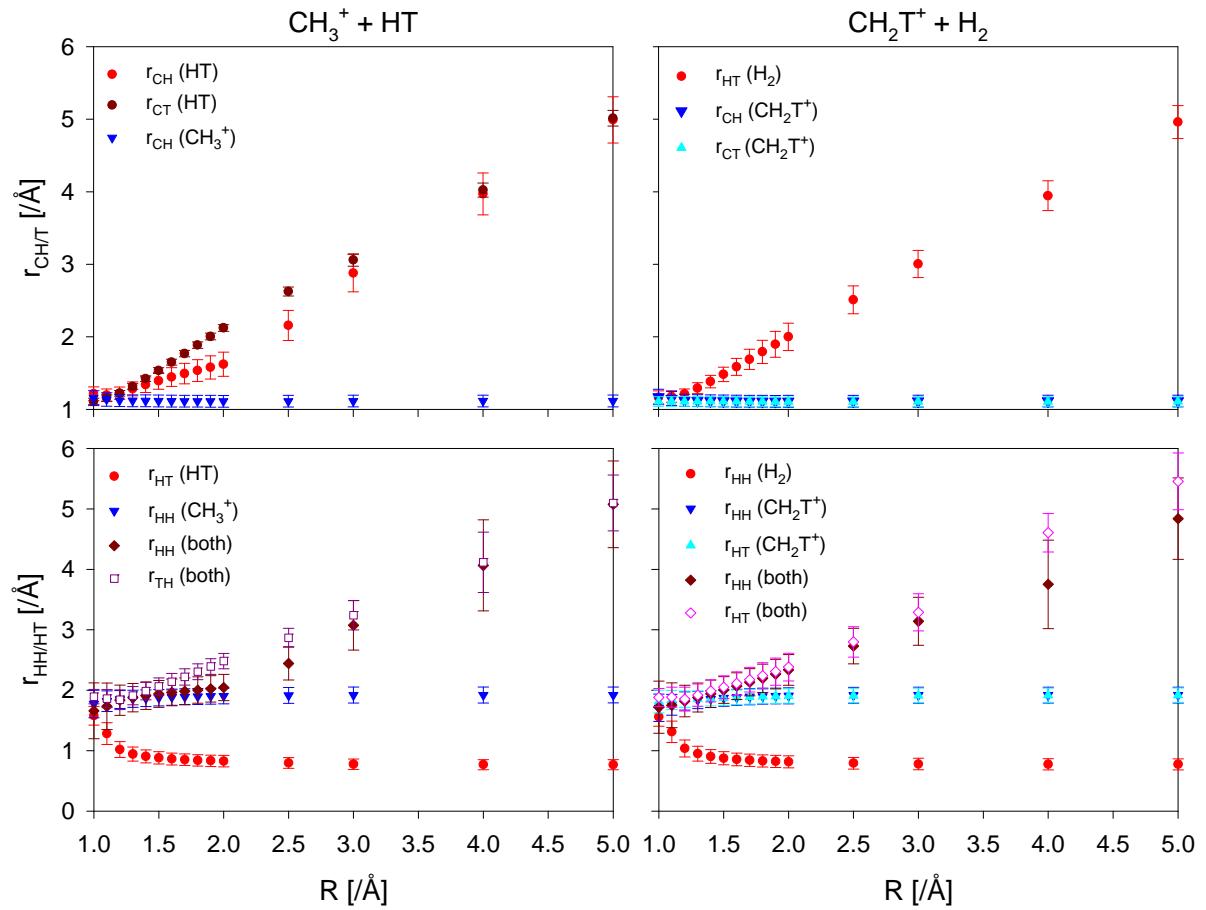


Figure S9: Projections of the probability amplitude for $\text{CH}_3^+ + \text{HT}$ [left], and $\text{CH}_2\text{T}^+ + \text{H}_2$ [right] onto r_{CH} or r_{CT} [top] and r_{HH} or r_{HT} [bottom] are plotted as functions of R . The symbols represent the average values of the quantities of interest, while the error bars provide the widths of the distributions.

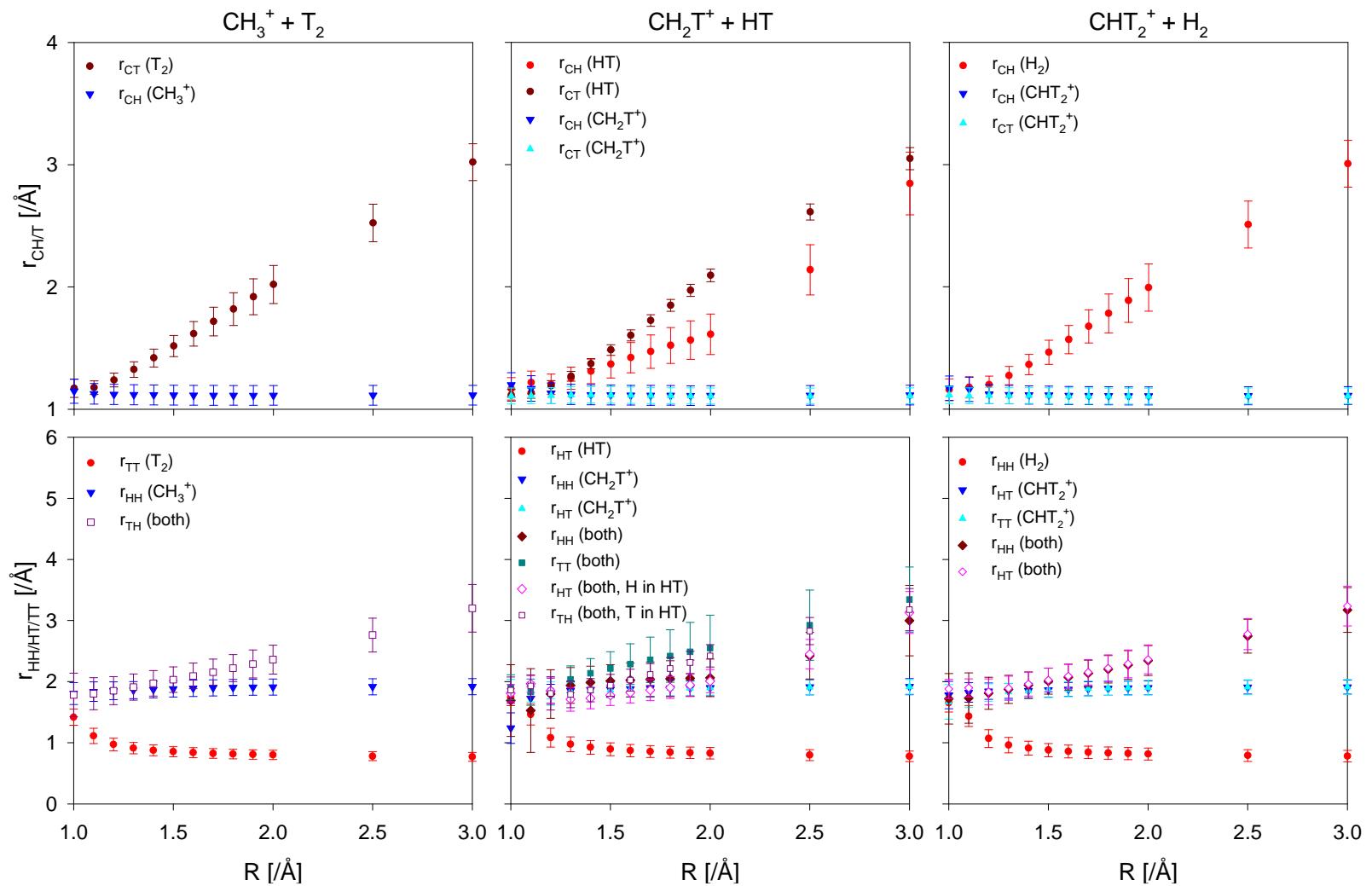


Figure S10: Projections of the probability amplitude for $\text{CH}_3^+ + \text{T}_2$ [left], $\text{CH}_2\text{T}^+ + \text{HT}$ [center], and $\text{CHT}_2^+ + \text{H}_2$ [right] onto r_{CH} or r_{CT} [top] and r_{HH} , r_{HT} or r_{TT} [bottom] are plotted as functions of R . The symbols represent the average values of the quantities of interest, while the error bars provide the widths of the distributions.

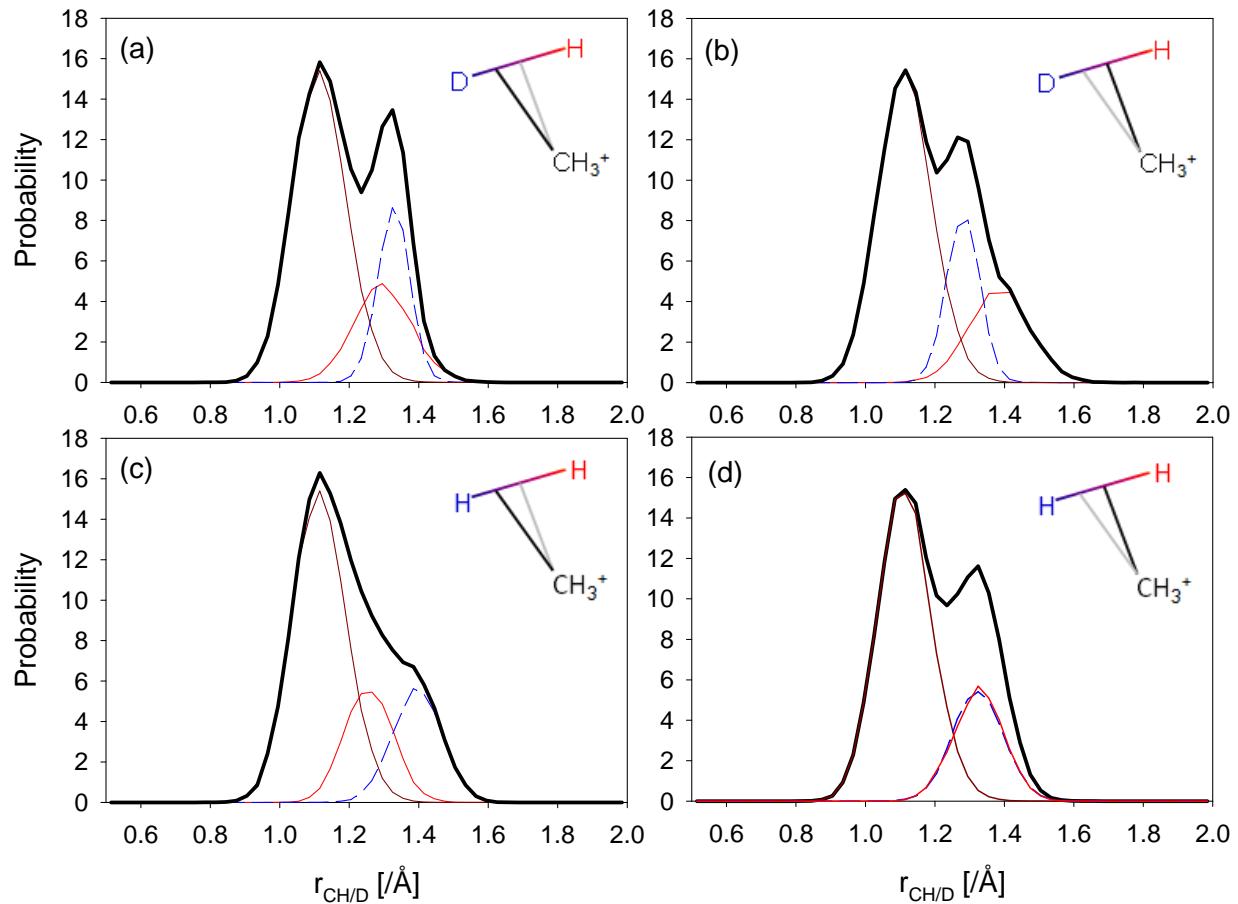


Figure S11: Projections of the probability amplitude for $\text{CH}_3^+ + \text{HD}$ [top] and $\text{CH}_3^+ + \text{H}_2$ [bottom] onto the CH/D distances for $R = 1.3 \text{ \AA}$. As is illustrated in the insets, in the left panels, the simulations were performed with origin of R placed at center of mass of HD, while in the right panels, it is at the center of the H_2 bond axis.

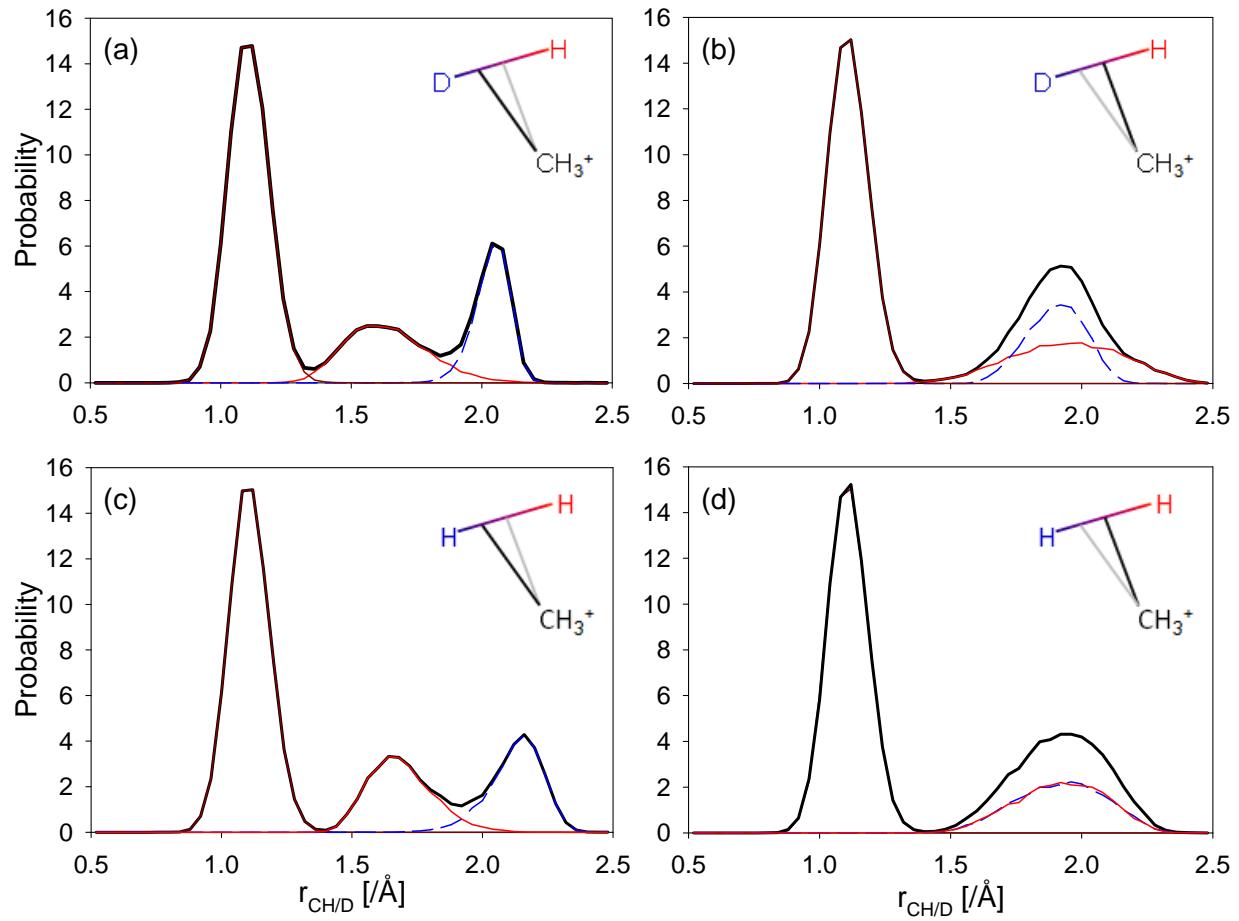


Figure S12: Same as Figure S11, but for $R = 1.9 \text{ \AA}$.