

Description of Additional Supplementary Files

Supplementary Movie 1: A representative AIMD trajectory leading to H_3^+ formation from $\text{CH}_3\text{Cl}^{2+}$.

Supplementary Movie 2: A representative AIMD trajectory leading to H_3^+ formation from $\text{CH}_3\text{OH}^{2+}$.

Supplementary Movie 3: An example of an AIMD trajectory obtained for CH_3F^{2+} , where the liberated H_2 fragment becomes positively charged and dissociates, so that the final products are the CH_2F^+ moiety and a proton.