

PROBING THE REACTION PATH OF $\text{CH}_3^+ + \text{H}_2 \rightarrow \text{CH}_5^+ \rightarrow \text{CH}_3^+ + \text{H}_2$ AND ISOTOPOLOGUES

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Protonated methane has long been of interest to astrochemists due to its presumed importance as a reaction intermediate in the reaction involving $\text{CH}_3^+ + \text{HD}$ within the interstellar medium. Within the interstellar medium there is a nonstatistical H/D isotopic abundance observed for isotopologues of CH_3^+ . While classical trajectory calculations have been performed dissociating CH_5^+ and CH_4D^+ into the fragments, $\text{CH}_3^+ + \text{H}_2$, $\text{CH}_2\text{D}^+ + \text{H}_2$ and $\text{CH}_3^+ + \text{HD}$ ^a, these calculations do not account for a large portion of the available energy being tied up in the zero point energy of the reactants and products. Earlier work in our group on CH_2D_3^+ ^b showed the deuterium atoms were localized to the CH_3^+ group, rather than the H_2 moiety. Classical calculations fail to account for this observed localization, instead showing full delocalization of D between both CH_3^+ and H_2 . With a quantum mechanical treatment, the energetics and wave functions will depend on which asymptotic channel is chosen, while in the classical treatment, these channels will be energetically equivalent. By performing Diffusion Monte Carlo simulations in Jacobi coordinates, we can constrain the distance between the CH_3^+ and H_2 subunits. Using this technique we have evaluated a one-dimensional reaction potential that includes the full anharmonic zero point energy in the remaining degrees of freedom and can determine how energetics of this reaction change upon partial deuteration of CH_3^+ or H_2 . We have also evaluated the probability amplitude associated with the wave functions that are obtained in the DMC simulations at various values of the reaction coordinate.

^aZ. Jin, B. J. Braams, J. M. Bowman, *J. Phys. Chem. A* 110, 1569 (2006).

^bA. B. McCoy, B. J. Braams, A. Brown, X. Huang., Z. Jin, J. M. Bowman, *J. Phys. Chem. A* 108, 4991 (2004).