# DIFFUSION MONTE CARLO CALCULATIONS OF MINIMUM ENERGY PATHS FOR THE ISOTOPIC VARIANTS OF THE $CH_3^+$ + $H_2$ $\leftrightarrow$ $CH_5^+$ $\leftrightarrow$ $CH_3^+$ + $H_2$ REACTION

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Protonated methane is of interest to astrochemists due to its presumed importance as a reaction intermediate in the reaction involving $CH_3^+$ + HD within the interstellar medium. However, within the interstellar medium there is a nonstatistical H/D isotopic abundance observed for the isotopologues of $CH_3^+$. Kinetic studies performed by Gerlich and co-workers determined that the reactions

$$\mathrm{CH_{3-n}D_n^+ + HD \rightarrow CH_{4-n}D_{n+1}^+ \rightarrow CH_{2-n}D_{n+1}^+ + H_2} \tag{1}$$

have identical net rate constants regardless of the value of n.[a] We have calculated zero-point corrected energies and wave functions of the $CH_3^+$ + $H_2$ system[b] and its deuterated analogs as functions of the center of mass separation between $CH_3^+$ and $H_2$, $R$. We can divide these simulations into distinct ranges of $R$; long-range interactions, complexation, and intermediate distances. Analysis of the wave functions associated with these three ranges of $R$ allows us to study how zero-point energy influences the approach geometries that are sampled during low-energy collisions.

[a]O. Asvany, S. Schlemmer, D. Gerlich, Astrophys. J. 617, 685 (2004).
[b]C. E. Hinkle, A. B. McCoy, J. Phys. Chem. Lett. 1, 562 (2010).