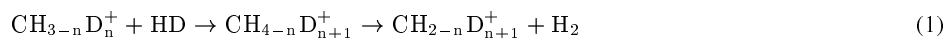


DIFFUSION MONTE CARLO CALCULATIONS OF MINIMUM ENERGY PATHS FOR THE ISOTOPIC VARIANTS OF THE $\text{CH}_3^+ + \text{H}_2 \leftrightarrow \text{CH}_5^+ \leftrightarrow \text{CH}_3^+ + \text{H}_2$ REACTION

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Protonated methane is of interest to astrochemists due to its presumed importance as a reaction intermediate in the reaction involving $\text{CH}_3^+ + \text{HD}$ 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



have identical net rate constants regardless of the value of n .^a We have calculated zero-point corrected energies and wave functions of the $\text{CH}_3^+ + \text{H}_2$ 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.

^aO. Asvany, S. Schlemmer, D. Gerlich, *Astrophys. J.* 617, 685 (2004).

^bC. E. Hinkle, A. B. McCoy, *J. Phys. Chem. Lett.* 1, 562 (2010).