

STUDIES OF VIBRATIONAL EXCITATIONS OF CH_5^+ BY DIFFUSION MONTE CARLO TECHNIQUES

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Understanding the vibrational spectrum of CH_5^+ is a question of great interest. There are currently only a few spectra of CH_5^+ . These include a high resolution spectrum observed by Oka^a, a high resolution, jet cooled spectrum that is only partially assigned, and the broad peaks in the low resolution spectrum that is assigned.^b The method that we employ for obtaining excited state structures of CH_5^+ is Diffusion Monte Carlo (DMC). DMC has been effectively applied to finding structural information about the ground state of CH_5^+ , and we are currently using extensions of this technique to probe CH excited states of CH_5^+ . Of particular interest is the broad CH stretching band observed between 2200 and approximately 3200 cm^{-1} , and a broad bending region centered at 1200 cm^{-1} .^c We will study the nature of states that have a single node along a single coordinate such as the CH stretching and bending motions.

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