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.

[a] E. T. White, J. Tang, T. Oka, Science 284, 135 (1999).
[b] X. Huang., A. B. McCoy, J. M. Bowman, L. M. Johnson, C. Savage, F. Dong, D. J. Nesbitt, Science 311, 60 (2006).
[c] O. Asvany, P. Kumar P, B. Redlich, I. Hesemann, S. Schlemmer, D. Marx, Science 309, 1219 (2005).