EXCITED STATES OF CH_5^+ BY DIFFUSION MONTE CARLO

CHARLOTTE E. HINKLE, ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

Understanding the spectrum of CH_5^+ is a problem of long standing interest. Of particular interest is gaining a better understanding of the two high resolution spectra; one observed by White et. al [a], and one that is partially assigned observed by the Nesbitt group. [b] Using excited state Diffusion Monte Carlo techniques in combination with symmetry adapted linear combinations of the internal coordinates of CH_5^+, obtained from group theoretical analysis of the G_{240} CNPI group, we investigate the nature of the vibrationally, and rotationally excited states of CH_5^+. By probing CH_5^+ using these methods, we find that we are able to gain insights into the effects of the internal rotor motions of vibrationally excited states of CH_5^+.

[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).