TOWARD A QUANTUM-MECHANICAL UNDERSTANDING OF THE HIGH-RESOLUTION INFRARED SPECTRUM OF CH_5^+

CHANDRA SAVAGE, FENG DONG, DAVID J. NESBITT, *JILA, National Institute of Standards and Technology and University of Colorado, Boulder, CO 80309*.

Our recent measurement of the infrared spectrum of CH_5^+ in the C-H stretching region (2825-3100 cm^{-1}) has provided new insight into the behavior of this highly fluxional molecule. Examining four-line combination differences matched to 40 MHz, we have tentatively assigned two vibrational band origins near 2950 and 3025 cm^{-1}. Using the most complete ab initio calculations to date, these features can be assigned to symmetric and asymmetric stretches of the hydrogen-like CH_2 component of CH_5^+. Furthermore, we have assigned several ro-vibrational progressions within these bands. Fits of these lines to a simple spherical-top Hamiltonian yield a ground-state rotational constant of approximately 3.92 cm^{-1}, in agreement with theoretical predictions. With these initial results, the mystery of CH_5^+ is beginning to be unraveled.