SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE OF METHACRYLONITRILE (C_4H_5N)

HOUSTON H. SMITH, SAMUEL M. KOUGIAS, DANNY J LEE, BRIAN J. ESSELMAN, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA*; BRYAN CHANGALA, MICHAEL C McCARTHY, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; R. CLAUDE WOODS, ROBERT J. McMAHON, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA*.

The detection of acrylonitrile (C_3H_3N) in Titan's atmosphere and the interstellar medium suggests methacrylonitrile may also have astronomical relevance. To aid in the astronomical observation, we synthesized methacrylonitrile *via* the hydrocyanation and subsequent dehydration of acetone and obtained its rotational spectrum from 6 – 40 GHz and 130 – 500 GHz. The ground vibrational state of the main isotopologue has been least-squares fit to a sextic Hamiltonian accounting for internal rotation splitting, and the resulting spectroscopic constants compare well with previous literature. The increase in the measured frequency range improved the determination of centrifugal distortion constants, and thus enhances the possibility of detection *via* radioastronomy. Additionally, a semi-experimental equilibrium structure (${r_e}^{SE}$) for methacrylonitrile is sought after due to its small molecular size and accessibility to a wide range of isotopologues. We analyzed the spectra from 6 – 40 GHz and 130 – 360 GHz of all singly-substituted heavy-atom isotopologues (^{13}C and ^{15}N), which were detectable at natural abundance, and least-squares fit them to sextic Hamiltonians accounting for internal rotation. The synthesis of methacrylonitrile was modified by using partially deuterated or fully deuterated acetone to yield samples of varying deuterium incorporation. We will present our analysis of 23 isotopologues, including the main isotopologue, and the resulting (${r_e}^{SE}$) structure.