SUB-DOPPLER SLIT JET DISCHARGE SPECTROSCOPY OF JET COOLED POLYACETYLENES: THE ANTI-SYMMETRIC CH STRETCH MODE OF TRIACETYLENE

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Growth of polyacetylenic molecules in acetylene flames is thought to play a central role in combustion chemistry and formation of soot, as well as the chemistry of gas clouds in the interstellar medium. In this talk, we present results from first sub-Doppler, high resolution infrared spectroscopic studies on triacetylene.[a,b] In particular, we explore the fundamental anti-symmetric CH stretching mode (v_5) of jet-cooled triacetylene in a pulsed slit discharge, where the $in-situ$ synthesis arises from a discharge of trace(0.1-1%) acetylene/rare gas mixtures followed by rapid CCH + HCCH chemistry in the supersonic expansion environment. The band origin of this mode is determined to be 3329.0544(2) cm^{-1}. At high resolution, a series of avoided energy level crossings arising from rotational perturbations are observed and ascribed to perpendicular Coriolis mixing with a near degenerate manifold of Π vibrational symmetry. The energy level patterns are successfully analyzed to reveal spectroscopic constants and Coriolis coupling matrix elements for the perturbing manifold. In addition, a weak Π-Π hot band progression due to thermal population in the slit jet is observed and assigned.

[a] D. McNaughton and D. N. Bruget, J. Mol. Spectrosc.150, 620 (1991)
[b] K. Matsumura, K. Kawaguchi, D. McNaughton, and D. N. Bruget, J. Mol. Spectrosc.158, 489 (1993)