

ROTATIONALLY-RESOLVED INFRARED SPECTROSCOPY OF THE POLYCYCLIC AROMATIC HYDROCARBON PYRENE (C₁₆H₁₀) IN THE MID-INFRARED USING A QUANTUM CASCADE LASER-BASED CAVITY RINGDOWN SPECTROMETER

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We have constructed a high-resolution infrared spectrometer based on a quantum cascade laser (QCL) which operates near 8.4 μm . The ultimate purpose of this spectrometer is to obtain a rotationally-resolved gas phase spectrum of buckminsterfullerene (C₆₀). We performed initial testing of the spectrometer with methylene bromide (CH₂Br₂), but to test the high-temperature capabilities of our instrument, we have observed a C-H bending mode of pyrene (C₁₆H₁₀) near 1184 cm⁻¹ (near the expected band center of the C₆₀ vibrational band). The observed spectra were rotationally resolved, and individual features had a linewidth (FWHM) of ~ 10 MHz. To our knowledge, pyrene is the largest molecule to be observed with rotational resolution by infrared absorption spectroscopy. Gas-phase pyrene was generated in a high-temperature (420 - 440 K) oven and cooled by a continuous supersonic expansion from a 150 $\mu\text{m} \times 1.6$ cm slit using argon as a carrier gas. The cooled pyrene was observed by continuous-wave cavity ringdown spectroscopy (cw-CRDS). We have collected 2 cm⁻¹ of the band, which is observed to be a b-type band. The observed spectra were fit to an effective asymmetric top Hamiltonian using PGOPHER^a. Using this fit and knowledge of the vibrational band strength, we estimate the vibrational temperature of the cooled pyrene to be ~ 70 K, while the rotational temperature was as low as 13 K.

^aPGOPHER, a Program for Simulating Rotational Structure, C. M. Western, University of Bristol, <http://pgopher.chm.bris.ac.uk>