ROTATIONALLY-RESOLVED INFRARED SPECTROSCOPY OF THE POLYCYCLIC AROMATIC HYDROCARBON PYRENE ($C_{16}H_{10}$) 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 (C_{60}). We performed initial testing of the spectrometer with methylene bromide (CH_2Br_2), but to test the high-temperature capabilities of our instrument, we have observed a C-H bending mode of pyrene ($C_{16}H_{10}$) near 1184 cm^{-1} (near the expected band center of the C_{60} vibrational band). The observed spectra were rotationally resolved, and individual features had a linewidth (FWHM) of $\sim$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 μm $\times$ 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 $\sim$70 K, while the rotational temperature was as low as 13 K.

[a]PGOPHER, a Program for Simulating Rotational Structure, C. M. Western, University of Bristol, http://pgopher.chm.bris.ac.uk