HIGH-RESOLUTION INFRARED SPECTRA OF THE ν1 FUNDAMENTAL BANDS OF 13C MONO-SUBSTITUTED PROPYNE IN A SUPersonic SLIT JET

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In the past few decades, many high-resolution spectroscopic studies have been dedicated to the C-H stretch vibrations in propyne (CH$_3$-C≡CH), aiming to understand the intramolecular vibrational redistribution in isolated small hydrocarbons. In this talk, we present the sensitive detection of the ν1 (acetylenic C-H stretch) fundamental bands of the three 13C mono-substituted isotopologues of propyne. The infrared absorption spectra are recorded using continuous-wave cavity ring-down spectroscopy (CRDS) in combination with a supersonic jet expansion of propyne/argon gas mixtures. A 0.05x30 mm slit nozzle is used in the present experiment to realize an effective rotational cooling to ≈14 K and a reduced Doppler width of ≈90 MHz. The high sensitivity of CRDS allows us to detect the three 13C isotopologues in their 1.1% natural abundance. Different infrared band intensities of ν1 are found for the three isotopologues. Detailed rotational analyses of the experimental spectra are performed to derive effective spectroscopic constants for the upper ν1 vibrational state. The 13C-substitution effect of the near/non-resonant perturbations to ν1 of propyne is discussed. In addition, more accurate infrared data of 12C-propyne, including the ν1 fundamental band, are also obtained from our experimental spectra.