

¹³C MONO-SUBSTITUTED ISOTOPOLOGUES OF PROPYNE (H₃CCCH): INVESTIGATING THE ACETYLENIC CH STRETCH PERTURBATION

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The acetylenic CH stretch (ν_1) fundamental band of propyne is known to have a "double-crossing" type perturbation that shifts the K' -subbands out of normal order. To further investigate this perturbation, we present a combined experimental and *ab initio* study on the jet-cooled high-resolution infrared spectra of the ν_1 fundamental band of the three mono-substituted ¹³C isotopologues of propyne: ¹³CH₃¹²C \equiv ¹²CH, ¹²CH₃¹³C \equiv ¹²CH, and ¹²CH₃¹²C \equiv ¹³CH. The experimental spectra are recorded using continuous wave cavity ringdown spectroscopy (cw-CRDS), with the isotopologues produced at natural abundance in a continuous supersonic expansion of regular propyne diluted in argon and helium. The $K' = 0$ and 1 subbands of all three isotopologues are measured near 3330 cm⁻¹.^b

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