INFRARED-MICROWAVE DOUBLE-RESONANCE ASSIGNMENT OF THE ACETYLENIC C-H STRETCH SPECTRA OF TRANS AND GAUCHE 1-PENTYNE

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The high-resolution infrared spectrum of the acetylenic C-H stretch of 1-pentyne has been assigned using infrared-microwave double-resonance spectroscopy in an electric-resonance, optothermal spectrometer. Both the trans and gauche conformations of the molecule are populated in the molecular beam expansion. The acetylenic C-H stretch spectrum consists of sets of transitions for each rotational level. The lineshape profile is approximately Lorentzian, although an asymmetry is observed in several spectra. This broadening of the spectrum comes from the intramolecular vibrational energy redistribution (IVR) of the acetylenic C-H stretch vibrational mode. Extremely slow, and K-dependent, IVR rates are found for the trans conformer. The lifetime for energy localization in the C-H stretch is about 1 ns. The measured IVR rates are discussed within the context of the rate of conformational isomerization predicted by RRKM theory.