MICROWAVE AND SUBMILLIMETER SPECTROSCOPY OF 2-PENTYNAL, CH_3CH_2CCCHO

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The barrier to internal rotation in a substituted acetylene is very small. We have observed the low resolution microwave band spectrum of 2-pentynal in a Stark-modulated spectrometer, its high resolution microwave spectrum in a pulsed-jet Fourier Transform spectrometer, and submillimeter spectra of the room temperature gas from 400-500 GHz. The low resolution Stark spectrum displays an intense near-symmetric top series of a-type R-branch bands consistent with B+C = 2639 MHz. The high resolution microwave spectrum in the low temperature pulsed-jet displays transitions of the torsional ground state as well as two nearly degenerate torsionally excited states. A model which fits these observations is a one-fold torsional potential function with such a low barrier, about 2 inverse cm, that there is only one bound state. The a- and b-type microwave transitions of the ground state are well fit (std. dev. = 1.5 kHz) by A = 13492.1199(9) MHz, B = 1396.2413(1) MHz, and C = 1288.3182(1) MHz plus five centrifugal distortion constants. The submillimeter spectra are dominated by a-type Q-branches of many (21 as of this writing) vibrational states. No b-type transitions have been identified in the submillimeter spectrum.