ROTATIONAL SPECTRUM AND STRUCTURE OF 3-HEXYN-2-ONE

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3-Hexyn-2-one, $CH_3CH_2CCCOCH_3$, is expected to have a very low internal rotation barrier about the central carbon-carbon triple bond. The low resolution Stark-modulated microwave spectrum displays a single a-type band series characteristic of a nearly prolate symmetric top with B+C = 2072 MHz. The rotational spectrum of the sample cooled in the pulsed jet of a Fourier Transform microwave spectrometer displays transitions of a single stable conformation with a heavy-atom-planar structure. Tunneling splittings from internal rotation of the acetyl methyl group are observed, assigned, and are consistent with a 3-fold barrier of 355 cm^{-1}. The rotational spectrum of the A-state species of this internal rotor can be fit with a conventional Hamiltonian with a standard deviation of less than 2 kHz. The rotational parameters determined are A = 7235.122(5) MHz, B = 1086.857(1) MHz, C = 964.530(1) MHz, plus three centrifugal distortion constants. It appears that the internal rotation potential about the acetylenic C-C triple bond is predominantly 1-fold. Thus, the acetylenic torsional ground state, the only one observed, displays no splitting and yields no information about that potential barrier. NUTS.