

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

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3-Hexyn-2-one,  $\text{CH}_3\text{CH}_2\text{CCCOCH}_3$ , 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  $355\text{ cm}^{-1}$ . 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.