

LOW BARRIER METHYL ROTATION IN 3-PENTYN-1-OL AS OBSERVED BY MICROWAVE SPECTROSCOPY

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It is known that the barrier to internal rotation of the methyl groups in ethane (**1**) is about 1000 cm^{-1} .^a If a C-C-triple bond is inserted between the methyl groups as a spacer (**2**), the torsional barrier is assumed to be dramatically lower, which is a common feature of ethynyl groups in general.

To study this effect of almost free internal rotation, we measured the rotational spectrum of 3-pentyn-1-ol (**3**) by pulsed jet Fourier transform microwave spectroscopy in the frequency range from 2 to 26.5 GHz. Quantum chemical calculations at the MP2/6-311++G(d,p) level of theory yielded five stable conformers on the potential energy surface. The most stable conformer, which possesses C_1 symmetry, was assigned and fitted using two theoretical approaches treating internal rotations, the rho axis method (*BELGI- C_1*) and the combined axis method (*XIAM*). The molecular parameters as well as the internal rotation parameters were determined. A very low barrier to internal rotation of the methyl group of only $9.4545(95)\text{ cm}^{-1}$ was observed.

^aR. M. Pitzer, *Acc. Chem. Res.*, **1983**, *16*, 207–210.

