TORSIONAL ANALYSIS OF 2-BUTYNOL

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Microwave spectroscopic studies of substituted propynes, CH_3-C≡C-X, have increased our understanding of the nature and origin of the potential barriers for internal rotation. Specifically, the potential barriers have been measured for the groups, -CD_3[a], -CH_2Cl[b], -SiH_3[c], and -COF[d], bonded to the propynyl fragment, with reported 3-fold barriers of 5.62(16), 10.05(9), 3.77(70) and 2.20(12) cm^{-1} respectively. We report here a study of the rotational spectrum of 2-butynol, CH_3-C≡C-CH_2OH. 2-butynol has two low energy rotational conformers with the OH group either anti or gauche with respect to the propynyl moiety. The study of 2-butynol was performed with a pulsed-jet, Fourier Transform Microwave Spectrometer. The rotational spectrum of one species including tunneling splittings has been assigned and is consistent with the gauche conformer. A preliminary value of the 3-fold barrier is 12.5(4) cm^{-1}. Unassigned transitions in the spectrum may be due to the other conformer.

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