TORSIONAL ANALYSIS OF 2-BUTYNOL AND 2-PENTYNE

RANGA SUBRAMANIAN, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*; ROBERT K. BOHN, *Department of Chemistry, University of Connecticut, Storrs, CT 06269* ; and STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*.

The microwave spectrum of 2-butynol, CH_3-C≡C-CH_2OH, has been investigated in the frequency range of 6 to 26.5 GHz. The spectra of the *A* and *E* torsional states were observed using Fourier transform microwave spectroscopy. Due to the presence of the cylindrically symmetric -C≡C- "spacer" between the methyl group and the rest of the molecule, the barrier to internal rotation, V_3, is only 7 cm^{-1}. One conformer of 2-butynol was observed and assigned. The spectrum was analyzed with the ρ-axis method using a very flexible Hamiltonian which gives a fit an order of magnitude better than that obtained with more standard code for internal rotation. The spectroscopic constants for 2-butynol are 23744.(18), 2093.429(1), 1966.358(1), and -400.34(2) MHz for *A, B, C,* and D_{ab} ; 0.48(1) kHz, -30.3(4) kHz, and 4.5(5) MHz for Δ_J, Δ_{JK}, and Δ_K; and 0.1406(6), 6.93(9) cm^{-1}, -33.4(7) kHz, and 192.0(9) GHz for ρ, V_3, L_V, and F, respectively. The root mean squared error of the fit is 14 kHz. The angles between the internal rotor axis and the principal axes are θ_a = 12°, θ_b = 78°, with θ_c held fixed at 90°. A preliminary fit for the torsional states of 2-pentyne, CH_3-C≡C-CH_2CH_3, will also be presented.