

ROTATIONAL SPECTROSCOPY AND RING-PUCKERING CONFORMATION OF 3-HYDROXY-TETRAHYDROFURAN

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The ring puckering conformation of 3-hydroxytetrahydrofuran, a five-membered heterocyclic ring, has been determined from rotational spectroscopy. Rotational constants for the normal isotopomer are $A = 5581.8230$ (7), $B = 3638.8316$ (7), and $C = 2924.7410$ (7) MHz; rotational spectra were also recorded for four ^{13}C isotopic species in natural abundance. The best fit structure is a $\text{C}_{4'}$ endo conformation with an intramolecular hydrogen bond from the hydroxyl to the ring oxygen. Projections of the dipole moment on the inertial axes, $\mu_a = 0.956$ (1) D, $\mu_b = 0.875$ (2) D, and $\mu_c = 1.050$ (2) D, were determined from Stark effect measurements. The experimental structure is nearly identical to the lowest energy ab initio conformation (MP2/6-31+G**).