STRUCTURAL ANALYSIS OF 2-FLUOROPHENOL AND 3-FLUOROPHENOL USING FTMW SPECTROSCOPY

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The ground states of 2-fluorophenol (2-FPh) and 3-fluorophenol (3-FPh) were studied using Fourier transform microwave (FTMW) techniques to record their rotational spectra in the range of 6 to 26 GHz. Two planar conformers of similar energy were observed for 3-FPh (cis, trans) while only the lowest energy conformer (cis) of 2-FPh was observed due to the stabilizing effect of an intramolecular interaction between fluorine and OH. Rotational constants derived from spectra of the ^{13}C analogs, observed in natural abundance, were used to calculate the substitution (r_s) and effective ground state (r_0) parameters for cis-2-FPh and trans-3-FPh in order to study the effect of fluorination at sites along the benzene backbone. Geometry optimization at the MP2/6-311++G(2d,2p) level was used obtain the equilibrium (r_e) structures for comparison. Furthermore, natural bond order (NBO) calculations provided supporting information of a OH•••F interaction in cis-2-FPh.