ROTATIONAL SPECTRA AND STRUCTURES OF THE MONO- AND DI-FLUORINATED PYRIDINES

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The ground state rotational spectra of a series of fluorinated pyridines have been measured using a Balle-Flygare Fourier transform microwave (FTMW) spectrometer and a chirped pulse Fourier transform microwave (cp-FTMW) instrument between 8 and 23 GHz. The species under investigation include 2- and 3-fluoropyridine as well as 2,3-, 2,4-, 2,5-, 2,6- and 3,5-difluoropyridine. In addition to the parent species, the spectra of the ^{13}C and ^{15}N singly-substituted isotopologues were recorded in natural abundance and used to calculate relevant geometric parameters of the pyridine ring backbone. Analysis of the ^{14}N hyperfine structure provided an additional source of information about the electronic structure surrounding the nitrogen atom as a function of fluorine substitution. The experimental results are compared with those from *ab initio* theory and are consistent with a bonding model that involves donation of electron density from fluorine into the π-system of pyridine.