

## ROTATIONAL SPECTROSCOPIC AND COMPUTATIONAL INVESTIGATION OF 2-FLUOROANILINE

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The rotational spectrum of 2-fluoroaniline was investigated using chirped pulse and Balle-Flygare Fourier transform microwave (FTMW) spectroscopy in the 8-19 GHz range. The spectrum contains transitions due to the  $^{13}\text{C}$  and  $^{15}\text{N}$  minor isotopologues which were detected in natural abundance for the first time. The ground state  $r_0$  geometry of 2-fluoroaniline was derived from the spectrum and compares well with the  $r_e$  geometry derived from quantum chemical calculations at the B3LYP-D3BJ/cc-pVTZ level of theory. Previous room temperature microwave spectra,<sup>a,b</sup> report a tunneling splitting due to  $\text{NH}_2$  inversion but this is not consistent with our FTMW results nor with computational estimates of the tunneling barrier.

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<sup>a</sup>J. Mol. Struct.41(1977)315-317

<sup>b</sup>J. Mol. Spectrosc.114,13-22(1985)