

A MICROWAVE STUDY OF 3,5 DIFLUOROPYRIDINE \cdots CO₂: THE EFFECT OF META-FLUORINATION ON INTERMOLECULAR INTERACTIONS OF PYRIDINE

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The rotational spectrum of the weakly bound complex 3,5-difluoropyridine \cdots CO₂ has been observed using pulsed-nozzle Fourier transform microwave spectroscopy. Spectroscopic constants are reported for the parent and the ¹³CO₂ isotopologues. The data indicate a structure in which the nitrogen approaches the carbon of the CO₂ with the C₂ axis of the difluoropyridine perpendicular to the CO₂. The N \cdots C van der Waals bond distance is 2.827(17) Å and the oxygen \cdots ortho-hydrogen distance is 3.045(3) Å. The amplitude of the zero point bending vibrational motion of the difluoropyridine moiety away from the C₂ axis of the complex is estimated from ¹⁴N nuclear hyperfine structure to be 8.8°. The N \cdots C van der Waals bond length is 0.029 Å longer than that previously determined for pyridine-CO₂, but is still considerably shorter than the 2.997(1) Å distance in HCN \cdots CO₂. Density functional theory calculations place the binding energy of the complex at 3.2 kcal/mol.