WEAK C-H···N HYDROGEN BOND AND INTERNAL ROTATION IN THE PYRIDINE-TRIFLUOROMETHANE COMPLEX

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The investigation of the rotational spectrum of benzene-trifluoromethane has shown that this complex is a symmetric top, with the two moieties held together through a C-H···π interaction. When replacing the benzene with pyridine, two high electronic density sites become available in the ring. The molecular beam Fourier transform rotational spectra in a supersonic expansion of several isotopologues of pyridine-trifluoromethane show that trifluoromethane acts as a proton donor to the N lone pair. The carbon atom of trifluoromethane is in the plane of pyridine and one of its fluorine atoms makes a contact with the ring hydrogen in position 2. In addition, all rotational transitions are split due to the internal rotation of the HCF$_3$ group, corresponding to a barrier $V_3 = 0.45(3)$ kJ/mol.

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