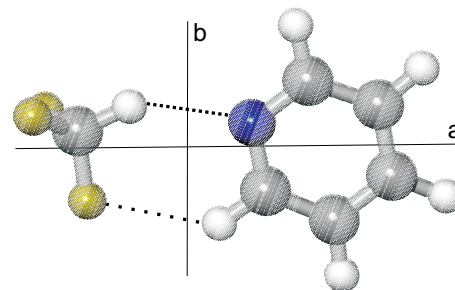


WEAK C-H...N HYDROGEN BOND AND INTERNAL ROTATION IN THE PYRIDINE-TRIFLUOROMETANE COMPLEX

B. M. GIULIANO, A. MARIS, S. MELANDRI, P. OTTAVIANI, W. CAMINATI, *Dipartimento di Chimica "G. Ciamician" dell'Università, Via Selmi 2, I-40126 Bologna, Italy*; L. B. FAVERO, *Istituto per lo Studio dei Materiali Nanostrutturati (ISMN, Sezione di Bologna), CNR, Via Gobetti 101, I-40129 Bologna, Italy*; B. VELINO, *Dipartimento di Chimica Fisica e Inorganica dell'Università, Viale Risorgimento 4, I-40136 Bologna, Italy*.

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.^a 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 HCF₃ group, corresponding to a barrier $V_3 = 0.45(3)$ kJ/mol.



^aJ. C. López, J. L. Alonso and W. Caminati, *Angew. Chem. Int. Ed. Engl.* 2006, 45, 290.