WEAK C-H$\cdots$N HYDROGEN BOND AND INTERNAL ROTATION IN THE PYRIDINE-TRIFLUOROMETANE COMPLEX

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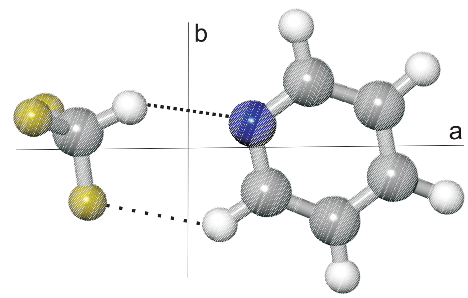
The investigation of the rotational spectrum of benzene-trifluoromethane has shown that this complex is a symmetric top, with the two moieties held together through a C-H$\cdots\pi$ interaction.[a] When replacing the benzene with pyridine, two high electronic density sites become available in the ring. 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 HCF_3 group, corresponding to a barrier V_3 = 0.45(3) kJ/mol.



[a] J. C. López, J. L. Alonso and W. Caminati, Angew. Chem. Int. Ed. Engl. 2006, 45, 290.