WEAK C-H$\cdots\pi$ HYDROGEN BOND AND FREE INTERNAL ROTATION IN THE BENZENE-TRIFLUOROMETANE DIMER

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The pure rotational spectra of the normal and benzene-^{13}C species of the benzene-trifluoromethane complex have been measured using molecular beam Fourier transform microwave spectroscopy. The normal species is a symmetric top, with the symmetry axes, C_3 of CHF_3 and C_6 of benzene, lying along the same line. The rotational spectrum of the benzene-^{13}C isotopomer is that of a slightly asymmetric top. Both species are characterized by an almost free rotation of the two subunits with respect to each other. From the present data the calculated length of the C-H$\cdots\pi$ hydrogen bond is 2.366(2) Å. The analysis of the structural and energetic features of the C-H$\cdots\pi$ interaction allow us to classify it as a weak hydrogen bond.