OBSERVATION OF A C–H$\cdots$AROMATIC INTERACTION IN THE FLUOROBENZENE$\cdots$HCCH WEAKLY BOUND COMPLEX

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Chirped-pulse Fourier-transform microwave (CP-FTMW) spectroscopy has been used to determine the structure of the $C_6H_5F\cdots$HCCH weakly bound complex. Assignment of spectra for the parent and all six unique ^{13}C isotopologues in natural abundance has allowed a full structure determination, using both Kraitchman substitution and least-squares methods. The acetylene lies nearly perpendicular to the fluorobenzene ring, approximately above the ring center, and in the dimer ab symmetry plane. There is a slight tilt of the hydrogen atom nearest the fluorobenzene away from the carbon atom bonded to the fluorine. The distance between the centers of mass of the two monomers is approximately $4.18(1)$Å, with C–H$\cdots$C distances of between $2.81(1)$Å and $2.92(1)$Å. The experimentally determined structure is in reasonable agreement with the minimum energy configuration from an MP2/6-311++G(2d,2p) *ab initio* calculation. Comparison will also be made with similar complexes of aromatic compounds with potential hydrogen bond donors.