C–H...π and C–F...H–C INTERACTIONS IN THE ACETYLENE–FLUOROFORM DIMER

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Rotational spectra for four isotopomers of the HCCH–HCF_3 complex have been identified by Fourier-transform microwave spectroscopy. The spectra exhibit considerable fine splittings, presumably arising from the internal motion of one or both subunits; both first- and second-order Stark effects have been observed. A fit of selected K=0 and 1 components for the normal isotopomer (assigned using second-order Stark effect data) gave an rms of around 4 kHz and provided rotational constants $A = 5450.236(4)$ MHz, $B = 1381.3361(9)$ MHz, $C = 1375.1333(12)$ MHz. These rotational constants and the planar moments are consistent with a structure of C_s symmetry exhibiting C–H...π and C–F...H–C interactions and are in excellent agreement with a structure obtained from optimizations at the MP2/6-311++G(2d,2p) level.