MICROWAVE SPECTROSCOPIC INVESTIGATIONS OF THE C–H$\cdots\pi$ CONTAINING COMPLEXES $CH_2F_2\cdots$PROPYNE AND $CH_2ClF\cdots$PROPYNE

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The spectra of the $CH_2F_2\cdots$propyne and $CH_2ClF\cdots$propyne complexes have been studied by chirped-pulse and resonant cavity Fourier-transform microwave spectroscopy and by *ab initio* calculations at the MP2/6-311++G(2d,2p) level. Both complexes contain C–H$\cdots\pi$ contacts, with the halogen atoms angled towards the methyl group end of the propyne. While $CH_2F_2\cdots$propyne has C_s symmetry, $CH_2ClF\cdots$propyne has C_1 symmetry, with the fluorine and chlorine atoms straddling the propyne.

Investigation of four single ^{13}C and the DC≡CCH_3 isotopologues in $CH_2F_2\cdots$propyne has allowed a detailed structural determination, while only the ^{35}Cl and ^{37}Cl isotopologues have so far been assigned for $CH_2ClF\cdots$propyne. Experimental data will be compared with *ab initio* results and with the analogous acetylene complexes, both of which have C_s symmetry structures, with double C–H$\cdots\pi$ interactions.