

MICROWAVE SPECTROSCOPIC INVESTIGATIONS OF THE C-H $\cdots\pi$  CONTAINING COMPLEXES  
CH<sub>2</sub>F<sub>2</sub> $\cdots$ PROPYLENE AND CH<sub>2</sub>ClF $\cdots$ PROPYLENE

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The spectra of the CH<sub>2</sub>F<sub>2</sub> $\cdots$ propyne and CH<sub>2</sub>ClF $\cdots$ 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<sub>2</sub>F<sub>2</sub> $\cdots$ propyne has *C<sub>s</sub>* symmetry, CH<sub>2</sub>ClF $\cdots$ propyne has *C<sub>1</sub>* symmetry, with the fluorine and chlorine atoms straddling the propyne.

Investigation of four single <sup>13</sup>C and the DC $\equiv$ CCH<sub>3</sub> isotopologues in CH<sub>2</sub>F<sub>2</sub> $\cdots$ propyne has allowed a detailed structural determination, while only the <sup>35</sup>Cl and <sup>37</sup>Cl isotopologues have so far been assigned for CH<sub>2</sub>ClF $\cdots$ propyne. Experimental data will be compared with *ab initio* results and with the analogous acetylene complexes, both of which have *C<sub>s</sub>* symmetry structures, with double C-H $\cdots\pi$  interactions.