MICROWAVE SPECTROSCOPIC INVESTIGATIONS OF THE C–H···π CONTAINING COMPLEXES CH₂F₂···PROPYNE AND CH₂ClF···PROPYLE

REBECCA A. PEEBLES, SEAN A. PEEBLES, CORI L. CHRISTENHOLZ, ANTHONY A. ERNST, and YASSER J. DHAHIR, Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920.

The spectra of the CH₂F₂···propyne and CH₂ClF···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···π contacts, with the halogen atoms angled towards the methyl group end of the propyne. While CH₂F₂···propyne has Cs symmetry, CH₂ClF···propyne has C₁ symmetry, with the fluorine and chlorine atoms straddling the propyne.

Investigation of four single ¹³C and the DC≡CCH₃ isotopologues in CH₂F₂···propyne has allowed a detailed structural determination, while only the ³⁵Cl and ³⁷Cl isotopologues have so far been assigned for CH₂ClF···propyne. Experimental data will be compared with ab initio results and with the analogous acetylene complexes, both of which have Cs symmetry structures, with double C–H···π interactions.