

OBSERVATION OF C—H··· π INTERACTIONS: MICROWAVE SPECTRA AND STRUCTURES OF THE CH₂FX···HCCH (X=F,Cl) WEAKLY BOUND COMPLEXES

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With an interest in characterizing C—H··· π interactions, CH₂F₂···HCCH and CH₂ClF···HCCH have been examined by Fourier-transform microwave (FTMW) spectroscopy. These interactions involve the π bond in acetylene acting as a hydrogen bond acceptor to both hydrogen atoms of CH₂FX. In addition, there is a secondary contact between one hydrogen atom from acetylene and the X atom in the halomethane (X=F in CH₂F₂, X=Cl in CH₂ClF).

Initial assignments for the most abundant isotopologues of both species were completed using the chirped-pulse FTMW spectrometers at the University of Virginia (CH₂ClF···HCCH) and at Eastern Illinois University (CH₂F₂···HCCH). Rotational constants obtained from experiment are in good agreement with those of the most stable orientations predicted by ab initio calculations at the MP2/6-311++G(2d,2p) level. Multiple isotopically substituted species for each complex were measured using a Balle-Flygare cavity FTMW spectrometer at Eastern Illinois University. Spectroscopic parameters for all observed isotopologues will be presented, and a comparison of the C—H··· π interactions in these and related complexes will be discussed.