OBSERVATION OF C$-$H$\cdots\pi$ INTERACTIONS: MICROWAVE SPECTRA AND STRUCTURES OF THE $CH_2FX\cdots HCCH$ (X=F,Cl) WEAKLY BOUND COMPLEXES

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With an interest in characterizing C$-$H$\cdots\pi$ interactions, $CH_2F_2\cdots HCCH$ and $CH_2ClF\cdots HCCH$ 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 CH_2FX. In addition, there is a secondary contact between one hydrogen atom from acetylene and the X atom in the halomethane (X=F in CH_2F_2, X=Cl in CH_2ClF).

Initial assignments for the most abundant isotopologues of both species were completed using the chirped-pulse FTMW spectrometers at the University of Virginia ($CH_2ClF\cdots HCCH$) and at Eastern Illinois University ($CH_2F_2\cdots HCCH$). 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$\cdots\pi$ interactions in these and related complexes will be discussed.