THE $HCClF_2$–HCCH COMPLEX: MICROWAVE SPECTRUM, STRUCTURE AND C–H$\cdots\pi$ INTERACTIONS

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The HCF_3–HCCH complex was recently found to have a weak C–H$\cdots\pi$ interaction between the fluoroform and acetylene, as well as having a secondary interaction between the fluorine atoms and one of the acetylene hydrogen atoms;[a] however, extensive splittings due to large amplitude motions within the complex have complicated our efforts at making a full assignment of the HCF_3–HCCH spectrum. In an attempt to remove some of the ambiguity in the HCF_3–HCCH study, we have substituted a chlorine atom for one fluorine atom and undertaken an investigation of the $HCClF_2$–HCCH complex. This eliminates the possibility of internal rotation of the methane subunit, while still maintaining a C–H$\cdots\pi$ interaction.

Using the chirped-pulse Fourier-transform microwave (CP-FTMW) spectrometer at the University of Virginia and the Balle-Flygare FTMW spectrometer at Eastern Illinois University, the spectra of four isotopologues of $HCClF_2$–HCCH have been assigned, with no indication of internal motions within the complex. The structure has been determined from the experimental moments of inertia, confirming that this dimer has the expected weak C–H$\cdots\pi$ interaction. In addition, the off-diagonal χ_{ab} quadrupole coupling constant has been used to determine the angle between the C–Cl bond and the a-axis of the complex. This, and Kraitchman coordinates for the chlorine atom, help confirm the structural details from the inertial fit. The structural results will be compared with other complexes showing C–H$\cdots\pi$ and C–H$\cdots$O interactions.

[a] S. A. Peebles, M. M. Serafin, R. A. Peebles, 61^{st} International Symposium on Molecular Spectroscopy, Talk MH13, June 19, 2006.