FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF THE 1-CHLORO-1-FLUOROETHYLENE MONOMER AND THE ACETYLENE–1-CHLORO-1-FLUOROETHYLENE COMPLEX

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Guided by previous studies of the $^{35}$Cl and $^{37}$Cl isotopomers of 1-chloro-1-fluoroethylene, we have collected the spectra of these and four additional naturally occurring isotopomers in the 7–21 GHz region with a Fourier transform microwave spectrometer. The rotational transitions are split by both the chlorine nuclear quadrupole and the nuclear spin-rotation hyperfine interactions. The rotational constants, together with the hyperfine coupling constants and guidance from $ab$ initio calculations, allow a precise determination of the structure of the 1-chloro-1-fluoroethylene monomer, which in turn aids our work on structure determination for complexes involving this molecule. For the acetylene–1-chloro-1-fluoroethylene complex, we have collected the rotational spectra for five of its isotopomers. The transitions are once again split by chlorine nuclear quadrupole coupling. The spectroscopic constants are consistent with a planar structure in which a hydrogen bond is formed between an H atom in HCCH and the F atom in 1-chloro-1-fluoroethylene with a second interaction between the H atom located cis to the hydrogen-bonded F atom in 1-chloro-1-fluoroethylene and the acetylenic bond.

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