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,[a] 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.

[a] R. G. Stone and W. H. Flygare, J. Mol. Spectrosc. **32,** 233 (1969); J. L. Alonso, A. G. Lesarri, L. A. Leal, and J. C. López, J. Mol. Spectrosc. **162,** 4 (1993).