THE STRUCTURE OF THE 1-CHLORO-1-FLUOROETHYLENE–ACETYLENE COMPLEX

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The insensitivity of the moments of inertia to certain geometric parameters for the limited set of isotopologues studied led to unexpected results for a preliminary structure of the complex formed between 1-chloro-1-fluoroethylene and acetylene presented three years ago.[a] The availability of this chlorofluoroethylene with a single deuterium substitution in both (*E*) and (*Z*) isomeric forms[b] allows us to supplement the original data set with microwave spectra of (*E*)-CHDC^{35}ClF–HCCH and (*Z*)-CHDC^{35}ClF–HCCH. Supported by the results of *ab initio* calculations, a planar, chemically reasonable structure is obtained for this complex, in which the acetylene forms a hydrogen bond with the fluorine atom of 1-chloro-1-fluoroethylene. The hydrogen bond bends to allow a secondary interaction with the hydrogen atom *cis* to this fluorine atom. Comparisons with the structure of the analogous complexes formed with vinyl fluoride and 1,1-difluoroethylene reveal the effects of chlorine substitution geminal to the acceptor atom of the hydrogen bond.

[a] H.O. Leung and M.D. Marshall, The 62nd OSU International Symposium on Molecular Spectroscopy, Talk RG10 (2007)

[b] Kindly provided by Prof. Norman Craig, Oberlin College