THE STRUCTURE OF THE *TRANS*-1,2-DIFLUOROETHYLENE–HF COMPLEX

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To understand the effects of fluorine substitution in ethylene on intermolecular interactions, we have expanded our work on the Fourier transform microwave spectroscopy of *trans*-1,2-difluoroethylene–HF reported last year[a] to include six isotopomers: the most abundant, its DF counterpart, and four singly substituted ^{13}C species in natural abundance. The spectra are analyzed with the inclusion of the hydrogen-fluorine spin-spin coupling interaction in the HF subunit, or for those complexes containing DF, the deuterium nuclear quadrupole coupling interaction. Analysis of the rotational and hyperfine constants gives a planar complex, with a hydrogen bond formed between HF and one of the F atoms in *trans*-1,2-difluoroethylene. As with similar complexes, the hydrogen bond bends to allow the F atom in HF to interact with an H atom in the ethylene subunit. Although there are two possible sites for this secondary interaction, namely the H atoms vicinal and geminal to the hydrogen bonded F atom, only the interaction involving the former H atom is observed. The structure of this complex will be compared with those of similar complexes with different patterns of F atom substitution in the ethylene subunit.

[a] B. K. Amberger, H. O. Leung, and M. D. Marshall, The 63rd OSU International Symposium on Molecular Spectroscopy, Talk WF04 (2008).