DOES A SECOND HALOGEN ATOM AFFECT THE NATURE OF INTERMOLECULAR INTERACTIONS IN PROTIC ACID-HALOETHYLENE COMPLEXES? IN (*E*)-1-CHLORO-2-FLUOROETHYLENE-HYDROGEN CHLORIDE IT DEPENDS ON HOW YOU LOOK AT IT

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As part of a systematic study of the effect of chlorine substitution on the structures of protic acid haloethylene complexes, the structure of the (*E*)-1-chloro-2-fluoroethylene-hydrogen chloride complex has been investigated using *ab initio* quantum chemistry calculations and microwave spectroscopy. Although theory predicts a non-planar equilibrium structure for this species, it is only 7 cm^{-1} lower in energy than the planar geometry connecting the two equivalent minima on either side of the haloethylene plane, and the observed spectrum is consistent with a planar, average structure, likely the result of zero-point averaging. The geometry is very similar to the fluorine binding, vinyl fluoride-hydrogen chloride complex, suggesting that the substitution of chlorine for a hydrogen *trans* to the fluorine atom has very little effect on intermolecular interactions in this case. On the other hand, vinyl chloride-hydrogen chloride adopts a non-planar, chlorine binding configuration so that alternatively one could say that the presence of fluorine has a large effect on protic acid-chlorine interactions.