DOES A SECOND HALOGEN ATOM AFFECT THE NATURE OF INTERMOLECULAR INTERACTIONS IN PROTIC ACID-HALOETHYLENE COMPLEXES? IN (*Z*)-1-CHLORO-2-FLUOROETHYLENE-HYDROGEN CHLORIDE IT MOST CERTAINLY DOES!

HANNAH K. TANDON, HELEN O. LEUNG, MARK D. MARSHALL, *Chemistry Department, Amherst College, Amherst, MA, USA*.

As part of a systematic study of the effect of chlorine substitution on the structures of protic acid-haloethylene complexes, the structure of the (*Z*)-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 6 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 unlike that of any previously characterized protic acid-haloethylene complex with a bifurcated primary interaction in which the hydrogen of the acid interacts with both the fluorine and the chlorine atoms on the haloethylene and there is no evidence for a secondary interaction involving the electron rich region of the acid. This structure can be contrasted to those of vinyl fluoride-hydrogen chloride (fluorine bound, planar "top-binding," across the double bond), vinyl chloride-hydrogen chloride (chlorine bound, non-planar) and (*Z*)-1-chloro-2-fluoroethylene-acetylene (chlorine bound, planar "side-binding," at one end of the double bond).