

A NOVEL STRUCTURE FOR THE GAS PHASE HETERODIMER FORMED BETWEEN (Z)-1-CHLORO-3,3,3-TRIFLUOROPROPENE AND ACETYLENE

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Our characterization of the structures of gas phase heterodimers formed between haloethylenes and the three protic acids, hydrogen fluoride, hydrogen chloride, and acetylene, provided a wealth of information regarding intermolecular forces and the relative effects of electrostatic, dispersion and steric forces. By and large all of these species shared the common structural feature of a hydrogen bond formed between the protic acid donor and a halogen acceptor on the ethylene. The extension of the carbon chain by one atom via the addition of a trifluoromethyl group provides a wider variety of possible interactions and binding sites. For the heterodimer formed between (Z)-1-chloro-3,3,3-trifluoropropene and acetylene, a novel structure with no hydrogen bond but rather an interaction between the acetylenic triple bond and the two hydrogen atoms of the propene is obtained from the analysis of the microwave rotational spectra of the  $^{35}\text{Cl}$  and  $^{37}\text{Cl}$  isotopologues of the complex.