



26<sup>th</sup> April 2018 - 10:00

Building 99, Seminar Room I+II (EG)

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**From Microwave Spectroscopy to Understanding Intermolecular Interactions: Using Structural Characterization of Bimolecular Heterodimers Formed Between Protic Acids and Haloethylenes to Examine the Forces Contributing to Non-Covalent Bonding**

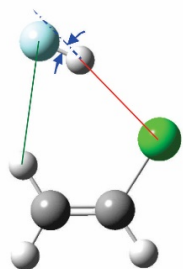
In the early 2000's, the work of Cole and Legon,<sup>a,b</sup> combined with that done earlier by Kisiel, Fowler, and Legon,<sup>c</sup> demonstrated that comparisons among the complexes of HF, HCl, and HCCH each with vinyl fluoride could provide information concerning the strength of intermolecular interactions. Building on this foundation, we undertook a systematic characterization of the molecular structures of complexes formed between these three acids and the remaining polar fluoroethylenes, leading to a full appreciation of the competition between electrostatic and steric forces in determining the lowest energy configuration for the heterodimer. In expanding the study to chlorofluoroethylenes, the first few examples confirmed earlier conclusions but subsequent complexes provided unexpected results that signaled an increasing importance of the dispersion interaction in determining the geometry of the complex as well as the fundamental differences in the electron distributions surrounding the halogens in a C–F versus a C–Cl bond. Our work with these species has allowed us to investigate fundamental questions regarding intermolecular interactions.

<sup>a</sup>G.C. Cole and A.C. Legon, *Chem. Phys. Lett.* 369, 31-40 (2003).

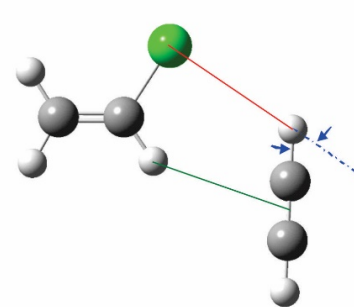
<sup>b</sup>G.C. Cole and A.C. Legon, *Chem. Phys. Lett.* 400, 414-424 (2004).

<sup>c</sup>Z. Kisiel, P.W. Fowler, and A.C. Legon, *J. Chem. Phys.* 93, 3054-3062 (1990).

Vinyl chloride-HF



Vinyl chloride-HCCH



Vinyl chloride-HCl

