IR SPECTROSCOPIC STUDIES ON MICROSOLVATION OF HCl BY WATER

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Acid dissociation reactions are at the heart of chemistry. These reactions are well understood at the macroscopic level. However, a microscopic level understanding is still in the early stages of development. Questions such as *'how many* H_2O *molecules are needed to dissociate one HCl molecule?'* have been posed and explored both theoretically and experimentally.[1−5] Most of the theoretical calculations predict that four H_2O molecules are sufficient to dissociate one HCl molecule, resulting in the formation of a solvent separated $H_3O^+(H_2O)_3Cl^-$ cluster.[1−3] IR spectroscopy in helium nanodroplets has earlier been used to study this dissociation process.[3−5] However, these studies were carried out in the region of O-H and H-Cl stretch, which is dominated by the spectral features of undissociated $(HCl)_m$-$(H_2O)_n$ clusters. This contributed to the ambiguity in assigning the spectral features arising from the dissociated cluster.[4,5] Recent predictions from Bowman's group, suggest the presence of a broad spectral feature (1300-1360 cm^{-1}) for the $H_3O^+(H_2O)_3Cl^-$ cluster, corresponding to the umbrella motion of H_3O^+ moiety.[6] This region is expected to be free from the spectral features due to the undissociated clusters. In conjunction with the FELIX laboratory, we have performed experiments on the $(HCl)_m(H_2O)_n$ (m=1-2, n≥4) clusters, aggregated in helium nanodroplets, in the 900-1700 cm^{-1}region. Mass selective measurements on these clusters revealed the presence of a weak-broad feature which spans between 1000-1450 $cm^{-1}$and depends on both HCl as well as H_2O concentration. Measurements are in progress for the different deuterated species. The details will be presented in the talk.

References: **1)** C.T. Lee et al., *J. Chem. Phys.*, **104**, 7081 (1996). **2)** H. Forbert et al., *J. Am. Chem. Soc.*, **133**, 4062 (2011). **3)** A. Gutberlet et al., *Science*, **324**, 1545 (2009). **4)** S. D. Flynn et al., *J. Phys. Chem. Lett.*, **1**, 2233 (2010). **5)** M. Letzner et al., *J. Chem. Phys.*, **139**, 154304 (2013). **6)** J. M. Bowman et al., *Phys. Chem. Chem. Phys.*, **17**, 6222 (2015).