

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 H₂O 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 H₂O molecules are sufficient to dissociate one HCl molecule, resulting in the formation of a solvent separated H₃O⁺(H₂O)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-(H₂O)_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 H₃O⁺(H₂O)₃Cl⁻ cluster, corresponding to the umbrella motion of H₃O⁺ 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(H₂O)_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 H₂O 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).