IONIC REACTIVITY OF SMALL GAS PHASE MOLECULAR CLUSTERS

NICOLA M TONGE, EWAN C Mac MAHON and MARTIN C R COCKETT, *University of York, Department of Chemistry, Heslington, YO10 5DD, United Kingdom*.

The study of ionised molecular clusters provides an insight into ion-molecule chemistry; ubiquitous in atmospheric, flame and plasma processes. The neutral fluorobenzene-ammonia system, essentially unreactive in the gas phase, will react in solution under high temperature and pressure conditions. However, fluorobenzene$^+$ will react, via nucleophilic substitution to form aniline$^+$ and HF. In combination with the aquisition of REMPI spectra, we have observed the following reactions, post-ionisation, of fluorobenzene$^+$-$(NH_3)_n$ (n=1,2) clusters:

$$C_6H_5F^+.(NH_3)_2 \longrightarrow C_6H_5NH_2{}^+$$

$$C_6H_5F^+.NH_3 \longrightarrow NH_3{}^+ + C_6H_5F$$

While nucleophilic substitution satisfactorily accounts for the formation of aniline$^+$, it is more difficult to rationalise the formation of $NH_3{}^+$ on thermodynamic grounds. By performing *ab initio* calculations we hope to be able to postulate a mechanism for this reaction.