IONIC REACTIVITY OF SMALL GAS PHASE MOLECULAR CLUSTERS

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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⁺-(NH₃)_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.