Chemical reactivity, bonding and structure of the nucleophilic substitution of p-chlorofluorobenzene ions by ammonia

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ABSTRACT
The chemical reactivity within gas phase p-chlorofluorobenzene-ammonia heterocluster cations ([CIFC₆H₄⁺]+(NH₃)₃) have been investigated via a triple quadrupole mass spectrometer and through DFT calculations. Collision induced dissociation (CID) experiments were performed in which mass selected cluster ions are accelerated into a cell containing argon gas and the resulting products then subsequently mass analyze. Two interesting reaction results are observed. The first is that the 1:1 peak is missing. Further investigation is underway to find out why this is the case. The second is survey from the CID experiments display the magic number for (CIFC₆H₄)₆⁺, with helium gas. The reactions between p-chlorofluorobenzene cation and ammonia involve intra-cluster proton transfer of ammonia giving clusters of high stability.

OBJECTIVES
• Triple quadrupole mass spectrometer
• Collision induced dissociation (CID)
• Metastable decay
• “Magic number” for (CIFC₆H₄)₆⁺

METHODS
Collision-Induced Dissociation:
• Powerful technique to study parent ions and chemical reactions within mass-selected cluster ions
• A mechanism to fragment molecular ions in the gas phase
• Fragment ions can be analyzed by a mass spectrometer
• Useful in determine partial or complete structure
• Achieve more sensitive and specific detection

Metastable Decay
• To make a qualitative comparison with CID experiments for decomposition processes of individual cluster ions of the series
• Identical to those employed for the CID mass spectra except with no collision gas in the collision cell

RESULTS
The collision induced dissociated proton transfer reaction within the p-chlorofluorobenzene-ammonia cluster ions is size-restricted at 2≤n≤5, for n=5 clusters, ammonia monomers must be evaporated off at least n=4 for this reaction to occur

ONGOING RESEARCH
To find out the reason why 1:1 peak on CID is missing
To study detail reactivity of “magic number” cluster size ion (CIFC₆H₄)₆⁺

REFERENCES

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