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## Study on Molecular Mechanisms in Dissolution and Deliquescence Processes of Salt Nanocrystals

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### Summary

Adsorption reaction of water on alkali halide nanocrystals gives a model of initial stage of dissolution or deliquescence of bulk salt crystals. We have investigated for three years how the adsorption reactivity of polar molecules, ROH, on sodium halide cluster ions,  $\text{Na}_n\text{F}_{n-1}^+$  and  $\text{Na}_n\text{I}_{n-1}^+$ , depends upon their sizes and geometrical structures by mass spectrometry coupled with a laser photodissociation technique in the ultraviolet region and also by theoretical calculations based on density functional theory. This year we discussed on the reactivity of  $\text{Na}_{13}\text{X}_{12}^+$  and  $\text{Na}_{19}\text{X}_{18}^+$ , in which the extraordinary reactivity was observed in the adsorption mass spectrometry. Also we have developed an experimental apparatus for adsorption reactions of isomer-separated cluster ions.

In our report about  $\text{Na}_{13}\text{X}_{12}^+$  reactivity last year, we found that the “net” adsorption reaction rate is ten to several tens higher for basket isomer than those for the other isomers. From the consideration of the potential energy surfaces along the adsorption reaction coordinate, this anomalous reactivity is presumably due to the existence of the reaction barrier. Once an adsorbate molecule enters the basket, the kinetic energy is dissipated to the vibrational modes of the nanocrystals. Thus the molecule is efficiently trapped inside without desorption. For  $\text{Na}_{19}\text{X}_{18}^+$  ions, we observed high adsorption reactivity of two ROH molecules in the mass spectrometric measurement. This time we obtained an optimized structure of  $\text{Na}_{19}\text{F}_{18}^+$  with two  $\text{H}_2\text{O}$  molecules trapped inside of two different cage sites.

Finally we have also developed an apparatus for the next stage of this research project, isomer-resolved reactivity measurements, by using an ion-mobility spectrometer coupled with reflectron-type time-of-flight mass spectrometer. With this new machine, we checked the performance of the instrument by observing the well-known structural change in carbon cluster ions  $\text{C}_n^+$ , from linear to cyclic at around  $n=7-10$ , and from cyclic to fullerene at around  $n=30$ .