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Study of the Incorporation Effects of Impurity Ions into Salt Nanocrystals

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Summary

In order to obtain salt crystals from seawater, it is necessary to prevent the incorporation of impurity ions such as K^+ and Br^- into the crystals. For this reason, studies on the influence of impurity ions on the crystal growth of NaCl have been conducted. However, those studies have been targeted at particles with a particle size larger than mm, and have not been discussed at the nanoparticle or molecular level. Therefore, we aimed to investigate how the uptake of impurity ions into NaCl clusters (nanocrystals) changes with the cluster size (number of constituent particles) and how the structure changes with the incorporation of impurity ions. To this end, we are using a home-made equipment to investigate both the composition (mass, number of constituent particles, cluster size) and geometric structure information (bulkiness, collisional cross-section) of nanocrystalline ions by ion mobility-mass spectrometry. As a method for the generation and introduction of nanocrystalline ions in this study, we have been using an electrospray ionization (ESI) from an aqueous compound solution. However, there is a problem that it is difficult to stably generate cluster ions with ordinary ESI sources. Therefore, from this year, we conducted a new experiment using a high-pressure electrospray ion source. As a result, we succeeded in producing nanocrystalline ions stably in the size region which were difficult to generate by a conventional ESI source. Furthermore, we began to investigate the effect of replacing alkali metal positive ions with K^+ instead of Na^+ using this ion source. First of all, the generation of monovalent positive ions, $Na_nCl_{n-1}^+$, $K_nCl_{n-1}^+$, and divalent positive ions, $Na_{n'}Cl_{n'-2}^{2+}$, $K_{n'}Cl_{n'-2}^{2+}$, was found to be generated from the experiments of nanocrystalline positive ions of sodium chloride and potassium chloride. Next, the geometric structure change was discussed from the dependence of the collision cross section of these ions on the cluster size. Finally, we observed ions in which some Na^+ ions of NaCl nanocrystalline ions were replaced with K^+, using a NaCl sample mixed with 1% KCl. We will obtain the equilibrium structures and their collision cross sections of the ions by quantum chemical calculations, and identify the geometric structures of the ions by comparing them with those obtained in the experiment.