Development and Computational Modeling of Novel Calixarenes for Separation of Valuable Metals in Seawater

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Summary

In the field of clinical and food industries, there is a high demand for selective recognition of a target salt ion. Therefore, attempts are being made to develop highly selective molecules that can recognize the target salt ion in an aqueous solution containing various salt ions. In a salt analysis, as the extractant has a crucial effect on separation and concentration efficiency, it is important to develop an efficient ligand for a target salt ion, and the selection of the ligand often decides the success of the analysis system. Apart from the large amount of works on extraction of base metals, relatively few papers have reported on salt extraction. Furthermore, in most works commercially available extractants have been employing as the host molecules for salt ions and little attention has been paid to the development of novel host compounds.

In the present study, we have synthesized novel host compound calixarenes, which is a new cyclic ligand connecting with some phenol rings. Using the newly synthesized ligands, separation and concentration of various salt ions were conducted. The extraction behavior is also discussed with computational modeling. The extraction behavior of alkaline and alkaline earth ions was systematically investigated with the cyclic host compound calixarene. The calixarene derivatives showed high extractability for all the salt ions compared to that of a noncyclic monomer analog. The extraction behavior of alkaline and alkaline earth metals is closely related to the cavity size of the cyclic ligands; thus, the tetramer selectively extracted sodium and calcium ions, while the hexamer did so for cesium and barium ions. These results indicate that the cyclic structure is effective for the recognition of alkaline and alkaline earth ions. All of the salt ions were confirmed to be extracted with the cyclic ligands by forming a 1 : 1 complex, which was also supported by the results of computational modeling. It is concluded that cyclic ligands are useful and show high selectivity when the cavity size fits the ionic size of a target ion.