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Oil for Extraction of Metals from High-concentration Salt Solutions: Search for Compounds Suitable for Ionic Solvation Extraction by Machine Learning

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Summary

Extraction based on ionic solvation, which can extract metal chloride from an aqueous solution rapidly, with high capacity, as well as high metal selectivity, is expected as a separation and recovering technique for rare metals from water resources including seawater. In recent years, the authors have found a candidate solvent (2-nonanone) that has the similar Au(III) extractability compared with commercial extractants. The solvent is expected to reduce wastewater pollution and extractant costs due to the lower water solubility. However, optimization of solvents for ion solvation extraction has not been achieved, because there are thousands of candidate compounds. In the present study, the relationship between the metal extractability for various solvents and physical properties of the solvents was analyzed by machine learning, in order to find the powerful solvents from a number of candidate solvents, with better physical properties than the commercial extractants. From the results of the extraction tests for Au(III) and Ga(III) at high HCl concentration, solvents were categorized by the metal extractability. Ketones commonly showed high extractability, whereas there was a wide distribution of metal extractabilities for ethers. Additionally, the authors found that there is a certain correlation between the Hansen solubility parameters (HSPs) and the metal extractability, but that there are also exceptions. By machine learning using the results of Au(III) extraction tests, models with high prediction accuracy for hydrocarbons, carboxylic acids, and ketones were constructed. However, in the model there was a large error for ethers. From the results of HSPs relationship and machine learning, dicyclohexyl ketone (DCHK) was selected as a candidate solvent for Au(III) extraction. The extraction test for Ga(III) from simulated seawater using 2-nonanone was also performed. Ga(III) was recovered by increasing HCl concentration.