Solvation of Lanthanide ion (III) in Water saturated Ionic Liquids by Molecular Dynamics Study

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We have studied the solvation structure behavior of lanthanide (Ln) ions in water saturated ionic liquids (ILs) via molecular dynamics simulation. All 15 Ln ions, which are La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, were considered with three ILs mixed from one cation molecules of 1-methyl-3-octyl imidazolium([OMIM+]) and three anion molecules of Tetrafluoroborate((BF_4-]), nonafluorobutyl sulfonate([NfO-]), bis(trifluoromethanesulfonyl) imide([Tf_2N]). In this study, we have built two representative systems, which are ILs/water model to obtain saturated water contents in pure ILs and IL/water model containing one type of Ln ion to figure out the ion concentration at interface of ILs/water. It is found that more hydrophobic anion makes more water residing in the first solvation shell from coordination of Ln ions. For the smaller Ln ion, NO_3- ion more easily construct sharing form between Ln ions. From these results, we could obtain Ln ion movement before extraction was occurred and postulate that hydrophobic anion (NfO and Tf_2N) have higher capability than hydrophilic anion (BF_4) to extract Ln.