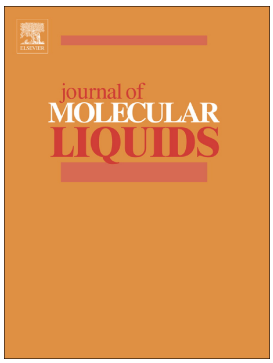

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Trihexyl Phosphate to Trihexyl Phosphine Oxide: Diverse Effect on Extraction Behavior of Actinides

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Abstract

To delineate the effect of P-C bond of phosphorous esters on the extraction of actinides, diverse organophosphorus esters (trihexyl phosphonate (THP), dihexylhexyl phosphonate (DHHP), hexyldihexyl phosphinate (HDHP) and trihexylphosphineoxide (THPO)) were synthesized and spectroscopically characterized. The physical properties such as density, viscosity are reported in subsequent sections. The extraction behaviour of the ligands were evaluated for U(VI), Th(IV) and Am(III), as well as acid uptake as a function of nitric acid ranging from 0.01- 6M. Distribution ratios for U(VI), Th(IV) and Am(III) indicate a large difference in solvent strength among these compounds. Replacement of P-O-C group by P-C group *i.e.* introduction of electron donating group greatly increases the solvent strength. The P=O stretching frequency can be correlated with the solvent strength of these compounds, and the conclusions are further supported by density functional theory calculations.

Keywords: Actinides; Organophosphorus compounds; Phosphate; Phosphine oxide; Solvent extraction; Density functional theory.