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# The Role of Solvent and Neutral Organophosphorus Extractant Structure in their Organization and Association

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## Abstract

The choice of organic solvent is known to impact metal ion partitioning in solvent extraction systems, although an understanding based on molecular interactions has been largely qualitative. To provide a more quantitative and molecular scale understanding of extractant and solvent association in liquid-liquid solvent extraction systems, molecular dynamics studies of binary extractant/solvent systems are conducted for several organophosphorus solvating extractants across a range of organic solvents. Classical molecular dynamics potentials for the extractants are optimized in pure phase simulations. These potentials are then validated with binary extractant/solvent solutions by comparison to experimental data for percent volume change on mixing and mixing enthalpies. Trends in association free energy, mixing enthalpy and deviations from ideal mixing volume are reported for each extractant and solvent binary mixture. Contributions to those properties depending on extractant and solvent molecular structure are investigated, including the rel-

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