Supplementary material: Molecular mechanisms induced by phase modifiers used in hydrometallurgy: consequences on transfer efficiency and process safety

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1. Surface tension measurements

The surface tension measurements are then transformed to surface area per polar head. The surface concentration excess $\Gamma$, is then determined from the Gibbs equation:

$$\Gamma = -\frac{1}{RT} \cdot \frac{d(\gamma)}{d(\ln[\text{extractant}])} \quad (S1)$$

where, $\gamma$ is the surface tension (N·m$^{-1}$), [extractant] is the concentration of the extractant in the organic phase (mol·L$^{-1}$), $R$ is the perfect gas constant ($R = 8.314472$ J·mol$^{-1}$·K$^{-1}$), and $T$ is the temperature (K).

This excess surface concentration $\Gamma$ can be related to the surface area occupied by each extractant by the relation:

$$\sigma = \frac{1}{N_A \cdot \Gamma} \quad (S2)$$

with $N_A$ is the Avogadro constant ($N_A = 6.02214 \times 10^{23}$ mol$^{-1}$).
Supplementary Figure S1. The cac values (solid black line) as well as the surface area per extractant molecule (dashed grey line) for two different extraction systems as a function of the amount of PnP added. The extractants studied are: (a) HDEHP and (b) DMDOHEMA.

Supplementary Figure S2. SANS spectra of organic phases containing 0.6 M HDEHP in deuterated dodecane.

Supplementary Figure S3. SANS spectra of organic phases containing 0.6 M DMDOHEMA in deuterated dodecane.

2. Neutron scattering experiments

We systematically compare sample with co-extracted water in the polar core of the micelle present as H₂O or as D₂O: this way of plotting allows detection of possible microemulsions if H₂O and D₂O w/o microemulsion have profoundly different signature patterns by scattering.
Supplementary Figure S4. SANS spectra of the n-octanol/dodecane binary not contacted or previously contacted with H\textsubscript{2}O or D\textsubscript{2}O for n-octanol volume fractions of: (a) 3\%, (b) 9\% and (c) 27\%.