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

Document complémentaire : Mécanismes moléculaires induits par les modificateurs de phase utilisés en hydrométallurgie : conséquences sur l'efficacité du transfert et la sécurité des procédés

Asmae El Maangar *, [a], **Sylvain Prévost** [b], **Sandrine Dourdain** [a] **and Thomas Zemb** *, [a]

[a] ICSM, CEA, CNRS, ENSCM, Univ Montpellier, Marcoule F-30207, France
[b] Institut Max von Laue-Paul Langevin, CS 20156, Grenoble Cedex 9, F-38042, France
E-mails: y.asmae.elmaangar.t@gmail.com (A. El Maangar), sylvain.prevost@ill.fr (S. Prévost), sandrine.dourdain@cea.fr (S. Dourdain), thomas.zemb@icsm.fr (T. Zemb)

1. Surface tension measurements

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

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

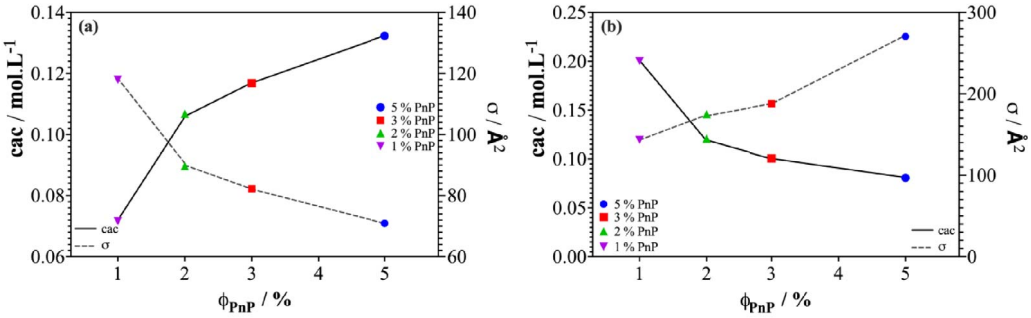
where, γ is the surface tension (N·m^1), [extractant] is the concentration of the extractant in the organic phase (mol·L^{-1}), R is the perfect gas constant (R = 8.314472 J·mol^{-1}·K^{-1}), and T is the temperature (K).

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

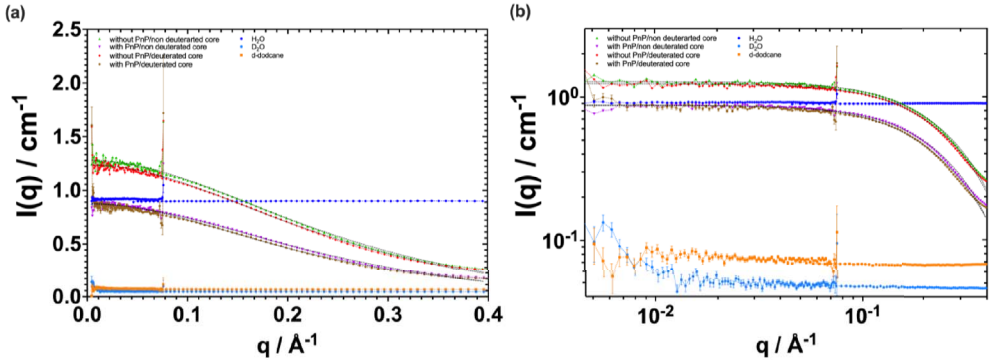
$$\sigma = \frac{1}{N_A \cdot \Gamma} \tag{S2}$$

with N_A is the Avogadro constant ($N_A = 6.02214 \times 10^{23}$ mol^{-1}).

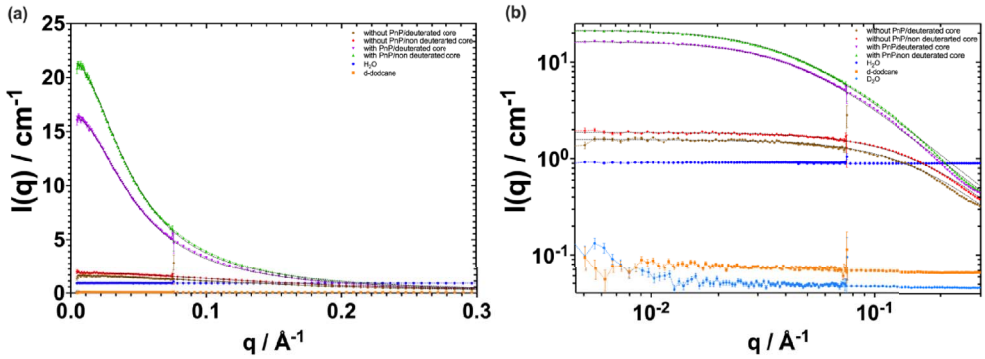
* Corresponding authors.



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.



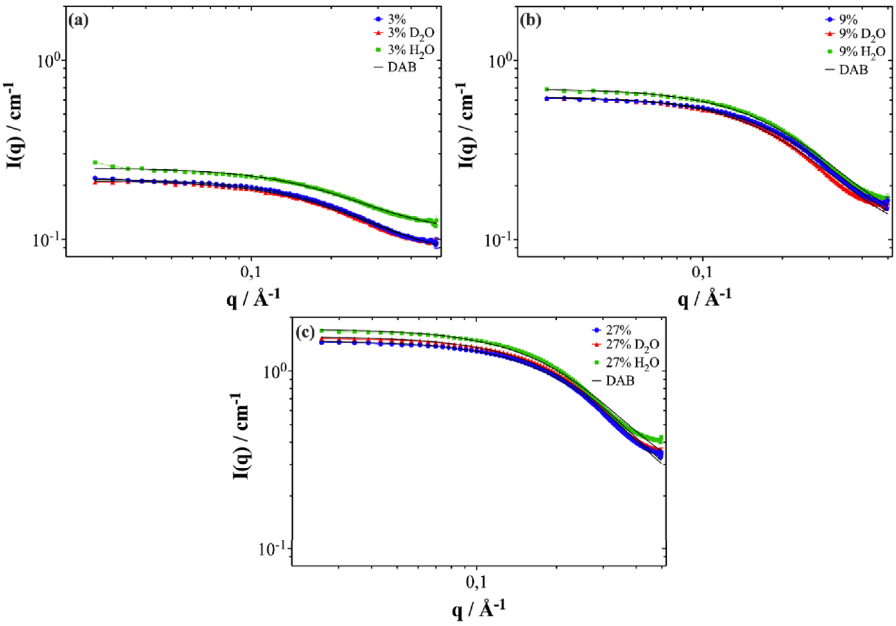
Supplementary Figure S2. SANS spectra of organic phases containing 0.6 M HDEHP in deuterated dodecane.



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 H_2O or as D_2O: this way of plotting allows detection of possible microemulsions if H_2O 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_2O or D_2O for n-octanol volume fractions of: (a) 3%, (b) 9% and (c) 27%.