

# Aqueous solubilization of hydrophobic compounds by inorganic nano-ions: An unconventional mechanism

Monday, 2 June 2025 18:45 (15 minutes)

Solubilization of hydrophobic compounds in water is commonly performed by the addition of organic solubilizers through (i) micellar or hydrotropic solubilization using amphiphilic molecules[1], (ii) co-solvency using water-soluble solvents, and (iii) host–guest complexation using macrocycles[2]. In this study, we show that the 3,3'-commo-bis[closo-1,2-dicarba-3-cobaltadodecaborane] derivatives (COSANs)—fully inorganic and non-amphiphilic ionic boron clusters with nanometric size and superchaotropic properties—efficiently solubilize model hydrophobic compounds, such as medium-chain alcohols ( $0.6 < \log P < 1.5$ ), in water. Unlike micellar solubilization using surfactants, COSAN acts as an efficient solubilizer in its monomeric state, i.e., at concentrations well below the critical aggregation concentration. The solubilization mechanism of COSAN differs significantly from the surfactant-based solubilization. COSAN induces the bi-dimensional anisotropic growth of COSAN/alcohol co-assemblies, whereas surfactants typically induce isotropic swelling of micelles. This unconventional solubilization mechanism, based on the formation of thermodynamically stable COSANs/alcohol anisotropic co-assemblies, was revealed through spectroscopic and scattering techniques (SWAXS and SANS). We have also shown that the COSAN/2-butanol co-assemblies can be used to solubilize more hydrophobic compounds with  $\log P$  values up to around 6. These findings suggest that ionic boron clusters have significant potential for solubilizing hydrophobic compounds across a broad hydrophobicity scale in various applied fields.

- [1] P. Bauduin, A. Renoncourt, A. Kopf, D. Touraud, W. Kunz, Unified concept of solubilization in water by hydrotropes and cosolvents, *Langmuir*. 21 (2005) 6769–6775.
- [2] Y. Chevalier, T. Zemb, The structure of micelles and microemulsions, *Reports, Prog. Phys.* 53 (1990) 279–37.
- [3] I. Chazapi, O. Diat, P. Bauduin, Aqueous solubilization of hydrophobic compounds by inorganic nanoions: An unconventional mechanism, *J. Colloid Interface Sci.* 638 (2023) 561–568.

**Primary author:** Dr CHAZAPI, Ioanna (Laboratoire Léon Brillouin, Université Paris-Saclay, CEA-CNRS UMR 12 CEA Saclay, 91191 Gif sur Yvette, France)

**Co-authors:** Dr DIAT, Olivier (ICSM, CEA, CNRS, ENSCM, Univ Montpellier, Bagnols sur Cèze, France); Dr BAUDUIN, Pierre (ICSM, CEA, CNRS, ENSCM, Univ Montpellier, Bagnols sur Cèze, France)

**Presenter:** Dr CHAZAPI, Ioanna (Laboratoire Léon Brillouin, Université Paris-Saclay, CEA-CNRS UMR 12 CEA Saclay, 91191 Gif sur Yvette, France)

**Session Classification:** Posters