

## Solubility of Polycyclic Aromatic Hydrocarbons in Ionic Liquids and Ionic Liquid Aqueous Solutions

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Polycyclic Aromatic Hydrocarbons (PAHs) are common compounds consisting of two or more fused aromatic rings. The interest in these compounds is twofold: a) they are pollutants that can be found mainly in soils and sediments as a result of fuel combustion; b) they represent the pathway from benzene to carbon-nanomaterials. The development of novel bioremediation processes to reduce the risk of exposure to these compounds is limited by their very low solubility in water, which declines with the increasing number of aromatic rings [1]. To date many works on surfactant micellar solubilization of hydrophobic compounds have used conventional surfactants [2,3]. Ionic liquids are known as designer solvents with solubility behaviour that can be tuned through changes in both cation and/or anion. Moreover, they can also present surfactant behaviour that enhances their potential as co-solvents. In this context we have used ionic liquids as solubilisers of hydrophobic PAHs. The PAHs solubility behaviour was mapped in all range of concentrations of ionic liquid in water, from more diluted solutions to pure ionic liquids. Several distinct families of ionic liquids have been used in this work. As expected the best results in aqueous solutions appear with ionic liquids that present surfactant-like behaviour. The model compounds chosen were naphthalene, anthracene, phenanthrene, pyrene and coronene. HPLC was used to measure the solubility of the PAHs in both pure ionic liquid as well as ionic liquid aqueous solutions. Ab-initio calculations and Molecular Dynamics simulations have been used as valuable tools to unravel the interactions between the aromatic moieties and the selected surface active ionic liquids.

### References

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- [2] Chun et al, 2002: *Environmental Pollution* 118 (2002) 307–313.
- [3] Markiewicz et al, 2013: *Environmental Science & Technology*, 47, 6951–6958.