Solubilities of Solid Polycyclic Aromatic Hydrocarbons and Polycyclic Aromatic Heterocycles in Pressurized Hot Water

P. Karasek, J. Planeta and M. Roth[C, S]
Institute of Analytical Chemistry, Academy of Sciences of the Czech Republic, Brno, Czech Republic
roth@iach.cz

Pressurized hot water (PHW), i.e., liquid water at temperatures between the normal boiling point and the critical point, has recently received an increasing attention as a green and temperature-tunable solvent with applications in environmental remediation, extraction of plant materials, and sample treatment procedures for analytical chemistry. However, despite the growing use of PHW, the solubility data base in PHW has not yet been sufficiently robust to allow reliable estimations of solubilities of heavy organic nonelectrolytes within a wide range of temperature and pressure, and predictive correlations in this field are virtually absent.
This contribution is concerned with three topics related to application of PHW as a solvent:

1. A review of recent experimental results from this laboratory on aqueous solubilities of several 2- to 4-ring solid polycyclic aromatic hydrocarbons (PAHs), with emphasis on comparison with literature data and on the temperature dependence of solubility of the individual PAHs.

2. Correlation of aqueous solubility of PAHs as a function of temperature and pressure employing only pure component properties. The required properties of water are cohesive energy density, internal pressure and static relative permittivity, all at the particular temperature and pressure. The required properties of PAHs include triple-point temperature, enthalpy of fusion, molar volume of the subcooled liquid and molar volume of the solid. Performance of the correlation is illustrated including extrapolation from PHW domain to environmentally relevant conditions of 298 K and 0.1 MPa.

3. New experimental results on aqueous solubilities of several sulfur- and nitrogen-containing heterocyclic analogs of anthracene. Effects of heteroatom(s) on solubility are shown and discussed.