

## Solubility of Solids in Mixed Solvents: Modeling and Data Reduction

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The solubility of solids in mixed solvents is important for the design and operation of chemical processes and for the functioning of medical, agrochemical and other chemical products. Traditionally, reliable modeling of mixed solvent solubility requires access to a wide variety of data, such as: Pure solute properties (e.g. melting temperature, heat of fusion, heat capacities), pure solvent properties (e.g. molar volume, heat capacity) and solubility of the solute in the pure solvents. Often these properties are not available, leading to the use of estimated or hypothetical values, which are subject to considerable uncertainty. A modelling framework has been presented previously<sup>1</sup>, which is able to describe the mixed solvent solubility behavior for wide ranges of solutes using transferable parameter values, but does not require all of the above properties. This semi-rigorous method is based on statistical mechanical fluctuation solution theory (FST), which employs integrals of total correlation functions to obtain composition derivatives of the solute/solvent infinite dilution activity coefficient and excess Henry's constants for solvent mixtures relative to pure solvents. Parameters involving the solute may be obtained either from mixed solvent solubility data (ternary) or directly from binary solute/solvent solubility. Solvent parameters are found from nonideality of the solvent mixture via a  $G^E$ -model, independent of the solute. We present a data base covering experimental solubilities of solid solutes in pure and binary solvent mixtures at various solvent compositions for more than 400 mixtures. Extensive comparisons with available data show that the FST method is successful in describing the whole variety of observed mixed solvent solubility behavior, including nearly ideal systems with small excess Henry's constants, solute-independent excess Henry's constants, and systems which deviate from these simple rules. Suggestions are made for classification of solute-solvent systems to provide a basis for estimating solubilities in unmeasured systems.

[1] M.E. Christensen, J. Abildskov, J.P. O'Connell. *Method for predicting solubilities of solids in mixed solvents*. AIChE Journal (2008). *Accepted for publication*.