

WATER ACTIVITY MODELS FOR CHARACTERIZING TRANSITIONS BETWEEN DEEP EUTECTIC SOLVENTS AND REGULAR SOLUTIONS

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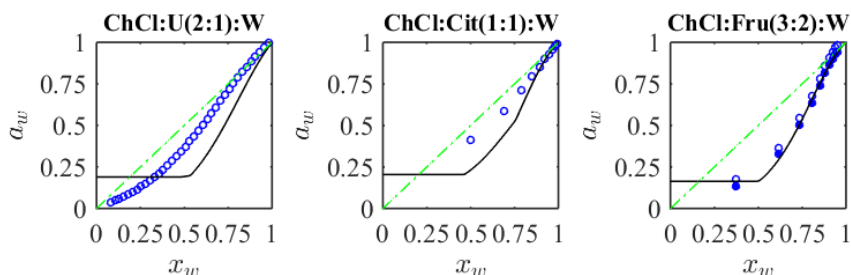
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Many applications of deep eutectic solvents (DES) require their dilution with water to reduce viscosity and improve practical efficiency. However, this raises the question of what fraction of water still allows such a ternary mixture to be considered a DES rather than merely a strongly non-ideal solution, and how these two thermodynamic entities can be distinguished.

In contrast to sophisticated experimental methods such as NMR, as well as numerical analyses based on quantum-chemical estimates, it has recently been argued [1] that studying the water activity of such ternary systems can serve as a demonstrative indicator when experimental data are compared with the predictions of relatively simple thermodynamic models. In the present work, the applicability of the Ross method, complemented by the Caurie and Norrish models for the corresponding binary subsystems, can serve as a criterion for assessing the extent to which donor–acceptor interactions between DES components are compromised by the addition of excessive water.

The validity of the proposed approach is tested with a wide range of systems for which corresponding experimental data are available; see some examples in the figure below. The results are compared with microstructure-characterizing chemical indicators, and practical rules for testing DES-candidate mixtures are proposed.



Examples of systems exhibiting strong, range-limited, and absent properties of deep eutectic solvents indicated by the deviation of experimental data on the water activity (markers) from a theoretical model for a ternary regular mixture (black curve).

1. Postnikov E.B., Vanina A.S., Wasiak M., Sychev A.V., Chorążewski M. Thermodynamic properties of natural deep eutectic solvents and their aqueous solutions exemplified by fructose–citric acid–water mixtures // *Molecular Thermodynamics of Aqueous Systems: Binary and Ternary Solutions/Mixtures*, eds. T. Letcher and E. Wilhelm. RSC Press, 2026 (in press).