Thermophysical Properties of N-Cyclohexylpyrrolidone + N-Methyl-2-Pyrrolidone + Water Solvent Mixtures at 298.15 K

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Nowadays, cyclic amides with water are used as mixed selective solvents in industry, and, for this reason, the need for determining their thermophysical properties has increased.

In this work, we report a thermophysical study of the ternary system: N-cyclohexyl-2-pyrrolidone (CHP) + N-methyl-2-pyrrolidone (NMP) + water (W), in the full composition range at 298.15 K and atmospheric pressure. Density, speed of sound, dynamic viscosity, refractive index, and isobaric heat capacity were measured with highly accurate experimental techniques, and the experimental procedures were described in a previous paper [1]

The excess and mixing properties were calculated and correlated with composition. A highly non-ideal behavior is observed for these mixtures, due to an association by hydrogen bonding when CHP and NMP are mixed with W, through the carbonyl lonely electron pair of the lactam.

To predict the ternary properties from the binary systems, semiempirical models, such as Jacob-Fitzner, Köhler, Colinet, Tsao-Smith, Toop, and Scatchard, were used. The volumetric properties were correlated using the Soave (SRK) and Peng-Robinson (PR) cubic equation of state, with a set of ten different mixing rules, and with the SAFT molecular-based equation of state. It was observed that the complex behavior of these mixtures is reproduced more accurately by the SAFT model.

[1] B. García, S. Aparicio, R. Alcalde, M.J. Dávila, and J.M. Leal, *New J. Chem.* **29**, 817 (2005).