PVTx Behavior of the N-Methyl-2-Pyrrolidone/Carbon Disulfide Mixed Solvent

S. Aparicio,[C,S] M.J. Davila, R. Alcalde, R. Alcalde, B. Garcia, and Leal
Departamento de Química, Universidad de Burgos, Burgos, Spain
sapar@ubu.es

N-Methylpyrrolidinone (NMP) is considered one of the most important cyclic amides because of its applications in molecular biology, as a model molecule for more complex peptide compounds, and because this molecule, in a pure form or when forming mixtures with other solvents, is used in several industrial applications, such as extraction, distillation, absorption, and gas desulfurization.

Densities were measured by means of a high pressure Anton Paar DMA512 vibrating tube densimeter. The temperature of the cell was controlled by an external water bath and measured using a platinum resistance thermometer inside the cell thermostated jacket. The measurement cell was connected to a Ruska 7615 digital pressure controller [1]. An Anton Paar DMA 58 was used to register the vibrating period of the cell. The PVTx behavior of the x NMP + (1-x) CS_2 system was measured in the full composition range between 278.15 to 358.15 K and pressures up to 60 MPa, and from it were calculated the derived properties: isobaric thermal expansivities, isothermal compressibilities, internal pressures, and excess properties of the system.

The PVTx data were correlated using several cubic equations of state (EoS) proposed by Soave (SRK), Peng–Robinson (PR), Stryjek–Vera modification of Peng–Robinson (PRSV), Patel–Teja (PT), and Sako–Wu–Prausnitz (SWP), with different mixing rules. Moreover, the Statistical Associating Fluid Theory (SAFT) with different mixing rules was applied to correlate the PVTx data, and the results were compared to the cubic EoS.

[1] B. García, S. Aparicio, R. Alcalde, M.J. Dávila, and J.M. Leal, *Ind. Eng. Chem. Res.* **43**, 3205 (2004).