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DEPARTMENT : Chemistry

TITLE OF THE THESIS : Experimental and theoretical studies of molecular interactions in multicomponent systems containing industrially important organic solvents.

Abstract

The work presented in this thesis is divided into the following chapters.

Chapter 1. This is introductory chapter. It embodies the scope and objective of the proposed work. An upto date literature survey has been presented to illustrate the work being carried out in this field.

Chapter 2. Calibrations of the apparatus have been detailed out in this chapter. Ultrasonic velocity, density, and refractive index have been measured at different temperatures for pure liquids and liquid mixtures.

Chapter 3. The densities, ρ and viscosities, η of binary mixtures of methyl acrylate (MA) with benzene, toluene, *o*-xylene, *m*-xylene, *p*-xylene, and mesitylene, including those of pure liquids, over the entire composition range were measured at different temperatures and atmospheric pressure. From the experimental data, the excess molar volume, V_m^E, partial molar volumes, $\overline{V}_{m,1}^{\circ}$ and $\overline{V}_{m,2}^{\circ}$, and excess partial molar volumes, $\overline{V}_{m,1}^{\circ E}$ and $\overline{V}_{m,2}^{\circ E}$ at infinite dilution were calculated.

Chapter 4. The densities, ρ and refractive indices, n_D of binary mixtures of ethyl acrylate with 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol, including those of pure liquids, over the entire composition range were measured at different temperatures and atmospheric pressure. The interactions in these mixtures follow the order: 1-butanol < 2-butanol < 2-methyl-1-propanol < 2-methyl-

2-propanol. It is observed that the magnitude of V_m^E depends upon the position of hydroxyl and methyl groups in these alkanol molecules.

Chapter 5. The densities, ρ and ultrasonic speeds, u of binary mixtures of butyl acrylate (BA) with benzene, toluene, *o*-xylene, *m*-xylene, *p*-xylene, and mesitylene, including those of pure liquids, over the entire composition range were measured at the temperatures (288.15, 293.15, 298.15, 303.15, 308.15, 313.15, and 318.15) K and atmospheric pressure. The deviations in V_m^E values follow the order: benzene < toluene < *p*-xylene < *m*-xylene < *o*-xylene < mesitylene. It is observed that the magnitude of V_m^E, and Δu depends upon the number and position of methyl groups in these aromatic hydrocarbon molecules.

Chapter 6. The densities, ρ viscosities, η and speed of sound, u of binary mixtures of MA and butanol / hexanol / octanol / decanol, including those of pure liquids, were measured over the whole composition range at 303.15, 308.15, 313.15, 318.15 K and atmospheric pressure. The strength of interactions in these mixtures follow the order: butanol > hexanol > octanol > decanol.

Chapter 7. The densities, ρ viscosities, η refractive index, n_D and speed of sound, u of binary mixtures of dimethylacetamide (DMA), MA, EA, BA, including those of pure liquids, were measured over the whole composition range at 303.15, 308.15, 313.15, 318.15 K and atmospheric pressure. The derived functions, V_m^E, $\triangle\eta$, $\triangle u$, $\triangle\kappa_s$ and $\triangle n_D$, have been used to have a better understanding of the intermolecular interactions occurring between the component molecules of the present liquid mixtures.