

Supplementary Information

Studies on acoustical parameters, thermodynamical properties and theoretical evaluation of morpholine with *ortho* xylene in isopropanol at 303K, 308K and 313K using ultrasonic sound

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I Acoustical and thermodynamical parameters

The following acoustical and thermodynamics parameters were calculated:

1 Adiabatic compressibility (β) has been calculated from the ultrasonic velocity (U), and the density (ρ) of the medium using the Newton- Laplace equation as follows:

$$\beta = 1/U^2\rho \dots\dots\dots (1)$$

2. Intermolecular free length (L_f) has been determined as²³ follows:

$$L_f = K_T\beta^{1/2} \dots\dots\dots (2)$$

Where K_T is the temperature – dependent constant known as Jacobson’s constant ($K_T = 2.131 \times 10^{-6}$ at 318K), and β is the adiabatic compressibility.

3. Free volume (V_f) in terms of ultrasonic velocity (U) and the viscosity (η) of liquid²⁴ is as follows:

$$V_f = (M_{eff} U/ k\eta)^{3/2} \dots\dots\dots(3)$$

Where M_{eff} is the effective molecular weight of the mixture ($M_{\text{eff}} = \sum m_i X_i$, where m_i and X_i are the molecular weight and mole fraction of individual constituents, respectively), k is temperature independent constant which is equal to 4.281×10^9 for all liquids²⁵.

4. Internal pressure (Π_i) can be calculated using the relation²⁶ as follows:

$$\Pi_i = bRT(k\eta/U)^{1/2} (\rho^{2/3} / M_{\text{eff}}^{7/6}) \dots (4)$$

Where b stands for cubic packing, which is assumed to be 2 for all liquids, k is a dimensionless constant independent of temperature and nature of the liquids, its values is 4.281×10^9 . T is the absolute temperature in Kelvin, M_{eff} is the effective molar weight, R is the universal gas constant, η is the viscosity of the solution in Nsm^{-2} , U is the ultrasonic velocity in ms^{-2} and ρ is the density in kgm^{-3} of solution.

5. The Gibbs free energy can be determined using the relation as follows:

$$\Delta G = k_B T \ln(k_B T \tau / h) \dots (5)$$

Where τ is viscous relaxation time, T is the absolute temperature, k_B is Boltzmann's constant, and h is Planck's constant.

6. Acoustic impedance (Z) is given as follows:

$$Z = U \cdot \rho \dots (6)$$

2 Theoretical Studies

The following theoretical relations were compared with the experimental values of ultrasonic velocity.

Nomoto's Equation:

$$U_{\text{NR}} = \sum_{i=1}^n \frac{x_i R_i}{x_i V_{mi}} \dots (8)$$

Van Dael Ideal Mixing Relation:

$$U_{IMR} = (\sum_{i=1}^n x_i M_i)^{1/2} \left(\sum_{i=1}^n \frac{x_i}{M_i v_{Mi}^2} \right)^{1/2} \dots\dots\dots (9)$$

Junjie's Relation:

$$U_{JR} = (\sum_{i=1}^n x_i v_{mi}) (\sum_{i=1}^n x_i M_i)^{1/2} \left[\frac{\sum_{i=1}^n x_i v_{mi}}{\sum_{i=1}^n \rho_i U_i^2} \right]^{1/2} \dots\dots\dots (10)$$

Impedance Dependant Relation:

$$U_{IMP} = \frac{\sum_{i=0}^n x_i \rho_i U_i}{\sum_{i=0}^n x_i \rho_i} \dots\dots\dots (11)$$

Where x_i is Mole fraction, R_i is molar sound velocity, ρ_i is the density and V_{mi} is the molar volume

$$\text{Absolute Average Percentage Deviation (AAPD)} = \frac{1}{n} \sum \left[\frac{(U_{exp} - U_{the})}{U_{exp}} \right] \times 100 \quad (12)$$

$$\% \text{ Error (PE)} = \{(U_{exp} - U_{the}) / U_{exp}\} \times 100 \dots\dots\dots (13)$$