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Studies on liquid–liquid interactions of some ternary mixtures by density, viscosity and ultrasonic speed measurements

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ABSTRACT

The density, viscosity and ultrasonic velocity have been measured for the ternary mixtures of Methyl benzoate, cyclohexane with primary alcohol (1-propanol, 1-butanol, 1-pentanol and 1-hexanol) at 303.15, 308.15 and 313.15K. From the measured values, the acoustical parameters such as adiabatic compressibility (β), free length (L_f), free volume (V_f) have been computed. The excess parameters like excess adiabatic compressibility (β^E), excess free length (L_f^E), excess free volume (V_F^E) and excess internal pressure (π_i^E) were also calculated in order to investigate the molecular interaction between the components of liquid mixtures.

1. Introduction

The measurement of ultrasonic speed enables the accurate determination of some useful acoustical and thermodynamic parameters and their excess functions, which are highly sensitive to molecular interactions in liquid mixtures [1,2].

The nature and relative strength of the molecular interaction between the components of the liquid mixtures have been successfully investigated by the ultrasonic method by Ali et al. [1] and Kannappan and Palani [3]. These interactions helps in better understanding the nature of the solute and solvent i.e., whether the solute modifies or distorts the structure of the solvent. The structure, nature and prevailing conditions of the solvents and solutes, play an important role on resulting properties and interactions occurring in the solution.

The compositional and temperature dependence of thermodynamic properties have proved by Satyanarayan Rao et al. [4] and it was a very useful tool in understanding the nature and extent of pattern of molecular aggregation resulting from intermolecular interactions between components. Ultrasonic velocity of a liquid is fundamentally related to the binding forces between the atoms or the molecules and has been adequately employed in understanding the nature of molecular interaction in binary and ternary mixtures (Rai et al. [5]; Nikam et al. [7]; Peralta et al. [8]; Resa et al. [9]Nikam and Kharat [6]; Prasad et al. [10], [11]; Oswal et al. [12]).

Systematic studies of various relations have been made for binary liquid mixture, multi component liquid mixtures which are of great practical importance in many industrial processes as they provide a wide choice of solutions with appropriate composition and properties. The non-linearity may be explained on the basis of molecular dimensions and the forces acting between the molecules. Ultrasonic velocity together with density and viscosity data furnish a wealth of information about the interaction between ions, dipoles, H-bonding, multipolar and dispersive forces (Eyring and John [13]; Bhadja et al. [14]; Syamala et al. [15] Ramamoorthy et al. [32];Sarkar and Roy [16]).

Compressed liquid density measurements for Methyl benzoate, Cyclohexane or hexanol have been studied by Davila et al. [18]. They found that Methyl benzoate structure is disrupted by the globular shaped Cyclohexane, which is considered as an order destroyer(Prausnitz et al. [17]).

Therefore, in order to have a clear understanding of the intermolecular interactions between the component molecules, the author has performed a thorough study on the molecular interactions using ultrasonic velocity data. The present work deals with the measurement of ultrasonic velocity and computation of related parameters in the following ternary systems,

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Table 1
Values of density (ρ), viscosity (η) and ultrasonic velocity (U) for pure liquids.

Liquids	ρ kg m^{-3}			η × 10^3 N s m^{-2}			U m s^{-1}		
	Temperature (K)								
	303.15	308.15	313.15	303.15	308.15	313.15	303.15	308.15	313.15
Methyl benzoate	1078.1	1076.8	1073.6	1.5539	1.4662	1.3374	1346.66	1314.26	1286.99
Cyclohexane	768.80	762.40	757.10	0.80	0.72	0.66	1230.33	1211.55	1290.60
1-Propanol	800.6	794.9	789.5	1.6095	1.4162	1.2517	1193.40	1180.50	1163.65
1-Butanol	805.1	803.2	799.15	2.1604	1.8615	1.6309	1230	1212.1	1198.56
1-Pentanol	806.76	801.78	800.26	2.7656	2.4088	2.0934	1252.9	1241.91	1217.4
1-Hexanol	810.28	807.5	803.12	3.523	3.1814	2.7857	1288.49	1272.5	1255.1

System I: Methyl benzoate+Cyclohexane+1-Propanol
System II: Methyl benzoate+Cyclohexane+1-Butanol
System III: Methyl benzoate+Cyclohexane+1-Pentanol
System IV: Methyl benzoate+Cyclohexane+1-Hexanol

The experimentally determined values of density, viscosity and ultrasonic velocity for all the mixtures for different mole fractions were studied at T303.15, 308.15 and 313.15K. The acoustical and thermo dynamical parameters are calculated using standard equations.

2. Materials and methods

All the chemicals used in the present work are Analar grade. The purity of the chemicals was ascertained by comparing their density, viscosity and ultrasonic velocity at 303.15, 308.15, and 313.15K which agrees with the corresponding literature values. The mixtures of Methyl benzoate, Cyclohexane with primary alcohol (1-propanol,1-butanol, 1-pentanol and 1-hexanol) were prepared by weight. The ultrasonic velocity was measured by a single crystal interferometer with a high degree of accuracy operating at a frequency of 3MHz (model F-05, with digital micrometer) at 303.15, 308.15 and 313.15 K. The viscosity was measured by Ostwald's viscometer. An electronically operated constant temperature water bath was used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desired temperature. Densities of the mixtures have been found by relative measurement method.

3. Theory and calculations

Intermolecular free length (L_F) is calculated using the standard expression

$$L_F = K\beta^{1/2} \tag{1}$$

where K is a temperature dependent constant known as Jacobson constant and β is the adiabatic compressibility that can be calculated from the speed of sound (U) and the density of the medium (ρ) as

$$\beta = \frac{1}{U^2\rho}. \tag{2}$$

The relation for free volume in terms of ultrasonic velocity (U) and the viscosity (η) of the liquid as

$$V_F = \left(\frac{M_{eff}\,U}{\eta K}\right)^{3/2}. \tag{3}$$

3.1. Excess compressibility

$$\beta_T = \frac{n_1\beta_1 + n_2\beta_2 + n_3\beta_3}{n_1 + n_2 + n_3} \tag{4}$$

where n_1, n_2 and n_3 are the number of moles of the components and β_1, β_2, and β_3 are the compressibilities of the components, and β_T is the compressibility of the ideal mixture. In certain liquid mixtures which deviate from ideal behavior, the experimentally determined compressibility (β_s) will be different from that of calculated adiabatic compressibility (β_T).

3.2. Excess intermolecular free length

$$L_F^E = L_F^{exp} - \left(L_F^A X_A + L_F^B X_B + L_F^C X_C\right) \tag{5}$$

where L_F^A, L_F^B, L_F^C are the intermolecular free length, X_A,X_B,X_C are mole fractions of the components A, B and C, and L_F^{exp} is the experimental intermolecular free length of the mixture.

Table 2
Values of density (ρ), viscosity (η) and ultrasonic velocity (U) for System I: Methyl benzoate (X_1)+Cyclohexane (X_2)+1-Propanol (X_3).

Mole fraction		ρ kg m^{-3}			η × 10^3 N s m^{-2}			U m s^{-1}		
x_1	x_3	Temperature (K)								
		303.15	308.15	313.15	303.15	308.15	313.15	303.15	308.15	313.15
0.5996	0	957.90	957.00	953.00	0.9344	0.8826	0.8403	1282.80	1270.00	1246.00
0.4886	0.1204	930.00	928.70	926.30	0.9478	0.8956	0.8427	1278.60	1256.40	1227.00
0.3691	0.2419	889.20	886.60	883.00	0.958	0.9053	0.8528	1246.00	1220.00	1207.00
0.3003	0.3457	874.30	874.00	870.80	0.9674	0.9173	0.8653	1231.50	1208.00	1198.80
0.1829	0.4511	846.00	844.50	836.60	0.9977	0.9462	0.8782	1218.60	1197.60	1181.40
0.0893	0.5519	812.60	811.40	802.80	1.0056	0.9551	0.8989	1190.40	1177.00	1148.40
0	0.6491	778.90	775.20	771.30	1.1000	1.0225	0.9392	1174.80	1148.40	1118.00