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ACOUSTICAL STUDIES ON MOLECULAR INTERACTIONS IN TERNARY LIQUID MIXTURES AT 303 K

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ABSTRACT:
Ultrasonic velocity study of ternary liquid mixture has gained much importance in assessing the molecular interactions and association between the component molecules. Measurements of ultrasonic velocity, density and viscosity have been carried out for 1,4 Dioxane + n- Heptanol + Cinnameldehyde at different concentrations at 303 K temperature and 2 MHz frequency, to provide information about molecular environment and extent of molecular interaction by ultrasonic technique. Ultrasonic studies may throw more light on the molecular interaction to know the behaviour of solute and solvent molecules in liquid mixtures and solutions. Acoustical parameters such as adiabatic compressibility (βa), intermolecular free length (Lf), Acoustic Impedance (Z) and free length (τ)for 1,4 Dioxane + n-Heptanol + Cinnameldehyde were calculated from ultrasonic velocity and effect of concentration on molecular interaction was predicted.

Keywords :- concentration, cinnamaldehyde, n- Heptanol, 1,4 Dioxane, molecular, ultrasonic.

INTRODUCTION :

In the recent days, for the proper design of any chemical industrial processes knowledge of thermodynamic and transport properties liquid/liquid mixtures are completely necessary. In polymerization processes 1, 4-dioxane is used as a cyclic ether, an excellent solvent frequently used in the manufacture of special chemicals, pesticides, bulk drug intermediates [1-4].

A measurement of sound velocity, density of liquid mixtures allows one to obtain information about their adiabatic compressibility, acoustic impedance, intermolecular free length, and relaxation timeand changes in their properties.

Cinnamaldehyde is an industrially significant organic compound which consists of a phenyl group attached to an unsaturated aldehyde.Cinnamaldehyde is an organic compound. Occurring naturally as predominantly the trans(E) isomer, it gives cinnamon its flavor and odor. It is a phenylpropanoid that is naturally synthesized by the shikimate pathway. This pale yellow, viscous liquid occurs in the bark of cinnamon trees and other species of the genus Cinnamomum.

1-Heptanol is an alcohol with a seven carbon chain and the structural formula of $CH_3(CH_2)_6OH$. It is a clear colorless liquid that is very slightly soluble in water, but miscible with ether and ethanol. 1-Heptanol is often utilized in cardiac electrophysiology experiments to block gap junctions and increase axial resistance between myocytes. Increasing axial resistance will decrease conduction velocity and increase the heart's condition to reentrant excitation and sustained arrhythmias. It has a pleasant smell and is used in cosmetics for its fragrance [5-7].

Ultrasonic velocity, density of binary mixture 1,4-dioxane+ n- Heptanol + Cinnameldehyde have been measured at 303K temperature.

EXPERIMENTAL DETAILS :

By using an ultrasonic interferometer (Mittal type, Model F-81) working at 2MHz frequency

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and at temperature 308K. The ultrasonic velocity (U) in liquid mixtures prepared by taking purified AR grade samples, have been measured The accuracyof sound velocity was ±0.1 ms^{-1}. Tocirculate water through the double walled measuring cell made up of steel containing the experimental solution at the desire temperature. An electronically digital operated constant temperature water bath has been used. The density of pure liquids and liquid mixtures was determined using pycknometer by relative measurement method with an accuracy of ±0.1Kgm^{-3}. Forthe viscosity measurement of pure liquids and liquid mixtures an Ostwald"s viscometer was used with accuracy of ±0.0001NSm^{-2}. All the precautions were taken to minimize the possible experimental error.

RESULTS AND DISCUSSION :

From the experimental data of ultrasonic velocity (U), viscosity (η) and Density (ρ) various acoustical parameters such as adiabatic compressibility (β_a), free length (L_f), acoustical impedance(Z) and relaxation time (τ) were calculated by the following equations (1-4).

$\beta_a = (U^2 \rho)^{-1}$ ..... (1)

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

$Z = U\rho$ ..... (3)

$\tau = 4/3\ \eta\ \beta_a$ ..... (4)

Where, K_T is the temperature dependent constant, K is constant equal to $4.28*10^9$ in MKS system.

The measured parameters *viz.*, ultrasonic velocity (U), density (ρ), viscosity (η) and calculated parameters such as adiabatic compressibility (β_a), intermolecular free length (L_f) , acoustical impedance(Z) and relaxation time (τ) for the system: 1,4- Dioxane + n- Heptanol +Cinnamaldehyde at temperature 303K and 2MHz frequency are given Table 1.

Velocitydecreases with concentration of 1,4-dioxane and Cinnamaldehyde in n-Heptanol. This indicates that strong interaction observed at higher concentrations of X_1 and lower concentration of X_2. The density values also have the same trend with velocity in the given system.

Viscosity decreases in given system shows that more intermolecular association. It is observed that for a given ternary mixture concentration as the number of CH- group or chain length increases, the sound velocity increases [8-10].

The adiabatic compressibility and free length are the most important factors of the ultrasonic velocity in liquid systems. The Intermolecular free length (L_f)is found to be a predominant factor to determining the nature of ultrasonic velocity in liquid mixtures. The intermolecular free length (L_f) is the mean distance between the surfaces of neighboring molecule, also reflects the sametrend as that of β. This indicates significant interaction between solute and solvent molecules. From the Table it is observed that, the adiabatic compressibility and free length increases with increase of mole fraction of the X_1 and decreases X_2 in system-I. Increase in intermolecular free length in system-I leads to positive deviation in sound velocity and negative deviation in compressibility. This indicates that the molecules are nearer in the system.

Acoustical impendence (Z) and Relaxation time are decreases with increase in mole fraction of 1,4- Dioxane, suggesting strong specific interactions between the constituent molecules of ternary mixtures [11-12].

CONCLUSION :

The ultrasonic velocity, density, viscosity and other related parameters Adiabatic compressibility (β_a), Intermolecular free length (L_f), acoustical impedance(Z) and relaxation time (τ) were calculated. The existence of molecular interaction in is favored in the system, confirmed from the U, ρ, η, βa, L_f, Z and τ data. The variation in ultrasonic velocity (U), density (ρ) and viscosity (η) and other related thermodynamic parameters such as βa, L_f, Zand τ at various concentrations and at 303 K

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temperature in 1,4- Dioxane + n- Heptanol +Cinnamaldehyde shows the variation linear. Strong intermolecular interactions are confirmed in the systems investigated.

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Table 1: The experimentally measured values of Velocity (U), Density (ρ), Viscosity (η), the calculated values of Adiabatic compressibility (β_a), Intermolecular free length (L_f), acoustical impedance(Z) and relaxation time (τ) for the system 1,4- Dioxane + n- Heptanol +Cinnamaldehyde at temperature 303K and 2MHz frequency are givenTable 1.

X1	X2	X3	U (m/s)	ρ (kg/m3)	η*10^{-3} (CP)	βa *10^{-10} (Pa-1)	L_f *10^{-10} (m)	Z*10^{6} (kg/m^{2}s)	τ*10^{-12} (s)
0	0.3	0.7	1411.11	985.0	3.0891	5.0985	0.464702	1.3899	2.0999
0.1	0.3	0.6	1401.88	964.0	3.0232	5.2783	0.472891	1.3514	2.1276
0.2	0.3	0.5	1392.66	978.0	2.5206	5.2719	0.472609	1.3620	1.7718
0.3	0.3	0.4	1388.22	969.2	2.1822	5.3539	0.476261	1.3454	1.5577
0.4	0.3	0.3	1462.66	958.8	1.9717	5.5032	0.482865	1.3199	1.4467
0.5	0.3	0.2	1369.33	954.5	2.4657	5.5873	0.486542	1.3070	1.8369
0.6	0.3	0.1	1347.55	948.2	1.2225	5.8077	0.496045	1.2777	0.9466
0.7	0.3	0	1219.33	942.1	1.2099	7.1393	0.549981	1.1487	1.1517

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