COMPATIBILITY STUDIES AND EVALUATION OF ULTRASONIC VELOCITY AND PERCENTAGE DEVIATION OF TERNARY MIXTURE OF CYCLOHEXANE, TOLUENE AND 2-PROPANOL AT 303.15 K & 308.15 K.

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ABSTRACT:-

The Compatibility studies of the above liquids have been carried out at 303.15 K & 308.15 K and the data can be described with its compatibility studies over a wide range of composition ranging from 0-100% of above different liquids. The result of ultrasonic velocity and its derived percentage deviation have been used to discuss the statistical approach of the blend under study. These discussion revealed that the blend is weakly polar in an ideal mixing relation. Using this data, the interaction parameters of molecular radius (r_m), molar sound velocity (R_{mix}) and molar volume (V_{mix}) were computed. The ultrasonic velocity results are further confirmed by Density and Percentage deviation results. For the ternary mixtures, the observed results shows that the Nomoto method seems to give good results for the evaluation and compared to Van-Dael's method.

Key Words: *Ternary Mixtures, Acoustical Parameters, Ultrasonic Velocity, Polar liquids, Molecular interactions.*

INTRODUCTION:

The ultrasonic wave through the solution is used for knowing the nature and strength of intermolecular interaction in pure liquids and the mixtures. The Ultrasonic velocity in three ternary liquid mixtures of cyclohexane, toluene and 2-propanol have been measured by Kannappan and V. Rajendiran[1] of different proportions and also compared the relative merits of Flory's statistical theory and junjie's thermo dynamical approach for theoretical evaluation of sound velocity in mixtures. Nomato and bhimseenachel et al made successful attempts to evaluate the sound velocity on ternary liquid mixtures. Van Dael ideal mixing relation has also been carried out successfully to investigate the acoustical behavior. For theoretical evaluation of sound velocity; other researcher found that Van Deal ideal mixing relation gives minimum deviation from the experimental values.

In this paper a comparative study[2] of relative merits of the different methods becomes essential and the present work has been attempt in this direction. In this paper, it is aimed to find the suitable theoretical [3] method to evaluate the sound velocity on ternary mixtures of cyclohexane + toluene + 2-propanol at the temperature of 303.15 k & 308.15 k.

THEORETICAL STUDIES:

Nomoto's empirical formula for sound velocity in ternary liquids mixtures in terms of molar sound velocity R_{mix} and molar volume V_{mix} as

$$U_{mix} = \left\{ \frac{R_{mix}}{V_{mix}} \right\}^{3} \qquad (1)$$

$$U_{mix} = \left\{ \frac{X_1R_1 + X_2R_2 + X_3R_3}{X_1R_1 + X_2R_2 + X_3R_3} \right\}^{3} \qquad (2)$$

where,

$$R = \left(\frac{M}{\rho} \right) U^{1/3} \qquad (3)$$

Where,	R	-	Rao's constant
	X_1, X_2, X_3	-	Concentration of first, second & third Liquids.
	V_1, V_2, V_3	-	Sound Velocity
	ρ	-	Density of Liquids.

Van-Deals expression for sound velocity in ternary mixtures is

$$\frac{1}{X_1 M_1 + X_2 M_2 + X_3 M_3} \cdot \frac{1}{\left(U_{im}\right)^2} = \frac{X_1}{M_1 U_1^2} + \frac{X_2}{M_2 U_2^2} + \frac{X_3}{M_3 U_3^2} \quad (4)$$

Schaff's and Nutsch – Kunhkies expression for sound velocity in ternary liquid mixture is

$$U_{mix} = U\alpha \{ X_1S_1 + X_2S_2 + X_3S_3\} \left(\frac{X_1B_1 + X_2B_2 + X_3B_3}{V_m} \right) \quad (5)$$

Where,

$U\alpha = 1600\ ms^{-1}$

S_1, S_2, S_3 & B_1, B_2, B_3 are collision factors and actual volume of the molecules per mole of first, second and third components respectively.

r_m - molecular radius which can be obtained from the formula

$$d^{5/2} = \frac{1}{7.2x10^3} \quad \frac{V\sigma^{1/4}}{T_C^{1/4}} \quad (6)$$

σ = Surface tension

The degree of intermolecular attraction α is given by

$$\alpha = \frac{U_{exp}^2}{U_{im}^2} - 1 \quad (7)$$

The experimental value of ultrasonic velocity and density of the ternary mixtures cyclohexane + toluene + 2-propanol are taken from the work of G. Arul etal[4].

DISCUSSIONS:

Ultrasonic velocity and density[5] for the pure Components cyclohexane, toluene, and 2-propanol are given in table (1). Ultrasonic velocity and percentage derivation of ternary mixture cyclohexane + toluene + 2-propanol at the temperature of 303.15 k & 308.15 k is evaluated in table (2, 3). The variation of ultrasonic velocity with concentration of cyclohexane and 2-Propanol is given in fig. 1 to 4.

The percentage deviations of theoretically calculated[6] ultrasonic velocity from the experimental results are also given in table 1, 2. The calculated values

$$\left(\frac{U_{exp}^{2}}{U_{idl}^{2}}\right) ; \quad \text{Alpha, Excess Velocity } U^{E}\{\ ,\ \}$$

a excess impedance Z^E and excess volume V^E with mole fraction are given in table 3.

Cyclohexane is a Non-polar liquid [7,8] where as toluene is a weakly Polar and 2-Propanol is a polar liquid. The calculated values of alpha, excess velocity, and excess impedance are positive and decreases with increase in concentration of 2-ol[9] where as the excess volume is negative. The Negative excess volume indicates the formation of molecular clusters and complexes and may involve even charge transfer complexes[10]. As the components are poor and zero dipole moments, the dipole-dipole interaction is weak in the pure state. The decrease in magnitude of the excess parameters suggests the close packing of molecules inside the shield, which may brought about by the increasing magnitudes of interactions[11]. The positive and decreases of excess parameters with increasing 2-ol concentration is due to a weak bond of a type between a conventional localized hydrogen bond and the formation of charge transfer complex occurring between the components of mixtures[11]. The excess volume studies also confirm the weakening of dipolar interaction between the components of the liquid mixture.

Table 1:

Ultrasonic velocity & Density of pure Components for ternary mixtures at 303.15 k & 308.15k

Component	*303.15 K*		*308.15K*	
	Density (ρ) 10^3 kg m^3	Velocity (V) ms^{-1}	Density (ρ) 10^3 kg m^3	Velocity (V) ms^{-1}
Cyclohexane	766.9	1229.5	767.7	1230.3
Toluene	587.8	1285.3	857.8	1287.2
2-Propanol	762.1	1112.0	762.1	1112.0

Table 2:

Ultrasonic velocity and percentage deviation of the ternary mixture

cyclohexane + toluene + 2-Propanol at 303.15k

Mole fraction (x_1)	Mole fraction (x_3)	Density $\rho_{mix}{}^*$ (kg m^3)	Ultrasonic Velocity				Percentage Deviation		
			$U_{Expt}{}^*$ (ms^{-1})	U_{nomoto} (ms^{-1})	$U_{Van-dael}$ (ms^{-1})	U_{cft} (ms^{-1})	$\left(\Delta U/U\right)$ Nomoto	$\left(\Delta U/U\right)$ VanDael	$\left(\Delta U/U\right)$ Cft
0.5000	0.0990	798.53	1208.6	1244.2	1221.7	1243.9	-2.94	-1.09	-2.02
0.3990	0.2020	800.69	1205.8	1234.7	1196.8	1234.1	-2.40	0.74	-2.35
0.3000	0.3000	802.95	1201.3	1225.4	1176.7	1224.5	-2.01	2.04	-1.93
0.2000	0.3990	806.97	1197.2	1215.5	1159.5	1214.3	-1.53	3.15	-1.43
0.0990	0.4990	810.13	1194.2	1204.9	1144.8	1203.5	-0.89	4.14	-0.78
0.0000	0.6008	813.54	1190.6	1193.1	1132.4	1191.6	-0.21	4.89	-0.09

	-1.66	2.31	-1.58

X_1, X_3 - refers mole fractions of cyclohexane & 2-propanol

* - *Experimental values taken from the work of G.Arul etal [3].*

Table 3:

Ultrasonic velocity and percentage deviation of the ternary mixture

cyclohexane + toluene + 2-Propanol at 308.15k

Mole fraction (x_1)	Mole fraction (x_3)	Density ρ_{mix}* (kg m^3)	Ultrasonic Velocity				Percentage Deviation		
			U_{Expt}* (ms^{-1})	U_{nomoto} (ms^{-1})	$U_{Van-dael}$ (ms^{-1})	U_{cft} (ms^{-1})	$(\Delta U/U)$ Nomoto	$(\Delta U/U)$ VanDael	$(\Delta U/U)$ Cft
0.5000	0.0990	794.37	1197.8	1228.3	1206.0	1228.1	-2.55	0.69	-2.53
0.3990	0.2020	794.98	1191.1	1219.2	1181.7	1218.7	-2.36	0.79	-2.31
0.3000	0.3000	797.78	1182.5	1210.3	1162.0	1209.4	-2.35	1.73	-2.28
0.2000	0.3990	802.30	1179.6	1200.8	1145.2	1199.6	-1.79	2.92	-1.70
0.0990	0.4990	807.43	1172.9	1190.5	1130.8	1189.2	-1.50	3.59	-1.39
0.0000	0.6008	810.97	1169.6	1179.2	1118.7	1177.7	-0.82	4.36	-0.69
Average							-1.90	2.12	-1.81

X_1, X_3 - refers mole fractions of cyclohexane & 2-propanol

* - *Experimental values taken from the work of G.Arul etal [3].*

RESULT:

In this study a trial has been made to evaluate the theoretical parameters of ultrasonic waves when it passes through ternary liquid mixtures. Three methods have been chosen namely (Nomoto's method, Van Dael's ideal method and Schaff's collision factor theory) for the theoretical evaluation. Also an attempt is made to identify the suitable method to compute the ultrasonic velocity theoretically. Suitable interpretations are based on hydrogen bonding of dipole-dipole interaction and charge transfer complexes. The work gives very interesting results and out of three different methods the Nomoto method is found to be the best for ternary mixtures due to the closeness in values obtained with respect to the experiment.

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