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Theoretical ultrasonic velocity studies of pentanol containing methyl benzoate and benzene at 301K

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ABSTRACT

Theoretical ultrasonic velocity for the binary mixtures of pentanol with benzene and ternary mixtures of pentanol with methyl benzoate in benzene systems have been predicted at 301K using various theoretical relations . The experimental values are compared with the theoretical values of ultrasonic velocity of Nomotos relation, Van Dael relations, Impedance relations, Junjies relation, Impedance relations, Rao relations. The deviation of theoretical values of velocity from the experimental values shows that the molecular interaction is taking place between the unlike molecules in the liquid mixture. The deviation in the variation of U^2_{Exp} / U^2_{mix} from unity has also been evaluated for explaining the non-ideality in the mixtures. It is observed that the Nomoto's relation give the better results followed the other theoretical models for these systems.

Key words: Ultrasonic velocity, mixing model, binary, sound velocity, percentage deviation.

INTRODUCTION

Theoretical ultrasonic velocity for liquid mixtures used to predict the molecular interaction. [1] Ultrasonic velocities of liquid mixtures containing organic liquids are of importance to understanding intermolecular interaction between component molecules due to applications in industrial and technological processes. [2] Ultrasonic velocities in liquid mixtures have been predicted through different theoretical models [3-4]. From theoretical ultrasonic velocities with those obtained experimentally is expected to reveal the nature of interaction between components molecules in the mixtures are studies various investigators [5-6]. Theoretical findings are useful defining a comprehensive theoretical model for a specific liquid mixture. They are also testing validity various theories of liquid state [7]. Many researchers compared the experimental values of ultrasonic velocities with theoretically evaluated values for organic liquid mixtures using different theories [8-11]. Our research investigates the nature solute – solvent and other type of interactions using various techniques including theoretical methods [12-20]. The aim of the present investigation is to compare the experimentally determined ultrasonic velocity binary and ternary liquid mixtures for various theoretical relations at various compositions.

MATERIALS AND METHODS

The ultrasonic velocity was measured using a single crystal interferometer (Mittal type, M-80) with an accuracy of 0.001 m/s operating at 2 MHz frequency. The chemicals pentanol, methyl benzoate and benzene were used without further purification.

THEORY

The following theoretical relations for used for the find the ultrasonic velocity in the binary mixtures.

Nomotos (NR) established the mixtures relation by assuming molar sound velocity

$$u = \left[\frac{\sum x_i R_i}{\sum x_i V_i} \right]^3 \quad \ldots (1)$$

Where x is the mole fraction of specie and R is the molar sound velocity related to the molecular weight and density i.e.,

$$R_i = \left[\frac{m_i}{\rho_i} \right]^3 u^{1/3} = v_i u_i^{1/3} \ldots (2)$$

The molar volume is given by $V_i = \frac{m_i}{\rho_i}$

Van Dael etal. (VVD) obtained the re

lation for ultrasonic velocity in the liquid mixtures as

$$\left[\frac{1}{m_1 x_1 + m_2 x_2} \right] \left[\frac{1}{u^2} \right] = \frac{x_1}{m_1 u_1^2} + \frac{x_2}{m_2 u_2^2} \ldots (3)$$

Junjies relations (JR) given by

$$u_{JM} = \left[\frac{\sum x_i v_i}{(x_i m_i)^{1/2}} \right] \left[\frac{x_i v_i}{\rho_i u_i^2} \right] \ldots (4)$$

Impedance relation (IR) written as

$$u = \frac{\sum x_i Z_i}{\sum x_i \rho_i}, \ldots (5)$$

Z is the acoustic impedance

From the Rao constant (RR) obtained the ultrasonic velocity of the mixtures

$$R_i = \left[\frac{m_i}{\rho_i} \right] u^{1/3} = v_i u_i^{1/3}$$

$$u = \left[\frac{x_i \rho_i R_i}{m_i} \right]^3 = \left(\frac{x_i R_i}{V_i} \right)^3 \ldots (6)$$

X, V, m, and ρ are the mole fraction, molar volume, molecular weight and density of constituent's species.

RESULTS AND DISCUSSION

The experimental ultrasonic velocity along with theoretical ultrasonic velocity find using the following relations, Nomotos , Van Dael and Vangeel, Junjes theory, Impedance relation, and Rao specific sound velocity of pentanol with benzene , pentanol with methyl benzoate in at 301 K are given in table 1 to 2 also reported the percentage deviations of all the binary mixtures. The average percentage error reported in table 3. Check the validity of the theoretical relation in terms of average percentage deviation for alcohols with benzene mixtures.

It can be seen from table 1 to 2 that the theoretical values of ultrasonic velocity computed by various relations shows the deviation from experimental values. The limitation and approximations incorporated in these relations are responsible for it. It is assumed that all the molecules in spherical shape which is not true every time. In Nomotos relations, it is supposed that the volume does not change on mixing, there is no interaction between the components of liquid mixtures has taken into account.

Similarly, the assumption for the formation of ideal mixing relation is that the ratios of specific heat of ideal mixtures and the volume are equal. Again no molecular interaction is taken into account. But on mixing more than one liquids, the interaction between two liquids taken place because of the presence of various type of forces such as

dispersion forces, charge transfer, hydrogen bonding, dipole-dipole, dipole-induced dipole interaction, thus the observed deviation of theoretical ultrasonic velocity from experimental values shows that the molecular interactions is taking place between the unlike molecule in the liquid mixtures.

X2	uExp	Theoretical Ultyrasonic Velocity					Percentage Deviation				
		NR	VVR	JR	IR	RR	NR	VVR	JR	IR	RR
		Pentanol + Benzene									
0.1	1273	1275	1274	1275	1275	1275	-0.16	-0.11	-0.12	-0.18	-0.17
0.2	1271	1274	1273	1273	1274	1274	-0.25	-0.16	-0.18	-0.28	-0.27
0.3	1268	1273	1272	1272	1274	1274	-0.41	-0.3	-0.33	-0.45	-0.44
0.4	1266	1272	1271	1271	1273	1273	-0.51	-0.38	-0.42	-0.55	-0.54
0.5	1263	1272	1270	1270	1272	1272	-0.68	-0.55	-0.59	-0.72	-0.71
0.6	1260	1271	1269	1270	1271	1271	-0.86	-0.73	-0.78	-0.9	-0.89
0.7	1258	1270	1269	1269	1271	1270	-0.96	-0.85	-0.89	-1	-0.99
0.8	1255	1269	1268	1269	1270	1270	-1.14	-1.06	-1.09	-1.17	-1.16
0.9	1253	1269	1268	1268	1269	1269	-1.25	-1.2	-1.22	-1.27	-1.26
Pentanol + methyl benzoate + benzene											
0.05	1328	1350	1272	1332	1348	1340	-1.68	-1.68	4.19	-0.3	-1.49
0.1	1317	1351	1276	1332	1349	1341	-2.55	-2.55	3.15	-1.1	-2.42
0.15	1306	1351	1279	1331	1350	1342	-3.44	-3.44	2.08	-1.92	-3.37
0.2	1296	1351	1282	1331	1351	1343	-4.27	-4.27	1.06	-2.68	-4.25
0.25	1285	1352	1286	1330	1352	1344	-5.19	-5.19	-0.06	-3.53	-5.23
0.3	1274	1352	1289	1330	1353	1345	-6.12	-6.12	-1.2	-4.4	-6.22
0.35	1264	1352	1293	1330	1354	1346	-6.98	-6.98	-2.29	-5.2	-7.15
0.4	1253	1353	1297	1330	1355	1347	-7.95	-7.95	-3.49	-6.11	-8.18
0.45	1243	1353	1301	1329	1357	1348	-8.84	-8.84	-4.63	-6.94	-9.14
0.05	1328	1350	1272	1332	1348	1340	-5.22	-1.68	4.19	-0.3	-1.49

Table-2 Average percentage deviations of alcohols inbenzene systems

System	NR	VVR	JR	IR	RR
Pentanol+Benzene	-0.69	-0.59	-0.63	-0.72	-0.71
Pentanol+Methyl benzoate +Benzene	-5.22	-0.13	-3.58	-5.27	-4.64

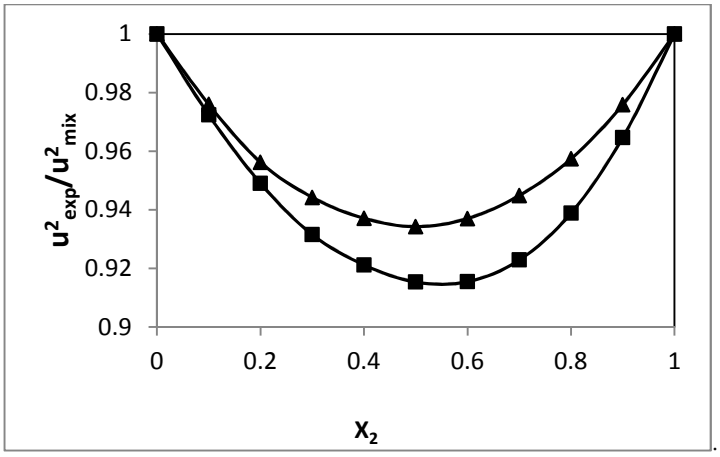

Fig.1 Plots of mole fraction of pentanol with u^2_{exp}/u^2_{mi}

The table 1 shows they in the systems of pentanol with benzene , there is good agreement between the experimental and theoretical values of Nomotos relations. Here ideal mixing relation provides between results then the results of Nomotos relation. However, higher values observed in Van Dael and Vangeel Relations, Junjies relation, Impedance relation, Rao Relations.

From the table 2, it is observed that in the system of pentanol with methyl benzoate in benzene, there is good agreement between the experimental and theoretical values of Nomotos relations followed by impedance relations. However, higher values observed in Junjies relation, Impedance relation, Rao Relations.

The good agreement between theoretical and experimental values of Nomotos relations in all the binary mixtures, suggests that R is additive property in all the systems. The higher deviation in some intermediate concentration range suggests the existence of strong tendency for association between the component molecules, in this concentration range as a result of hydrogen bonding. These values vary non linearly with the composition suggesting that there is association in some composition. The percentage deviation is shows maxima at an intermediate

concentration in all the binary mixtures. Figure 1 represents the variation $\frac{u^2_{Exp}}{u^2_{Mix}}$ with the mole fraction of pentanol. It is observed to be similar for all the systems.

The deviation of the ratio $\frac{u^2_{Exp}}{u^2_{Mix}}$ from unity and its variation as a function of pentanol in a direct measure of non ideality of the systems as a consequence of association or other type of interaction. The figure 1 shows the interaction parameter and variation of $\frac{u^2_{Exp}}{u^2_{Mix}}$ with the values of mole fraction of pentanol with benzene. From the figure it is observed that maximum positive deviations are observed are 0.5. The ratio of $\frac{u^2_{Exp}}{u^2_{Mix}}$ is an important component to measure the non ideality in the mixtures especially in such cases where the perhaps other than the sound velocity are known.

Figure 1 represents the variation of $\frac{u^2_{Exp}}{u^2_{Mix}}$ with the mole fraction of pentanol for binary and ternary mixtures. It is positive for the system and infers strong interaction between the mixing molecules. It is negative value indicate the dominance of dispersion forces arising from breakage of hydrogen bonds in the associates. The positive value of the systems clearly indicates the evidence of strong tendency for the formation of association in mixtures through dipole-dipole interaction.

The high values of percentage deviation point out maximum departure the particle theory from experiment at these particular concentrations finally determine the overall validation of these theories. The percentage deviation are given in table 2 on the whole, all the theoretical models fairly close to the experiment values for the binary and ternary mixtures represents in this work thus showing the validity of theoretical models for the binary mixtures. The order of percentage deviations of theoretical models are Nomotos relations < Impedance relations < rao relations < Junjies relations <Impedance relations.

The prediction ability of various ultrasonic theories discussed above depends on the strength of interaction providing in a system. These theories generally tool to predict accurately the ultrasonic velocity where strong interactions are supposed to exist and average absolute percentage relation deviation is small in system where the interaction is less.

CONCLUSION

From the experimental and theoretical ultrasonic velocity discuss about the solute-solvent interaction is the order of pentanol + benzene < pentanol + methyl benzoate + benzene. Different theoretical methods used to evaluate the ultrasonic velocity of the binary and ternary mixture also predict the percentage deviations. From this value check the validity of these relations. Nomotos relation is better than the other theoretical methods.

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