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Speed of Sound Studies And Behavior of Intermolecular Interactions of Benzyl Benzoate With Acetone At Different Temperatures

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Abstract: *The speed of sound (U), density (ρ) and viscosity (η) has been measured for the mixtures of benzyl benzoate with acetone at T = 303.15, 313.15 and 323.15K (10K interval). From these measured values the various speed of sound theoretical relations such as nomoto (NOM) relation, impedance (IMP) relation, ideal mixing relation (IMR), vandael and vangeel (VDV) relation, junjie (JUN) relation and rao's specific velocity (RAO) relation have been computed. The validity of these theories was checked by applying the chi-square test (χ)for goodness of fit and by calculating the average percentage error (APE).The results are discussed in terms of intermolecular interactions between the component molecules in these binary liquid mixtures.*

Keywords: *Theoretical speed of sound velocities, chi-square test, average percentage error, inter molecular interactions*

I. Introduction

Theoretical evaluation of ultrasonic velocity in binary liquid mixtures and its comparison with the experimental values reflects the molecular interaction in liquid mixtures, which is very useful to build comprehensive theoretical models for liquids. The effect shown by the molecules with other functional groups on these molecules plays a vital role in understanding the behavior of hydrogen bonding. In the present study, the experimental speed of sound values correlated with the Several relations, semi empirical formulas of Nomoto s relation, ideal mixing relation (IMR), impedance dependence relation (IDR), Rao s velocity relation (RVM) Junjie' s method (JM) ("equations 1-6")for the binary mixtures of benzyl benzoate with acetone**.** Further, the best suitable theory for the given molecular system under study is also picked out by calculating the average percentage error (APE) and chi-square test (χ) ("equation 7-8")

II. Experimental

The density was measured by using specific gravity bottle method and Viscosity was measured by using Ostwald's viscometer by the standard procedure.The speed of sound was measured at 303.15K to 323.15k using ultrasonic interferometer (M/s Mittal Enterprises, India) operating at a frequency of 2 MHz with an accuracy of ±0.1m/s. for the compounds of benzyl benzoate with acetone.

Table 01 Comparison of experimental densities (ρ), viscosities (η) and speed of sound (U) of pure liquids with literature values.

liquid	**Temp T (K)**	**Density(□)**kg m^{-3}		**Viscosity(□)**$kgm^{1}s^{-1}$		**Speed of sound(U)** $m.s^{-1}$	
		literature	**experimental**	**literature**	**experimental**	**literature**	**experimental**
Benzyl benzoate	303.15	1.1193[a]	1.1193	6.53[b]	6.56	1506.00[c]	1505.40
	313.15	1.1097[a]	1.1093	5.02[b]	5.03	1471.40[c]	1475.20
	323.15	1.1070[a]	1.1068	4.29[b]	4.22	1440.00[c]	1440.20
Acetone	303.15	0.776[d]	0.779	3.22[f]	3.22	1138.33[h]	1139.20
	313.15	0.764[d]	0.762	2.50[f]	2.51	1115.96[h]	1118.80
	323.15	0.758[e]	0.754	2.90[g]	2.43	- - -	1104.60

[a,b,c] Reference [1]
[d,f,h] Reference [4]
[e,g] Reference [5]

III. Theory

The predictive abilities of various Speed of sound theories depend upon the strength of interaction prevailing in a system. These theories generally fail to predict accurately the ultrasonic velocities where strong interactions are supposed to exist. The following empirical relations are used for the prediction of speed of sound in the binary liquid mixtures.

$$U_{NOM} = \left[\frac{X_1R_1 + X_2R_2}{X_1V_1 + X_2V_2}\right]^3 \quad (1)$$

where, Molar sound velocity, $R_1 = \frac{m_1}{d_1} U_1^{1/3}$; $R_2 = \frac{m_2}{d_2} U_2^{1/3}$

$V_1 = \frac{m_1}{d_1}$; $V_2 = \frac{m_2}{d_2}$

Where X, R and V are the mole fraction, molar sound velocity and molar volume of the mixture

3.1 Nomoto's relations(NOM)

3.2 Ideal mixture relation (IMR)

$$U_{IMR} = \left[\frac{1}{X_1m_1 + X_2m_2}\right]^{1/2} \left[\frac{X_1}{m_1U_1^2} + \frac{X_2}{m_2U_2^2}\right]^{-1/2} \quad (2)$$

Where X, m and U are the mole fraction, effective molecular weight and ultrasonic velocity of the mixture

3.3 Junjie's method(JM)

$$U_{JM} = \left[\frac{X_1V_1 + X_2V_2}{(X_1m_1 + X_2m_2)^{1/2}}\right] \left[\frac{X_1V_1}{d_1U_1^2} + \frac{X_2V_2}{d_2U_2^2}\right]^{-1/2} \quad (3)$$

Where X, d, U and V are the mole fraction, density, ultrasonic velocity and molar volume of the mixture

3.4 Impedance Relation (IMP)

$$U_{IMP} = \frac{X_1Z_1 + X_2Z_2}{X_1\rho_1 + X_2\rho_2} \quad (4)$$

Where X, ρ and Z are the mole fraction, density and acoustic impedance of the mixture.

3.5 The van dael and vangeel equation(VDV)

$$U_{VDV} = \left[\frac{1}{X_1m_1 + X_2m_2}\right]^{1/2} \left[\frac{X_1}{m_1U_1^2} + \frac{X_2}{m_2U_2^2}\right]^{-1/2} \quad (5)$$

Where X, m and U are the mole fraction, effective molecular weight and ultrasonic velocity of the mixture

Rao's relation

$$U_R = (R/V)^3 \quad (6)$$

Where R ,V are the Rao's specific sound velocity and molar volume of the mixture

IV. Results And Discussion

The comparison values of viscosity of acetone at 323.15K is differ to other two temperatures because author got viscosity data at high pressure compared to pressure of other two temperatures for Table 1 ,the evidence of literature papers also produced. The experimental values along with the theoretically calculated values using Nomoto's relation, ideal mixing relation, impedance dependence relation, Rao's velocity relation ,Junjie method for the systems of benzyl benzoate with acetone for different temperatures are given in Table 2, 3 & 4. The validity of these theories are checked by applying Chi-square test and by calculating average percentage error.

4.1 Chi-square test for goodness of fit

According to Karl Pearson, the Chi-square value is calculated using the formula,

$$(x^2) = \sum_{i=1}^{n} \frac{\left(U_{mix(obs)} - U_{mix(cal)}\right)^2}{U_{mix(cal)}} \quad (7)$$

For (*n*-1) degrees of freedom, where, n is the number of data used.

4.2 Average percentage error (APE)

The average percentage Error is calculated using the relation,

$$APE = \frac{1}{n}\sum \frac{(U_{mix(obs)} - U_{mix(cal)})}{U_{mix(obs)}} X100\% \quad (8)$$

Where,
n- number of data used. Umix (obs) = experimental values and Umix (cal) = computed values of ultrasonic velocities.

It can be seen from Table 2, 3 and 4 that the theoretical values of speed of sound studies computed by various theories show deviation from experimental values at different temperatures. The predictive abilities of various Speed of sound studies depend upon the strength of interaction prevailing in a system. The density and viscosity values are increasing with dependence of temperature and mass of the sample liquid.

Table 1. Experimental and computed values of *Speed of sound studies* for benzyl benzoate with acetone at 303.15 K temperature

X1	U_{NOM}	U_{NOM}	U_{IMR}	U_{IMP}	U_{JM}	U_{VDV}	U_R
0.0000	1139.2	1139.2	1139.2	1139.2	1139.2	1139.2	1139.2
0.0208	1167.2	1156.3	1118.9	1150.0	1144.5	1118.8	1126.0
0.0456	1186.0	1175.6	1097.2	1162.7	1151.4	1097.2	1223.2
0.0757	1296.6	1197.6	1074.4	1177.7	1160.5	1074.3	1281.3
0.1130	1331.0	1222.6	1050.5	1195.8	1172.6	1050.4	1426.5
0.1604	1398.6	1251.6	1026.0	1218.0	1189.1	1025.9	1359.2
0.2227	1422.8	1285.3	1002.1	1245.9	1211.8	1002.1	1385.2
0.3083	1442.8	1325.3	982.1	1282.1	1244.3	982.0	1460.2
0.4332	1469.6	1373.4	975.2	1330.8	1292.8	975.2	1543.2
0.6323	1502.0	1432.1	1018.8	1399.8	1369.6	1018.8	1528.6
1.0000	1505.4	1505.4	1505.4	1505.4	1505.4	1505.4	1505.4
APE		0.0263	0.0666	0.0323	0.0375	0.0666	0.0070
CHI TEST(χ)		1.727	13.533	2.676	3.692	13.533	0.114

Table 2. Experimental and computed values of *Speed of sound studies* for benzyl benzoate with acetone at 313.15 K temperature

X1	U_{NOM}	U_{NOM}	U_{IMR}	U_{IMP}	U_{JM}	U_{VDV}	U_R
0.0000	1118.8	1118.8	1118.8	1118.8	1118.8	1118.8	1118.8
0.0208	1172.6	1121.1	1122.9	1129.5	1119.4	1122.8	1173.9
0.0456	1214.4	1124.0	1127.8	1142.0	1120.2	1127.8	1409.4
0.0757	1223.2	1127.6	1134.0	1156.8	1121.2	1133.9	1563.4
0.1130	1252.6	1132.3	1141.9	1174.6	1122.6	1141.8	1601.1
0.1604	1269.4	1138.7	1152.3	1196.4	1124.5	1152.3	1761.9
0.2227	1272.6	1147.9	1166.9	1223.7	1127.5	1166.9	1994.9
0.3083	1332.6	1162.1	1188.5	1259.1	1132.7	1188.5	2005.1
0.4332	1426.8	1187.1	1223.9	1306.5	1143.4	1223.9	2247.7
0.6323	1446.2	1242.9	1291.9	1373.5	1174.6	1291.8	2128.9
1.0000	1475.2	1475.2	1475.2	1475.2	1475.2	1475.2	1475.2
APE		0.0257	0.0231	0.0144	0.0285	0.0231	-0.0970
CHI TEST(χ)		1.499	1.189	0.446	1.866	1.189	13.766

Table 3. Experimental and computed values of *Speed of sound studies* for benzyl benzoate with acetone at 323.15 K temperature

X1	U_{NOM}	U_{NOM}	U_{IMR}	U_{IMP}	U_{JM}	U_{VDV}	U_R
0.0000	1104.6	1104.6	1104.6	1104.6	1104.6	1104.6	1104.6
0.0208	1131.0	1106.8	1108.3	1114.7	1105.1	1108.3	1197.7
0.0456	1188.4	1109.5	1112.8	1126.6	1105.8	1112.8	1437.9
0.0757	1227.2	1112.9	1118.5	1140.6	1106.7	1118.4	1594.1
0.1130	1288.6	1117.3	1125.7	1157.5	1107.9	1125.7	1631.7
0.1604	1311.4	1123.3	1135.4	1178.1	1109.6	1135.3	1794.0
0.2227	1334.6	1131.9	1148.8	1203.9	1112.3	1148.8	2028.9
0.3083	1354.6	1145.2	1168.9	1237.3	1117.0	1168.9	2036.5
0.4332	1391.0	1168.7	1202.0	1282.0	1126.7	1201.9	2276.2
0.6323	1428.6	1221.1	1265.9	1345.0	1155.6	1265.9	2142.9
1.0000	1440.2	1440.2	1440.2	1440.2	1440.2	1440.2	1440.2
APE		0.0359	0.0336	0.0254	0.0385	0.0336	-0.0920
CHI TEST(χ)		3.150	2.728	1.508	3.669	2.728	12.983

An important reason for deviation from experimental and theoretical studies are the molecular association of Speed of sound studies, it effects are not taken into account in these theories. Because when two liquids are mixed, the interaction between the molecules of the two liquids takes place because the presence of various forces like dispersive force, charge transfer, hydrogen bonding dipole-dipole and dipole-induced dipole interactions. The chi square value compared at three temperatures it is more affective at Rao's relation the value too high when compared to others ,the chi value of IMR and VDV at 303.15 K and also RAO at three temperature gives high it indicates weaker bonding. And for APE value also get good result at all temperatures except Rao's value gives negative. The observed deviation shows that the molecular interaction is taking place between the unlike molecules in the liquid mixtures. Higher deviations are observed in some intermediate concentration range. This suggests that existence of strong tendency for the intermolecular interaction between compound molecules as a result of strong Hydrogen bonding .

Plot the Variation of speed of sound theories for the system benzyl benzoate with acetone at different temperatures against entire range of mole fraction(X1)

The predictive abilities of various speeds of sound theories depend upon the strength of interaction prevailing in a system .Experimental observations were taken from literature sources and compared with the calculated values .The calculations will be performed using Microsoft Excel and the results were imported and plotted in graphs from Fig 01 to Fig 03 using Origin Software.

Figure 01 Variation of speed of sound theories for benzyl benzoate with acetone at 303.15K

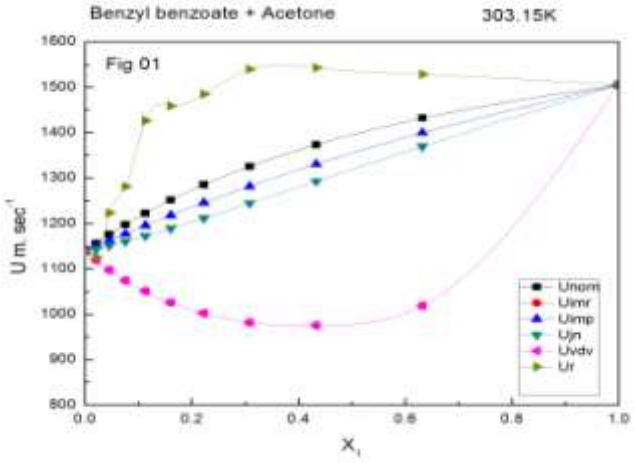


Figure 02 Variation of speed of sound theories for benzyl benzoate with acetone at 313.15K

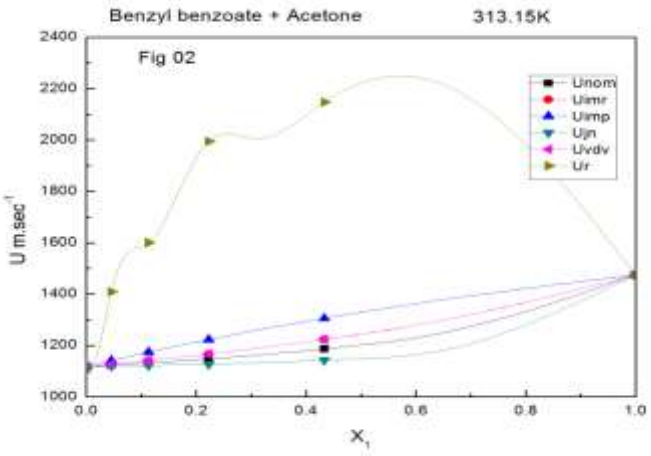
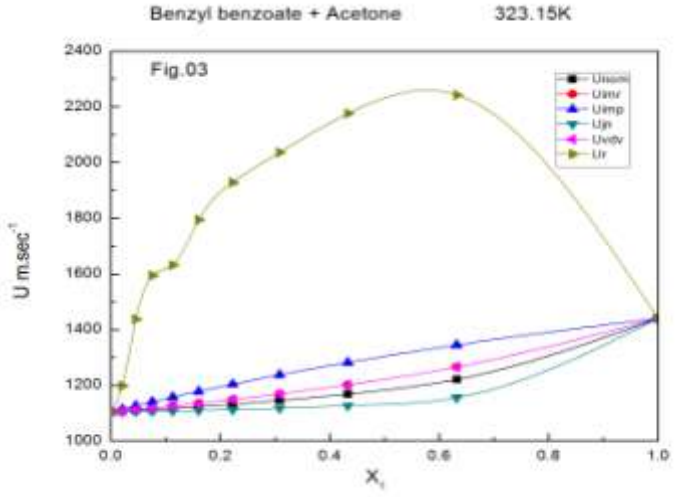


Figure 03 Variation of speed of sound theories for benzyl benzoate with acetone at 323.15K



We observe the three graphs all the theories are in same manner except the RAO relation. The observed deviation shows that the molecular interaction is taking place between the unlike molecules in the liquid mixtures.The extent of deviation may be attributed to the assumptions made in these theories for the non polar-polar and non polar-non polar interaction between the molecules.

V. Conclusion

Experimentally measured speed of sound studies at 303.15, 313.15 and 323.15K for the binary mixtures of benzyl benzoate with acetone are correlated using NOM, IMR, JM, IMP, VDV and RAO relations. It may be concluded that impedance dependence relation and Nomoto's relation are best suited for all the binary mixtures also Rao's relation give higher deviation under study.The APE and Chi square values also support this theory. The observed deviation of theoretical values of speed of sound from the experimental values are attributing in the presence of intermolecular association arising from the hydrogen bonding between the binary mixtures.

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