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Theoretical Prediction of Ultrasonic Velocity in Ternary Liquid Mixture of ethyl alcohol+ ethylene glycol + glycerol at 303.15, 308.15 and 313.15 K

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***Abstract*— Ultrasonic velocities of the ternary liquid mixture of ethyl alcohol, ethylene glycol and glycerol have been measured at the temperature of 303.15, 308.15 and 313.15 K, over the entire composition range of mole fractions. The experimental ultrasonic velocity have been analysed in terms of Nomoto's Relation (NR), Junjie's Method (JM), Van dael's Ideal Mixture Relation (IMR), Jacobson's Free Length Theory (FLT), Schaaff's Collision Factor Theory (CFT) and Impedance Dependence Relation (IDR). Theoretical ultrasonic velocity values were compared with the experimental ultrasonic velocity values and the validity of the theories was checked by calculating the Average Percentage Error (APE). The results are interpreted in terms of percentage deviation and the molecular interaction parameter (α) was computed by using the experimental and the theoretical ultrasonic velocity values. A good agreement has been found between experimental and Jacobson's Free Length Theory, Schaaff's Collision Factor Theory and Impedance Dependence Relation ultrasonic velocities. The variation of this parameter with composition of the mixtures has been discussed in terms of molecular interaction in these mixtures in the form of hydrogen bonding.**

Keywords*— *Ultrasonic velocities; Intermolecular interactions; Ternary mixtures; Average Percentage Error and Temperatures.

I. INTRODUCTION

The ultrasonic velocity measurement makes a comparative study with six different theoretical models. Ultrasonic velocities in liquid mixtures consisting of polar and non-polar components are of considerable importance in understanding the intermolecular interaction between component molecules and find applications in several industrial and technological process[1-3]. Measurement of ultrasonic velocity gives the valuable information about the physicochemical behavior of the liquid and liquid mixtures. Several relations, semi-empirical formula and theories are available for the theoretical computation of ultrasonic velocity in liquid and liquid mixtures[4-9]. Further, the best suitable theory for the given molecular system under study is also picked out by calculating the average percentage error.

The present investigation is to compare the ultrasonic velocity in ternary mixtures evaluated from various theories and relations. An attempt has been made to compare the merits of the relations for the ternary liquid mixtures investigated at different temperatures. The relative applicability of these theories to the present systems have been checked and discussed. The results are explained in terms of intermolecular interactions occurring in these ternary systems. The deviation of the ratio U^2exp/U^2imr from unity has also been evaluated for explaining the non-ideality in the mixtures.

II. EXPERIMENTAL TECHNIQUES

All the chemical used are of analytical reagent (AR) and spectroscopic reagent (SR) without further purification. The ternary liquid mixtures of different known compositions were prepared in stopper measuring flasks. The ultrasonic velocity are measured as a function of composition of the ternary liquid mixture at 303.15, 308.15 and 313.15K for mixed solvent systems in which glycerol was added to a binary mixtures of ethyl alcohol

and . For this purpose binaries with fixed volume ratios $X_1/X_2 \cong$ 1:1 were prepared. An ultrasonic interferometer having the frequency of 3 MHz (MITTAL ENTERPRISES, New Delhi, Model: F-81) with an overall accuracy of $\pm$ 0.1% has been used for velocity measurement. An electronically digital operated constant temperature bath (RAAGA Industries) has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desired temperature. The accuracy in the temperature measurement is $\pm$ 0.1 K.

III. THEORY AND CALCULATIONS

1. Nomoto's Relations (NR)

$$U_{NOM} = \left[\frac{X_1R_1+X_2R_2+X_3R_3}{X_1V_1+X_2V_2+X_3V_3}\right]^3 \quad \ldots(1)$$

2. Junjie's Method (JM)

$$U_{JM} = \left[\frac{X_1V_1+X_2V_2+X_3V_3}{X_1m_1+X_2m_2+X_3m_3}\right]^{1/2}\left[\frac{X_1V_1}{d_1U_1^2}+\frac{X_2V_2}{d_2U_2^2}+\frac{X_3V_3}{d_3U_3^2}\right]^{-1/2} \quad \ldots(2)$$

3. Ideal Mixing Relation (IMR)

$$U_{IMR} = \left[\frac{1}{X_1m_1+X_2m_2+X_3m_3}\right]^{1/2}\left[\frac{X_1}{m_1U_1^2}+\frac{X_2}{m_2U_2^2}+\frac{X_3}{m_3U_3^2}\right]^{-1/2} \quad \ldots(3)$$

4. Free Length Theory (FLT)

$$U_{FLT} = \frac{K}{L_{f_{mix}}\, d_{exp}^{1/2}} \quad \ldots(4)$$

5. Collision Factor Theory (CFT)

$$U_{CFT} = \frac{U_\infty \sum x_iS_i \sum x_iB_i}{V_{mix}} \quad \ldots(5)$$

Here, U_∞ = 1600 ms^{-1} , S is the collision factor and B the actual volume of molecule per mole.

6. Impedance Dependence Relation (IDR)

$$U_{IDR} = \frac{X_1Z_1+X_2Z_2+X_3Z_3}{X_1\rho_1+X_2\rho_2+X_3\rho_3} \quad \ldots(6)$$

7. Average Percentage Error (APE)[10]

$$APE = \frac{1}{n}\sum_{i=1}^{n}\frac{U_{exp}-U_{theo}}{U_{exp}} \times 100 \quad \ldots(7)$$

8. The degree of intermolecular interaction (α) is given by

$$\alpha = \frac{U_{exp}^2}{U_{The}^2} - 1 \quad \ldots(8)$$

IV. RESULTS AND DISCUSSION

The values of ultrasonic velocities computed theoretically using the relations of Nomoto, Junjie, Van Deal and Vangeel, Free length Theory, Collision Factor Theory and Impedance Relation together with experimental values also the average percentage error (APE) and molecular interaction term (α) for the ternary mixture of ethyl alcohol (X_1) + ethylene glycol (X_2) + glycerol (X_3) at the temperatures 303.15, 308.15 and 313.15K are summarized in Table 1.

Table-3: Experimental and Computed values of ultrasonic velocity and Molecular Interaction Parameter (α) in Ethyl alcohol(X1)+ Ethylene glycol (X2)+ Glycerol (X3) (X1/X2=1:1) at 303.15, 308.15 and 313.15 K.

Mole Fraction (X_3)	U_{EXP} ms^{-1}	U_{NOM} ms^{-1}	U_{JUNJ} ms^{-1}	U_{IMR} ms^{-1}	U_{FLT} ms^{-1}	U_{CFT} ms^{-1}	U_{IDR} ms^{-1}	α
303.15 K								
0.0000	1495.1	1372.5	1263.1	1278.8	1495.4	1423.4	1438.6	0.3669
0.0201	1491.6	1382.9	1268.1	1279.0	1492.0	1439.1	1448.6	0.3600
0.0399	1487.5	1393.2	1273.4	1279.5	1487.9	1439.9	1458.5	0.3516
0.0601	1481.7	1403.4	1278.8	1280.2	1482.0	1455.5	1468.3	0.3395
0.0801	1475.2	1413.6	1284.4	1281.2	1475.5	1460.7	1477.9	0.3258
0.1006	1464.0	1423.7	1290.2	1282.4	1464.4	1466.2	1487.4	0.3032
Average Percentage Error (APE)	-	5.67	13.90	13.64	-0.02	2.35	1.29	-
308.15 K								
0.0000	1492.6	1356.8	1247.0	1263.1	1492.9	1408.6	1423.3	0.3965
0.0201	1488.0	1366.5	1251.8	1263.2	1488.4	1427.3	1432.6	0.3876
0.0399	1480.7	1376.2	1256.8	1263.5	1481.1	1429.2	1441.7	0.3733
0.0601	1473.2	1385.7	1261.9	1264.2	1473.6	1441.2	1450.8	0.3581
0.0801	1468.2	1395.3	1267.2	1265.0	1468.6	1445.6	1459.7	0.3470
0.1006	1460.1	1404.7	1272.7	1266.1	1460.4	1451.0	1468.5	0.3298
Average Percentage Error (APE)	-	6.50	14.72	14.41	-0.02	2.92	2.09	-
313.15 K								
0.0000	1471.8	1448.4	1257.6	1171.5	1472.1	1658.8	1515.1	0.4204
0.0201	1485.9	1451.3	1261.6	1177.7	1486.2	1653.6	1517.6	0.4030
0.0399	1487.0	1454.3	1265.7	1183.9	1487.3	1652.1	1520.1	0.3869
0.0601	1496.7	1457.2	1269.9	1190.3	1497.1	1639.4	1522.5	0.3748
0.0801	1506.4	1460.2	1274.2	1196.7	1506.7	1639.3	1524.9	0.3602
0.1006	1511.8	1463.3	1278.5	1203.2	1512.1	1632.9	1527.4	0.3403
Average Percentage Error (APE)	-	6.78	15.25	14.89	-0.02	2.87	2.19	-

The theoretical values show anomalous deviation with the experimental values of ultrasonic velocities which confirms the existence of molecular interactions. A perusal of Table 1 indicates that free length theory (U_{FLT}) predicts the ultrasonic velocity best with minimum average percentage error (APE) of -0.02 on three temperatures followed by collision factor theory (U_{CFT}) which predicts ultrasonic velocity with an average percentage error in the range of (2.35 – 2.87) for all the three temperatures studied. The impedance dependence relation[11] (U_{IDR}) and Nomoto's relation (U_{NOM}) predicts the ultrasonic velocity with average percentage errors in the range (1.29 - 2.19) and (5.67 – 6.78) respectively. The which does not predicts ultrasonic velocity with average percentage error for the present ternary mixtures. Junjie's relation (U_{JM}) and Ideal mixing relation (U_{IMR}) does not predict the data well and shows maximum average percentage error in the range (13.90 – 15.25) and (13.64 – 14.89) for these ternary mixtures. Out of the six theories and relations tested free length theory, Nomoto's relation and impedance dependence relation fit the data well with the other providing the better fit.

An important reason for deviation from experimental values of ultrasonic velocity is that the molecular association effects are not taken into account in these theories. When two liquids are mixed, the interaction between the molecules of the two liquids takes place because of the presence of various forces like dispersive force, charge transfer, hydrogen bonding dipole-dipole and dipole-induced dipole interactions. Hence the observed deviation shows that the molecular interaction is taking place between unlike molecules in the liquid mixture[12]. Similar kinds of results were obtained by earlier works[13]. The agreement between experimental and theoretical velocities of free length theory in the ternary system suggests that the mixture is additive property in all the temperatures. Higher deviations are observed in some theories. This suggests the existence of strong tendency for the association between component molecules as a result of Hydrogen Bonding[14,15].

The deviation of the ratio U^2exp/U^2imr from unity (degree of interaction, α) and its variation as a function of mole fraction of ethyl alcohol is a direct measure of the non-ideality of the system as a consequence of association or other type of interactions. The positive values of α in all the temperature clearly indicate the existence of strong tendency for the formation of association in mixture through hydrogen bonded complexes.

V.CONCLUSION

The experimental ultrasonic velocity values predicted using NR, JM, IMR, FLT, CFT and IDR were compared with measured ultrasonic velocity values at a temperature of 303.15, 308.15 and 313.15K for the ternary mixture of ethyl alcohol + ethylene glycol + glycerol. It may be concluded that free length theory, collision factor theory and impedance dependence relation is best suited for the ternary mixtures of ethyl alcohol + ethylene glycol + glycerol at all the temperatures. The theoretical values of ultrasonic velocity from the experimental values are attributed to the presence of intermolecular interactions in the system studied. Further, the positive values of α indicate the strong molecular interactions exist between the components.

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