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Theoretical Evaluation of Ultrasonic Velocity in Binary Liquid Mixtures at 5MHz for Temperature 298K

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Abstract: *The ultrasonic velocity is very important parameter to find out the physic-chemical behavior of the liquids. Theoretical velocities of binary liquid mixtures at 5 MHz for the temperatures 298K have been evaluated as a function of concentration. The experimental values are compared with theoretical models of liquid mixtures such as Nomoto, Free length theory, Collision Factor Theory, Impedance Relation, Ideal Mixing Relation, Rao's Specific Velocity Method and Junjie's Relations. A good agreement has been found between experimental and theoretical values of ultrasonic velocity. The relative applicability of these theories to the present systems has been checked and discussed. The results are explained in terms of molecular interactions occurring in these binary liquid mixtures.*

Keywords:*Ultrasonic velocity, theoretical models of liquid mixtures, molecular interactions, Nomoto, Free length theory, Collision Factor Theory, Impedance Relation, Ideal Mixing Relation, Rao's Specific Velocity Method and Junjie's Relations, Acetonitrile (ACN), Methanol and Ethanol.*

I. Introduction

Ultrasonic study of liquids is a useful technique for understanding its Physico-chemical properties of the liquid mixtures[1-3]. The study of properties of liquid mixtures consisting of polar as well as non - polar components has wide applications in industrial and technological processes[4-7]. Ultrasonic study of Pure liquid and liquid mixtures has much importance during last two decades for investigate the nature of inter molecular interactions in binary as well as in ternary liquid mixtures[8-11]. In a medium, the ultrasonic velocity of sound waves is fundamentally related to the binding force between the molecules. Polar and non-polar component of the liquid mixtures gives importance in understanding the intermolecular interactions between the component of molecules which gives the application in several industrial and technological process. The speed of sound has been carried out by many researchers[12-16] from several years and correlating the experimental results with the theoretical relations of Nomoto's relation (U_{NOM})[17], Free length theory[18](U_{FLT}), Collision Factor Theory[19](U_{CFT}), Impedance Relation[20](U_{IR}), Ideal Mixing Relation[21](U_{IMR}), Rao's[22](U_R) Specific Velocity Method and Junjie's Relations[23](U_{JR}).In the present investigation comparative study of seven different theoretical models have been discussed. The relative applicability of these theories to the present system have been checked and discussed.

The binary liquid mixtures studied for evaluating theoretical velocities in this paper are

1) Acetonitrile (ACN) + Methanol
2) Acetonitrile (ACN) + Ethanol

II. Materials And Methods

The liquid mixtures of Acetonitrile + Methanol and Acetonitrile + Ethanol of various concentrations in mole fraction were prepared by taking AR grade chemicals. All the liquids used were further purified by standard procedure. The mixtures were preserved in well-stopper conical flasks. After the thorough mixing of the liquids, the flasks were left undisturbed to allow them to attain thermal equilibrium. In all the mixtures the mole fractions of Acetonitrile has been increased from 0.0 to 1.0 in methanol and ethanol. The ultrasonic velocities were measured by using a Multifrequency (1-10MHz) ultrasonic pulse interferometer (Model No. F-83,Mittal Enterprises, New Delhi). It consists of a high Multirange frequency generator (1 to 10MHz) and a measuring cell. The measurements of ultrasonic velocities were made at a fixed frequency of 5 MHz Temperature was controlled by circulating water around the liquid cell from thermostatically controlled constant temperature water bath. The densities of pure liquids and liquid mixtures were measured by using a specific gravity bottle with an accuracy of ± 0.5%. For the viscosity measurement of pure liquids and liquid mixtures, an Ostwald's viscometer was used with an accuracy of ± 0.001 NSm^{-2}**.**

III. Theory

The following empirical and semi-empirical relations were used for theoretical estimation of speed of sound in the studied binary mixtures.

i) Schaaff's collision factor theory (CFT) :-

Schaaff's and Nutsch-Kuhnlies developed the Collision factor theory for determination of ultrasonic velocity of binary liquid mixtures is,

$$U_{CFT} = U_{\infty}\left[\frac{(x_1S_1+x_2S_2)(x_1B_1+x_2B_2)}{V_m}\right] \quad \text{---------- (1)}$$

U_{∞} is the temperature dependent constant ($U_{\infty} = 1600\ m/s$)

Where,

$V_m = \left[\left(\frac{x_1m_1+x_2m_2}{\rho}\right)\right]$

$S = \left(\frac{U\,V}{B\,U_{\infty}}\right)$

Actual Volume, $B = \frac{4}{3}\pi r^3 N$

$r = \left(\frac{3b}{16\pi N}\right)^{1/3}$

where, b is the Vander Waal's Constant and N is the Avogadro Number.

ii) Jacobson's free length theory (FLT) :-

Free length theory was established by Jacobson's for ultrasonic velocity and which is calculated using the following formula as,

$$U_{FLT} = \left(\frac{K}{L_{fmix}\rho_{mix}^{1/2}}\right) \quad \text{---------- (2)}$$

Where K is Jacobson's constant and

$L_{fmix} = 2\left[\frac{V_m-(x_1V_{01}+x_2V_{02})}{x_1Y_1+x_2Y_2}\right]$ Molar Volume at absolute zero,

$V_{01} = V_1\frac{U_1}{U_{\infty}}$ &$V_{02} = V_2\frac{U_2}{U_{\infty}}$,

Surface area per mole, $Y_1 = \frac{2(V_1-V_{01})}{L_{f1}}$ & $Y_2 = \frac{2(V_2-V_{02})}{L_{f2}}$

L_{fmix} and ρ_{mix} are the intermolecular free length and density of the mixtures respectively.

iii) Nomoto's relation (NOM) :-

Nomoto establish the relation for ultrasonic velocity in binary liquid mixtures on the assumption of additivity of molar sound velocity with concentration of molar fraction as,

$$U_{Nom} = \left[\frac{x_1R_1+x_2R_2}{x_1V_1+x_2V_2}\right]^3 \text{---------- (3)}$$

Where, $R_1 = \frac{M_1u_1^{1/3}}{\rho_1}$, $R_2 = \frac{M_2u_2^{1/3}}{\rho_2}$, $V_1 = \frac{M_1}{\rho_1}$, $V_2 = \frac{M_2}{\rho_2}$

In above equations x_1 and x_2 are the mole fraction of component of liquids, M_1 and M_2 are molecular weight, u_1 and u_2 are the ultrasonic velocity and V_1 and V_2 are the molar volume of components of binary liquid mixtures.

iv) Van Deal ideal mixing relation (IMR):-

This theory was proposed by VanDeel and Vangeeland obtained the expression for the ultrasonic velocity in binary liquid mixture as,

$$U_{IMR} = \left[\left(\frac{x_1}{M_1u_1^2}+\frac{x_2}{M_2u_2^2}\right)\right]^{-1/2}[(x_1M_1+x_2M_2)]^{1/2} \quad \text{---------- (4)}$$

In above equations x_1 and x_2 are the mole fraction of component of liquids, M_1 and M_2 are molecular weight, u_1 and u_2 are the ultrasonic velocity and of components of binary liquid mixtures.

v) Impedance dependence (IR) relation:-

The ultrasonic velocity of liquid mixture are also given by Impedance dependence relation,

$U_{IDR} = \left(\frac{\Sigma x_i Z_i}{\Sigma x_i \rho_i}\right)$ ---------- (5)

Where, x_i, ρ_i and Z_i are the mole fraction, density and acoustic impedance.

vi) Rao's Relation (R):-

The Rao's relation is also called as Specific sound velocity and can be express as,

$U_R = (\Sigma x_i r_i \rho_i)^3$ ---------- (6)

Where, r_i is the Rao's specific sound velocity which is given by,

$r_i = \frac{U^{1/3}}{\rho_i}$

vii) Zhang–Junjie relation (JR) :-

The Junjie's relation for determination of ultrasonic velocity in binary liquid mixtures is,

$U_{JR} = \left(\frac{\Sigma x_i V_i}{\Sigma x_i M_i}\right)^{1/2} \left(\frac{\Sigma x_i V_i}{\Sigma \rho_i U_i^2}\right)^{-1/2}$ ---------- (7)

Where, M_i and ρ_i are the molecular weight and densities of the components.

IV. Result and Disccusion

Comparative study of theoretical values of ultrasonic velocities in present liquid mixtures explained the nature of intermolecular interaction between the molecules in the mixtures. The theoretical studies of liquid mixtures are useful in building the comprehensive theoretical model of liquid mixtures. The value of ultrasonic velocities computed theoretically using the relation Collision Factor Theory, Free Length Theory, Nomoto's Theory, Ideal Mixing Relation, Impedance Dependence Relation, Rao's Theory and Junjie's Relation with experimental values for binary system-I: Acetonitril + Methanol and system-II: Acetonitril + Ethanol at the temperature 298K are given in table-1 and table-2.The experimentally determined values of ultrasonic velocity (U) at 298K have been taken from our previous work[23]. From the fig.-1 and fig- 2, it is clear that the theoretical values of ultrasonic velocities calculated by using different theories shows the deviations from experimental values. Due to limitations and approximation of these theories are responsible for the deviation of theoretical values from experimental values. In Nomoto's theory, it is supposed that the volume does not change on mixing. But on mixing two liquids, the interaction between the molecules of the two liquid takes place because of the presence of various type of force such as hydrogen bonding, dipole-dipole, dispersive forces, charge transfer and dipole induces dipole interactions. The deviations of experimental values from theoretical values calculated using Van Dael and Vangeel equation might be due to the compressibility of the component liquids in the present mixtures. The deviation of experimental values and values calculated from impedance relation and Rao's Relation imply non-additively of acoustic impedance and Rao's velocity in the liquid mixtures. The deviation is observed in case of Junjie's relation. Thus the observed deviation of theoretical values of velocities from the experimental values shows that the molecular interaction are taking place[24-27] between the unlike molecules in liquid mixtures. This is due to breaking of hetero and homo molecular clusters at higher temperatures[28]. On increasing temperature, the ultrasonic velocity decreases in binary liquid mixtures. This is probably due to the fact that the thermal energy activates the molecules, which would increases the rate of association of unlike molecules. Based on theoretical values of ultrasonic velocities, it is worthwhile to state that NR method yield the best result for both system-I and CFT for system-II.

V. Tables And Graphs

Table-1: Experimental and theoretical values of velocities in binary liquid system-I: Acetonitril + Methanol at 298K temperature.

Mole Fraction ACN in Methanol	U_{EXP}	U_{CFT}	U_{FLT}	U_{NOM}	U_{IMR}	U_{IR}	U_R	U_{JR}
0	1098.01	1098.08	1098.00	1098.27	1098.00	1098.00	1098.00	1097.95
0.1	1123.02	1108.20	1097.11	1115.22	1106.53	1113.52	1112.24	1111.98
0.2	1142.03	1120.11	1101.02	1131.63	1116.16	1128.88	1126.61	1126.17
0.3	1158.01	1132.19	1105.43	1147.54	1126.97	1144.07	1141.09	1140.54
0.4	1176.01	1141.32	1101.11	1162.95	1139.04	1159.10	1155.71	1155.06
0.5	1187.02	1152.18	1101.64	1177.90	1152.50	1173.97	1170.44	1169.77
0.6	1198.03	1161.20	1096.39	1192.39	1167.46	1188.68	1185.30	1184.64
0.7	1210.02	1171.11	1093.59	1206.46	1184.09	1203.23	1200.29	1199.69
0.8	1216.03	1195.59	1137.28	1220.11	1202.57	1217.64	1215.40	1214.93
0.9	1236.02	1222.81	1195.45	1233.38	1223.12	1231.89	1230.64	1230.35
1	1246.04	1246.38	1246.03	1246.26	1246.00	1246.00	1246.00	1245.96

Table-2: Experimental and theoretical values of velocities in binary liquid system-II: Acetonitril + Ethanol at 298K temperature.

Mole Fraction ACN in Ethanol	U_{EXP}	U_{CFT}	U_{FLT}	U_{NOM}	U_{IMR}	U_{IR}	U_R	U_{JR}
0	1098.01	1129.80	1130.00	1129.71	1130.00	1130.00	1129.37	1129.97
0.1	1123.02	1141.81	1138.61	1138.67	1140.60	1141.82	1136.16	1138.46
0.2	1142.03	1150.95	1139.17	1148.97	1151.41	1153.56	1148.03	1147.46
0.3	1158.01	1165.90	1158.15	1159.64	1162.43	1165.21	1159.99	1157.02
0.4	1176.01	1176.26	1163.73	1170.68	1173.67	1176.78	1172.02	1167.20
0.5	1187.02	1188.28	1175.46	1182.14	1185.12	1188.26	1184.14	1178.05
0.6	1198.03	1199.49	1185.49	1194.01	1196.81	1199.67	1196.35	1189.64
0.7	1210.02	1215.43	1213.46	1206.34	1208.73	1210.99	1208.63	1202.06
0.8	1216.03	1225.34	1221.52	1219.13	1220.90	1222.24	1221.01	1215.40
0.9	1236.02	1237.03	1237.58	1232.43	1233.32	1233.41	1233.46	1229.77
1	1246.04	1246.38	1246.00	1246.26	1246.00	1244.50	1246.00	1245.28

Graphs: Fig.-1 and Fig.-2 shows theoretical Values of Ultrasonic velocity of the System-I: ACN + Methanol and the system-II: ACN + Ethanol with respective to the experimental Values of Ultrasonic velocity.

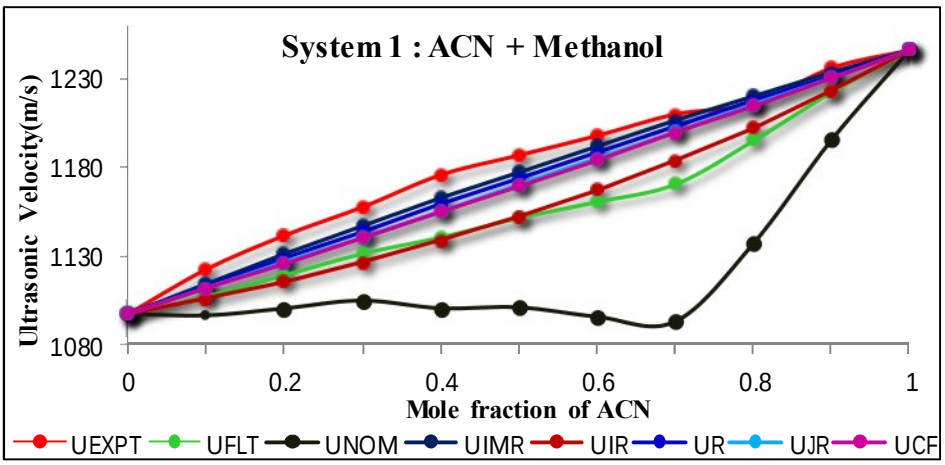

Figure 1- Theoretical Values of Ultrasonic velocity of System ACN + Methanol

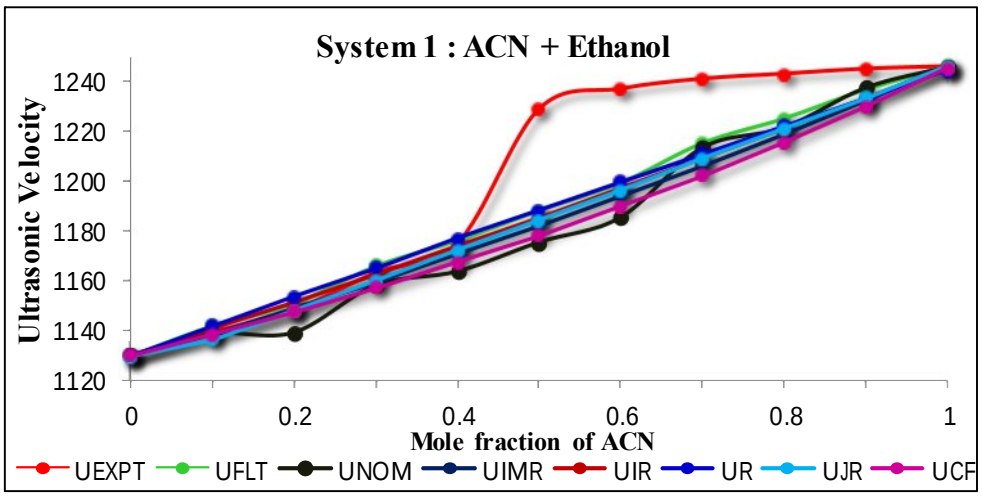

Figure 2- Theoretical Values of Ultrasonic velocity of System ACN + Ethanol

VI. Conclusion

Theoretical evaluations of ultrasonic velocity in binary liquid mixtures are determined and the validity of different theories has been checked. The ultrasonic velocities has been calculated using the relation CFT, FLT, NOM, IMR, IR, R and JR and compared with the experimental velocity at the temperature 298K in binary mixtures Acetonitril (ACN) + Methanol and Acetonitril (ACN) + Ethanol. The observed deviation of the theoretical values of ultrasonic velocity from experimental values is attributed to the presence of intermolecular interactions in the systems studied.

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