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Experimental and theoretical study of ultrasonic velocity in binary liquid mixture of chloroform and methanol

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ABSTRACT

Ultrasonic velocities and densities of binary mixture of chloroform and methanol has been measured at temperature 295 K and frequency 2 MHz over the entire range of mole fraction. Theoretical values have been measured using various theoretical models such as Nomoto, Junjie, Impedance, Van-Deal and Vangeel. The percentage error has been calculated to check the validity of theoretical models and found a good agreement in experimental and theoretical values. The deviation from experimental values has been interpreted in terms of molecular interactions between the components of the molecules of the binary mixture.

INTRODUCTION

The propagation of ultrasonic wave in the medium has been effectively employed to understand the physico-chemical behaviour of components of molecules in the liquid mixture.[1-4]The ultrasonic velocity measurement has become a very powerful tool to determine thermodynamic properties and for predicting the molecular interaction among the molecules of liquid or liquid mixture.[6-9] In this paper, ultrasonic velocity and density of chloroform and methanol and its mixtures has been calculated at temperature 295 K and frequency 2 MHz. Theoretical values of ultrasonic velocity are computed by using Nomoto's relation, impedance relation, Van-Deal and Vangeel ideal mixture relations and Junjie's relation. The deviation of theoretical velocity data from experimental values is interpreted in terms of molecular interaction[12-15] present in the system. The validity of theoretical models has been checked by applying Chi Square test and by calculating average percentage error.

MATERIALS AND METHODS

In the present investigations chemicals used are Chloroform and methanol having molecular weight 119.5 g/mol and 32 g/mol respectively of 99% AR grade. The ultrasonic velocity was measured at 295 K using ultrasonic interferometer (Mittal Enterprises) working at frequency of 2 MHz with an accuracy of ±0.1m/s. Density was measured using specific gravity bottle at temperature 295K.

Theory: The following relations has been used for computing theoretical values of ultrasonic velocity in experimental liquid mixtures.

Nomoto's Relation of sound velocity[5]:

$U_{NOM} = [(X_1 R_1+X_2R_2) / (X_1 V_1+X_2 V_2)]^3$

Where $R_1$and R_2 are molar sound velocities of pure component 1 and 2 respectively.

X_1 and X_2 corresponds to mole fractions of chloroform and methanol respectively.

Impedance dependent relation:
$U_{IMP} = (X_1 Z_1 + X_2 Z_2)/ X_1 \rho_1 + X_2 \rho_2$

Where $Z_1$and $Z_2$are acoustic impedance of pure component 1 and 2 respectively.

Van-Dael and Vangeel Ideal mixing relation[10]:

$U_{VDV} = [(X_1 /M_1U_1^2 + X_2/M_2U_2^2) (X_1M_1+X_2M_2)]^{-1/2}$

Where M_1 and M_2 are molecular weights are the molecular weights of pure component 1 and 2 respectively.

Junjie equation[11]:

$U_{JUN} = [(X_1M_1/\rho_1 + X_2M_2/\rho_2) / (X_1M_1+X_2M_2)^{1/2}][\{X_1M_1/\rho_1U_1^2+X_2M_2/\rho_2U_2^2\}]^{-1/2}$

Percentage deviation in ultrasonic velocity:
$(\Delta U/U)\ \% = ((U_{EXP}-U_{THEORY}) / (U_{EXP}))\ x100$

Where 1 and 2 represents the first and second component of the binary liquid mixture and other symbols have their usual meanings.

Chi-square test for goodness of fit: According to Karl Pearson, the Chi-square value is calculated by using the following formula:

$$(x^2) = \sum \frac{(U_{mix(\exp)} - U_{mix(cal)})^2}{U_{mix(cal)}}$$

Average Percentage Error (APE):Average percentage error has been calculated using following formula:

$$APE = \frac{1}{n} \sum \frac{U_{mix(\exp)} - U_{mix(cal)})}{U_{mix(exp)}}\ x\ 100$$

Where, n – number of mole fractions taken.
$U_{mix\ (exp)}$ – experimental values of ultrasonic velocity of binary mixture.
$U_{mix\ (cal)}$ – calculated values of ultrasonic velocity of binary mixture.

RESULTS AND DISCUSSION

The ultrasonic velocities of chloroform and methanol and their binary liquid mixtures which are measured experimentally at temperature 295K as well as theoretically using various theoretical models are given in **Table 1.** The percentage deviations in experimental and theoretical values of ultrasonic velocity are given in **Table 2.**To check the validity of theoretical models Chi Square test is applied and average percentage error has been calculated.

Table 1 shows the experimental values followed by theoretical values which are calculated by various theoretical models such as Nomoto's relation, impedance dependent relation, ideal mixing relation and from Junjie's equation. **Table 2**shows the percentage deviation of theoretical values from experimental values. It has been observed that there is much less deviation from experimental values. Formulae for average percentage error and chi square test has also been applied for each theoretical model and is given in **Table 2.** It can be clearly seen that for Junjie's model of ultrasonic velocity the value for average percentage error and chi square test is least. Hence Junjie's equation is the best suited model for theoretical interpretation of ultrasonic velocity. The effects of molecular association are not considered in theoretical models that is why deviation in theoretical ultrasonic velocitiesare observed.

Table1: Experimental and theoretical values of ultrasonic velocities in the binary liquid mixtures of chloroform and methanol over the entire mole fraction at temperature 295 K and frequency 2 MHz

Mole Fraction		U_{EXP} ms^{-1}	U_{NOM} ms^{-1}	U_{IMP} ms^{-1}	U_{VDV} ms^{-1}	U_{JUN} ms^{-1}
X1	X2					
1.0	0.0	1020.0	1020.16	1019.99	1020.00	1019.94
0.9	0.1	978.8	1024.10	1026.41	962.87	1021.20
0.8	0.2	981.2	1028.57	1033.34	925.94	1022.92
0.7	0.3	983.2	1033.68	1040.84	903.71	1025.28
0.6	0.4	992.4	1039.57	1049.00	893.41	1028.53
0.5	0.5	1008.4	1046.44	1057.89	893.86	1033.04
0.4	0.6	985.2	1054.56	1067.63	905.12	1039.40
0.3	0.7	1112.4	1064.29	1078.34	928.47	1048.56
0.2	0.8	1116.8	1076.18	1090.18	966.87	1062.15
0.1	0.9	1084.0	1091.03	1103.32	1026.13	1083.21
0.0	1.0	1118.0	1110.09	1118.01	1118.00	1117.92

Table 2: Percentage deviations between experimental and theoretical of ultrasonic velocities in the binary liquid mixtures of chloroform and methanol over the entire mole fraction at temperature 295 K and frequency 2 MHz

Mole Fraction		$\%U_{NOM}$	$\%U_{IMP}$	$\%U_{VDV}$	$\%U_{JUN}$
X1	X2				
1.0	0.0	-0.0157	0.0003	0.0000	0.0055
0.9	0.1	-4.6287	-4.8643	1.6271	-4.3318
0.8	0.2	-4.8283	-5.3139	5.6317	-4.2522
0.7	0.3	-5.1345	-5.8630	8.0844	-4.2802
0.6	0.4	-4.7535	-5.7034	9.9746	-3.6408
0.5	0.5	-3.7727	-4.9083	11.3580	-2.4437
0.4	0.6	-7.0402	-8.3673	8.1275	-5.5016
0.3	0.7	4.3244	3.0613	16.5336	5.7388
0.2	0.8	3.6368	2.3835	13.4243	4.8929
0.1	0.9	-0.6486	-1.7828	5.3379	0.07271
0.0	1.0	0.7069	-0.0011	0.0000	0.00633
APE		-2.0140	-2.8508	7.2817	-1.2485
Chi Square		168.6040	198.4622	965.6050	150.6533

CONCLUSION

The ultrasonic velocities computed from Nomoto's relation, impedance dependent relation, ideal mixing relation and from Junjie's equation were compared with experimentally obtained velocities at temperature 295K for binary mixtures of chloroform and methanol. From the results it can be concluded that Junjie's equation is the best suitable model for theoretical ultrasonic velocity. The deviation observed in theoretical values from experimental values is attributed to the presence of strong intermolecular in the binary mixture.

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