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Estimation of Acoustic Impedance of 1-Butanol + Dodecane and 2-Butanol + Dodecane Binary Mixtures from Various Models at Temperature Range 288.15 to 313.15

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Abstract: ***Densities and speed of sound were measured for the binary liquid mixtures formed by 1-butanol + dodecane and 2-Butanol + Dodecane at 288.15, 298.15, 308.15 and 318.15 K and atmospheric pressure over the whole composition range. From these data, acoustic impedance were obtained and analyzed in terms of Ramaswamy and Anbananthan model, model suggested by Glinski and Flory model to predict the associational behavior of polar and non-polar liquids. Furthermore, McAllister multi body interaction model was also used to correlate the binary properties. These models were compared and tested for different systems showing that the associated processes yield fair agreement between theory and experiment as compared to non-associated processes.***

Keywords: Speed of Sound, Acoustic Impedance, Flory, McAllister, Ramaswamy and Anbananthan

1. Introduction

Molecular interactions occurring in a variety of liquid mixtures and solutions can be studied with the help of ultrasonic velocity [1]. Sound velocity offers a convenient method for determining certain thermo dynamical properties of liquids and liquid mixtures, which are not obtained by other methods. As a part of research concerning the thermo chemical studies on new working fluid pair, we present here some useful data on acoustic impedance of binary liquid mixtures formed by 1-butanol + dodecane and 2-Butanol + Dodecane at 288.15, 298.15, 308.15 and 318.15 K and atmospheric pressure over the whole composition range. These data were analyzed in terms of Ramaswamy and Anbananthan (RS) model [2] model suggested by Glinski [3], Prigogine-Flory-Patterson (PFP) model [4-6], First two models, RS and model devised by Glinski are based on the association constant as an adjustable parameters where as PFP and others are based on the additivity of liquids. An attempt has also been made to correlate the experimental data with the McAllister multi body interaction model [7]

2. Experimental Section

High purity and AR grade samples of 1-butanol, dodecane,2-Butanol and Dodecane in this experiment were used and further purified by distillation in which the middle fraction was collected.The uncertainty in the density measurement was within ±6x10-4 g/cc .The densities of the pure components and their mixtures were measured with the bi-capillary pyknometer. The liquid mixtures were prepared by mass in an air tight stopped bottle using an electronic balance model SHIMADZUAX-200 accurate to within ±0.1 mg. The average uncertainty in the composition of the mixtures was estimated to be less than ±0.0001.Crystal controlled variable path ultrasonic interferometer supplied by M/s Mittal enterprises (model-05F), New Delhi (India), operating at a frequency of 2 MHz was used in the ultrasonic measurements with an accuracy ± 0.01m/s.The results are listed in Table 1 together with literature values [8-10] for comparison.

3. Modeling

3.1 Ramswamy and Anbananthan Model

Ramswamy and Anbananthan [2] proposed the model based on the assumption of linearity of acoustic impedance with the mole fraction of components. Further it is assumed, that an equilibrium physical property such as viscosity, refractive index, surface tension etc which are based on linearity can be predicted [11]. Glinski [3] assumed that when solute is added to solvent the molecules interact according to the equilibrium as:

$$A+B \leftrightarrow AB \tag{1}$$

and the association constant K_{as} can be defined as;

$$K_{as} = \frac{[AB]}{[A][B]} \tag{2}$$

where [A] is amount of solvent and [B] is amount of solute in the liquid mixture. By applying the condition of linearity in speed of sound with composition

$$z_{cal} = x_A \, z_A + x_{AB} \, z_{AB} \tag{3}$$

where x_A, x_{AB}, z_A and z_{AB} and z_{cal} are the mole fraction of A, mole fraction of associate AB, acoustic impedance of A, acoustic impedance of associate AB and calculated acoustic impedance respectively. The associate AB can not be obtained in its pure form. Following simplifications have been made in eq. (3), firstly, molar concentration term should be replaced by activities for concentrated solution and second, the equilibrium reaction is not complete by definition; i.e. there are also molecules of non associated component present in the liquid mixture even prevailing in the high solute content. The eq (3) takes the form,

$$z_{cal} = [x_A\, z_A + x_B\, z_B + x_{AB}\, z_{AB}] \quad (4)$$

On inspecting the results obtained from Ramaswamy and Anbananthan model, Glisnki [3] suggested the equation assuming additivity with the volume fraction, ϕ of the components, the refined version of Natta and Baccaredda model [12] as,

$$z_{cal} = \frac{z_A z_B z_{AB}}{\phi_A z_B z_{AB} + \phi_B z_A z_{AB} + \phi_{AB} z_A z_B} \quad (5)$$

where z_{cal} is the theoretical acoustic impedance of binary liquid mixture, ϕ_A, ϕ_B are the volume fractions of component A and B and z_A, z_B and z_{AB} are the acoustic impedance of components A, B and AB. The numerical procedure and determination of association constant, K_{as}, were similar to that described before and the advantage of this method as compared with the earlier one was that the data on densities of liquid mixture are not necessary except those of pure components needed to calculate the volume fractions

3.2 Prigogine-Flory-Patterson Model

With the particular (6,3) choice of m,n potentialFlory model takes the form as,

$$\tilde{\sigma}(\tilde{V}) = [M \tilde{V}^{-5/3} - (\frac{\tilde{V}^{1/3} - 1.0}{\tilde{V}^2}) \ln(\frac{\tilde{V}^{1/3} - 0.5}{\tilde{V}^{1/3} - 1.0})] \quad (6)$$

Thus on the basis of Flory theory, surface tension of liquid mixture is given by the

$$\sigma = \sigma^* \tilde{\sigma}(\tilde{V}) \text{ and } u = \left(\frac{\sigma}{6.3x10^{-4}\rho}\right)^{2/3} \quad (7)$$

$$z = u \times \rho_{mix} \quad (8)$$

All the notations used in the above equations have their usual significance as detailed out by Flory.

3.3 McAllister Multi body Interaction Model

Multi body interaction model of McAllister [7] is widely used for correlating the viscosity of liquid mixtures with mole fraction which is based on the assumption of additivity. In recent past [11, 13], we have applied this model successfully in the estimation of other equilibrium properties.

4. Results & Discussion

Relation between association phenomenon in liquids were analyzed earlier [11-12,] by considering van der Waals equation of state which was based only on simple averaged geometrical deviations without analyzing the system in terms of equilibrium. The association phenomenon has been related usually the deviation of different quantities from additivity. Ramaswami and Anbananthan derived the model based on the assumption of linearity of acoustic impedance with the mole fraction of components which was corrected [3] and tested to predict the associational behavior. The quantities analyzed were refractive index, molar volume, viscosity, intermolecular free length and many others. The results of fittings obtained from the model were utilized properly. The basic doubt regarding this model except the assumption of linearity of ultrasonic velocity with mole fraction is that these liquids have poor affinity to form dimmers. The calculations were performed using a computer program which allows fittings easily both the adjustable parameters simultaneously or the parameters were changed manually.

Values of thermal expansion coefficient (α) and isothermal compressibility needed in the PFP model were obtained from the equation which have already been tested in many cases by us [11,13]. The absolute average percent deviations (AAPD) in acoustic impedance obtained from different models are provided in Table 2 which shows that co relational models provide fairly good results as compared to PFP model. McAllister multi interactive model provides excellent agreement with the experimental findings. Higher deviation values in PFP model can be explained as the model was developed for non-electrolyte γ-meric spherical chain molecules and the system under investigation have interacting and associating properties. Moreover, the expression used for the computation of α and β_T are also empirical in nature. With the increase of mole fraction, the values of acoustic impedance obtained from all the models show irregular trend as evidenced by Table 2. Positive deviations in acoustic impedance are a result of molecular association and complex formation whereas negative deviations are due to molecular dissociation. The actual sign and magnitude of deviations depend upon relative strength of two opposite effect. The lacks of smoothness in deviations are due to the interaction between the component molecules as evident in figure1 & 2. Plots of Acoustic Impedance deviation, ΔZ with mole fraction x, for 1-Butanol + Dodecane and 2-Butanol + Dodecane at 288.15, 298.15, 308.15, and 318.15K indicate similar trend. Results of acoustic impedance obtained from different models have been compared and are also reported in Table 2. A careful perusal of the results clearly indicates the close proximity of our results with the observed findings.

Conclusively, associated process give more reliable results as compared to non-associated processes and helpful in deducing the internal structure of associates through the fitted values of acoustic impedance in a hypothetical pure associate and observed dependence of concentration on composition of a mixture.

5. Acknowledgment

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Table 1: Comparison of Density and Ultrasonic Velocities with Literature Data for Pure Component at 288.15, 298.15, 308.15, and 318.15K

		ρ(g/cc)		U (m/s)	
liquids	**T/K**	**exp**	**Literature[a]**	**exp**	**literature**
	288.15k	0.75236	0.75255	1317.27	-
Dodecane	298.15k	0.74517	0.74528	1278.2	1278[b]
	308.15k	0.73795	0.73799	1239.82	-
	318.15k	0.73069	0.73066	1201.88	-
	288.15k	0.81349	0.81328	1273.51	
1-Butanol	298.15k	0.80586	0.80569	1239.29	-
	308.15k	0.79804	0.79798	1205.5	1203[c]
	318.15k	0.79007	0.79011	1172.12	-
	288.15k	0.81025	-	1247.03	-
2-butanol	298.15k	0.80219	0.80255	1210.98	1212[b]
	308.15k	0.79375	0.79392	1174.53	-
	318.15k	0.78486	0.78492	1137.61	-

Ref[a] - 8, Ref[b] - 9, Ref[c] - 10

Table 2: Comparison of Absolute Average Percentage Deviation of Acoustic Impedance from Various Liquid Models for Binary Liquid mixtures at Different temperatures

1-Butanol+n-Dodecane

			Average% dev				
T/K	**K_{as}**	**$Z_{ab}10^{-6}$**	**Z_{PFP}**	**Z_{RS}**	**Z_{GLI}**	**Z(Mc3)**	**Z(Mc4)**
288.15	0.006	1.00	1.07	1.36	1.53	0.02	0.02
298.15	0.007	0.96	2.07	1.49	1.69	0.02	0.02
308.15	0.009	0.95	0.29	1.62	1.88	0.02	0.02
318.15	0.04	0.91	1.85	1.28	2.55	0.02	0.02

2-Butanol+n-Dodecane

288.15	0.02	1.00	1.30	1.00	1.61	0.04	0.02
298.15	0.03	0.96	1.80	1.00	1.92	0.03	0.03
308.15	0.04	0.92	0.40	0.99	2.20	0.04	0.03
318.15	0.03	0.88	2.13	1.24	2.16	0.05	0.03

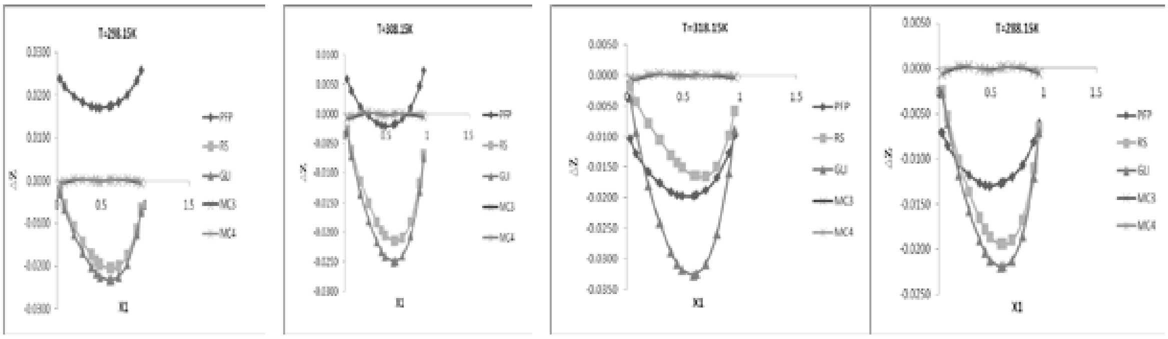

Figure 1: Plot of Acoustic Impedance deviation, ΔZ with mole fraction x, for (x) 1-Butanol+ (1-x) Dodecane at 288.15, 298.15, 308.15, and 318.15K.

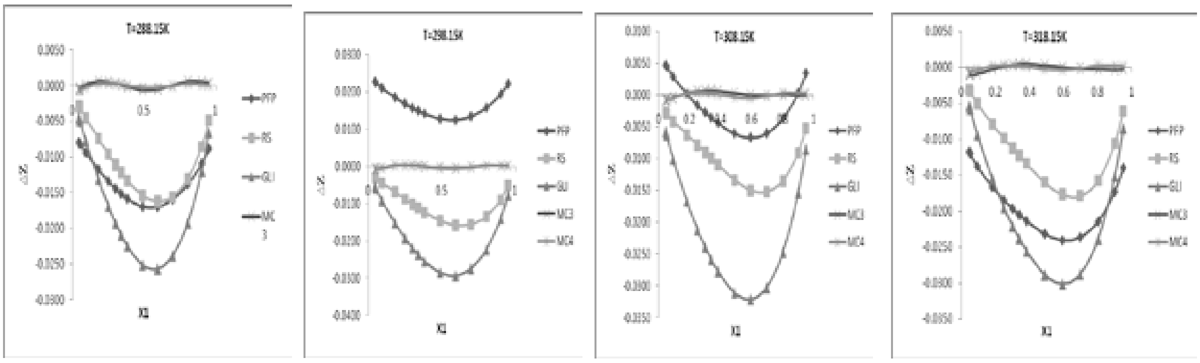

Figure 2: Plot of Acoustic Impedance deviation ΔZ with mole fraction x, for (x) 2-Butanol+ (1-x) Dodecane at 288.15, 298.15, 308.15, and 318.15K.