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Ultrasonic studies of molecular interactions in binary mixtures of n-Butanol with water at different temperatures (308K, 318K and 328K)

L. UMARALIKHAN[1*] DR. M. JAMAL MOHAMED JAFFAR[1]
[1]Department of Physics, Jamal Mohammed College, Trichy-620020
*Corresponding Author
E-mail address: **umarjor@gmail.com**

Abstract

The experimental ultrasonic velocity (u), density (ρ) and viscosity (ŋ) of butanol mixed with water has been measured over the full range of compositions at atmospheric pressure and at different temperatures (308, 318 and 328 K). From these experimental values the molar Isentropic compressibility (β_s), Intermolecular free length (L_f), Free volume (V_f) and Acoustic impedance (Z) are calculated.

Keyword

Ultrasonic sound velocity, Density, Viscosity, β_S, L_f, V_f, Z.

Introduction

The ultrasonic studies are extensively carried out to measure the thermodynamic properties and predict the inter-molecular interaction of binary mixtures. The sound velocity is one of those physical properties that helps in understanding the nature of Liquid state. Using the obtained values of sound velocity and density, the associated acoustical parameters such as Intermolecular free length, free volume, internal pressure, acoustic Impedance, and Excess parameters can be calculated. In recent years Ultrasonic method has become a powerful tool in providing information regarding the chemical properties of liquid system[1-4].

n-Butanol or butyl alcohol is a primary alcohol with a 4 carbon structure. n-Butanol occurs naturally as a minor product of the fermentation of sugars and other carbohydrates[5] and is present in many foods and beverages[6]. Hall. R. L, Oser. B. L. (1965)[7] reports used in butter, cream, fruit, rum, whiskey, ice cream and ices, candy, baked goods and cordials. It is mostly used as a solvent, as an intermediary in chemical synthesis, and as a fuel. It is also used as a paint thinner and a solvent in other coating applications where it is used as a relatively slow evaporating latent solvent in lacquers and ambient- cured elements. It finds other uses such as a component of hydraulic and brake fluids.

In the present investigation is linked on thermodynamic properties of binary liquid mixture of n-Butanol + water which is an organic solvent with low boiling point and evaporate easily or can be removed by refinement, thereby leaving the dissolved substance behind. Solvents should therefore not react chemically with the dissolved compounds they have to be inert.

Experimental

Ultrasonic measurements

Aqueous solutions of 1-butanol were prepared by dissolving in double distilled water (the solvent). The molar solutions of 1-butanol (0.006, 0.01, 0.02 and 0.03M) were prepared by standard procedure. Measurement of ultrasonic velocity is generally made either by continuous wave method or by pulse methods. In the present study, continuous wave variable path interferometer is used. The accuracy of ultrasonic velocity determination in non–aqueous solutions is 0.001%. The ultrasonic measurements are carried out on these solutions for various acoustical parameters at different temperatures (308K, 318K, and 328K) and different concentrations.

Ultrasonic sound velocities for the aqueous solutions were measured using 2 MHz ultrasonic interferometer with a reproducibility of ±0.2m/s.0The temperature was constantly maintained by circulating water from a thermostatically controlled water bath with an accuracy 0of ±0.1 °C. The density measurements were made by using a 10 ml specific gravity bottle with an accuracy of $\pm 0.0001\times 10^3$ kg m^{-3}. The viscosity measurements were made by using Ostwald's viscometer of ±0.1% accuracy.

Result and discussion

The measured and other calculated parameters namely ultrasonic sound velocity(u), density(ρ) and viscosity(η), Isentropic compressibility (β_s), Intermolecular free length (L_f), Free volume (V_f) and Acoustic impedance (Z) are calculated for aqueous n-Butanol solutions are presented in Table 1.

Velocity (u), viscosity (η) and density (ρ), isentropic compressibility (β_s), intermolecular free length (L_f) , free volume (V_f) and acoustic impedance (Z)

T	M	u	η	ρ	$\beta_s \times 10^{-10}$	$L_f \times 10^{-8}$	$V_f \times 10^{-8}$	$Z \times 10^5$
K	mol kg^{-1}	m sec^{-1}	N S m^{-2}	kg m^{-3}	N^{-1} m^2	cm	m^3	Kgm^{-2} s^{-1}
308	0.006	1529.6	0.8323	0.9918	4.309	2.41018	6.728	15.1705
	0.01	1536.4	0.8701	0.986	4.296	2.41	7.266	15.1489
	0.02	1557	0.8729	0.9799	4.209	2.408	7.476	15.2570
	0.03	1566	0.8957	0.9715	4.197	2.40676	7.869	15.2136
318	0.006	1546	0.6922	0.9891	4.23	2.40463	5.185	15.2914
	0.01	1556.8	0.7109	0.984	4.202	2.403	5.473	15.2862
	0.02	1561.6	0.7187	0.9788	4.192	2.40109	5.61	15.2724
	0.03	1569.6	0.7353	0.9674	4.195	2.40063	5.873	15.2406
328	0.006	1554	0.4799	0.9774	4.236	2.4028	3.016	15.1888
	0.01	1561.5	0.495	0.9743	4.209	2.4019	3.194	15.2136
	0.02	1566.4	0.5061	0.9713	4.196	2.40101	3.33	15.2144
	0.03	1573.2	0.532	0.9702	4.164	2.4	3.626	15.2445

Table 1: measured and other calculated parameters of n-Butanol.

Ultrasonic velocity

It can be observed from Figure. 1 that the ultrasonic velocity is found to increase from the increase in n-Butanol concentration. The increase in ultrasonic velocity in any solution shows the greater association with the molecules of a solution. The greater association is due to the intermolecular hydrogen bonding among the solute and solvent molecules.

When the Aqueous solution n-Butanol's temperature is increases, the ultrasonic velocity also increases. This action is similar to that of pure water. The ultrasonic velocity increases in increase in temperature of water. As the monomeric water molecules are formed into the water molecules break in the hydrogen bonds, this process occurs to increases in Temperature[8]. From the Table 1 we observed the ultrasonic velocity for the n-Butanol solutions increases in the increase in temperature for all concentrations. The plots of Ultrasonic velocities as a function of temperature are shown in Figure. 1.

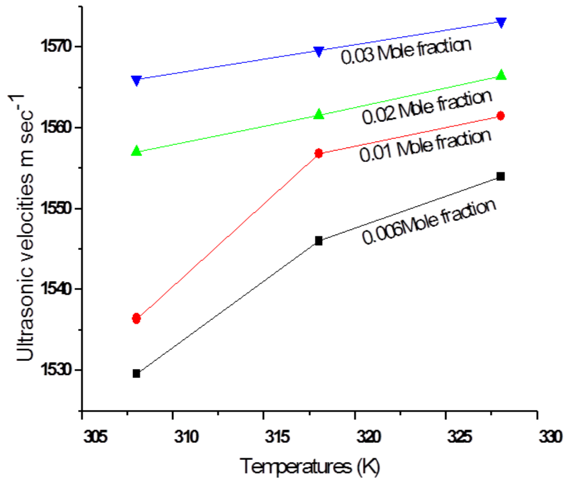

Figure 1: Variation of ultrasonic velocity (u m s^{-1}) with respect to Temperature T (K) in aqueous solutions of n-Butanol.

Isentropic compressibility

Every solvent has a limit of the density called the limiting compressibility value. The compressibility of a solvent is greater than that of a solution and decreases with the increase in concentration of the solution. With to increase from ionic solute concentration, their electrostrictive forces cause the water structure to break and the solute surrounded water molecules is more closely packed. The results are when the ionic solute concentration is increasing then the compressibility is decreases.

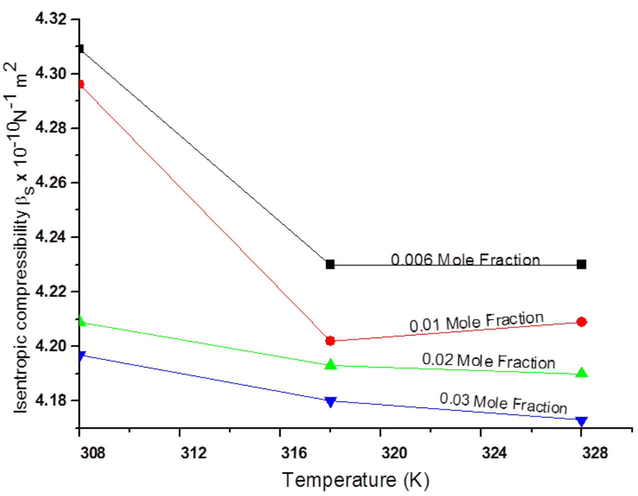

Figure 2: Variation of Isentropic compressibility ($\beta_s \times 10^{-10}$ N^{-1} m^2) with respect to Temperature T (K) in aqueous solutions of n-Butanol.

In the aqueous n-Butanol solutions, it is observed from the Figure 2 and Table 1 that isentropic compressibilities decrease with the increase in n-Butanol concentrations and temperature. This confirms the existence of strong solute- solvent interactions through dipole-dipole interactions of the -OH groups of n-Butanol with the surrounding water molecules.

Intermolecular free length

Intermolecular free length is the distance between the surfaces of the neighboring molecules. Generally, when the ultrasonic velocity increases, the values of the intermolecular free length decreases. The decrease in intermolecular free length indicates the interaction between the solute and solvent molecules due to which the structural arrangement in the neighborhood of the constituent ions or molecules gets affected considerably.

In the present investigation, it has been observed that intermolecular free lengths decrease on increasing the concentration of n-Butanol. This behaviour indicates significant interaction between the solute and solvent molecules suggesting a structure promoting tendency of the added n-Butanol.

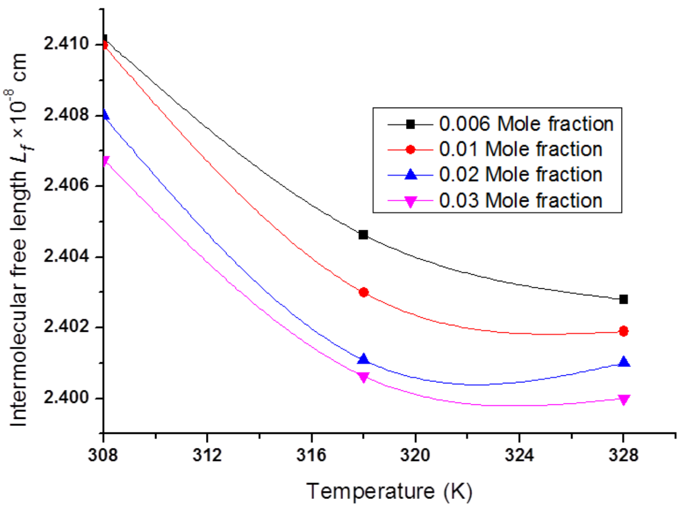

Figure 3: Variation of Intermolecular free length ($L_f \times 10^{-8}$ cm) with respect to Temperature T (K) in aqueous solutions of n-Butanol.

Free volume

The variation on free volume of mole fractions of n-Butanol at 308 K, 318 K and 328 K is represented in Figure 4. Free volume increases with increase in size of the molecule. From the figure 4, the free volume decreases of the increases in temperature. When the concentration increases then free volume also increases. As the temperature increases, the molecular moving area is decreases. As the temperature decreases, the molecular moving area is increases. It shows that the molecular repulsion is decreases of increases in temperature.

Acoustic impedance

The specific acoustic impedance in liquids can also be used to assess the strength of intermolecular attraction. As the strength of intermolecular attraction increases, the ultrasonic velocity also increases. Therefore, the acoustic impedance value also increases. The acoustic impedance values in pure liquids and binary liquid mixtures can be used to estimate the strength of intermolecular attraction.

Specific acoustic impedance is a characteristic property of a medium. V Vyas *et. al*[9] has reported the variation on this parameter with temperature and pressure in case of pure liquid systems.

Acoustic impedance is observed from Table 1 that the values of acoustic impedance differ linearly with the increase in n-Butanol concentrations. The linear variation on acoustic impedance with concentration confirms the presence of molecular association with the solute–solvent molecules through intermolecular hydrogen bonding

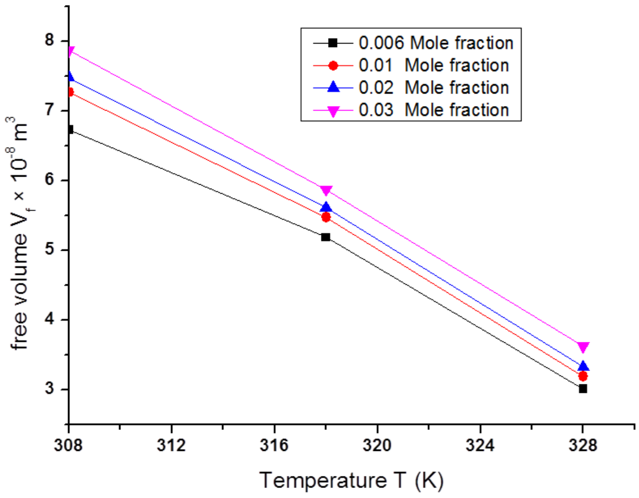

Figure 4: Variation of Free volume ($V_f \times 10^{-8}$ m^3) with respect to temperature, T (K), in aqueous solutions of n-Butanol

Conclusion

A systematic study of n-Butanol in water has been carried out at different concentrations and at different temperatures using ultrasonic experiments. The ultrasonic velocity data and other acoustical parameters give valuable information to understand the solute–solvent interactions in the aqueous solutions. Intermolecular free length indicates significant interaction between solute and solvent molecules due to which structural rearrangements take place. This depends on size and shape of molecules. The free volume plays an important role in ultrasonic wave propagation in liquids. The free volume of liquid molecules depends on particular temperature and pressure of the liquid at which it is measured. The free volume decreases with increases in temperature for butanol. These results will provide an additional information for future applications of n-Butanol with other mixture.

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