ISSN: 2277-9655
Scientific Journal Impact Factor: 3.449
(ISRA), Impact Factor: 2.114

IJESRT

INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY

Intermolecular Interaction in the Binary Mixture of valine with Water at 303.15 K

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Abstract

The ultrasonic velocity (u), density (ρ) and viscosity (η) have been measured at 2 MHz frequency in the binary mixtures of valine with water over entire range concentration at 303.15 K using ultrasonic interferometer technique. The experimental data have been used to calculate acoustical parameter namely adiabatic compressibility (β_a), acoustic impedance (z), intermolecular free length (L_f) and relative association (R_A) with a view to investigate the nature and strength of molecular interaction in the binary liquid mixture. The obtained result support the occurrence of complex formation through intermolecular hydrogen bonding in there binary liquid mixtures and further used to interpret the hydrophilic part of the solute and molecular interactions in the solutions.

Keywords- Ultrasonic Velocity(u), Binary Mixture, Molecular Interaction, Hydrogen Bonding.

Introduction

In recent year, the measurement of ultrasonic velocity has been adequately employed in understanding the nature of molecular interactions in pure liquids and liquid mixtures. The ultrasonic velocity measurements are highly sensitive to molecular interactions and can be used to provide qualitative information about the physical nature and strength of molecular interaction in liquid mixture [1-3].Ultrasonic velocity in a liquid is fundamentally related to the binding forces between the atoms or the molecules and has been adequately employed in understanding the nature of molecular interaction in pure liquids [4-8]. The variation of ultrasonic velocity and related parameters throw much light on the structural changes associated with the liquid mixtures having weakly interacting components as well as strongly interacting components. The acoustical study provides information about the intermolecular processes and structure of liquid state [9-11].

In the present study; we report the value of ultrasonic velocity, viscosity and density of 0.00 to 0.043 mole concentration of valine with water solution at 303.15K. The various physical and thermodynamic parameters like adiabatic compressibility (βa), acoustic impedance (z), intermolecular free length (L_f) and relative association (R_A) were calculated from ultrasonic velocity, viscosity and density data. All these parameters were discussed in term of solute – solvent interaction accruing in the binary mixture of valine and water.

Experimental section

Valine used in the present work was of Analytic Reagent (AR) grades with minimum assay of 99.9%, having specific conductivity ~ 10^{-6} S cm^{-1}. The stock solutions of 1M concentration were prepared by weighing the valine on a digital balance with an accuracy of ± 1 x 10^{-4} g. The various concentration of solution was prepared by adding sufficient amount of solvent water to valine. The solutions were kept in the special air tight bottles and were used within 12 hrs after preparation to minimize decomposition due to bacterial contamination.

Ultrasonic velocity was measured with a single crystal interferometer (F- 81, Mittal Enterprises, New Delhi) at 2MHz The interferometer was calibrated against the ultrasonic velocity of water used at T = 303.15K. The present experimental value is 1508.80 ms^{-1} which is in good agreement with literature value 1509.55 ms^{-1}. Accuracy in the velocity measurement was ± 1.0 ms^{-1}.

The density measurements were performed with recalibrated specific gravity bottle with an accuracy of ± $2x10^{-2}$ kg m^{-3}. An average of triple measurements was taken into account. Sufficient care was taken to avoid any air bubble entrapment.

Viscosity was measured with recalibrated Ostwald type viscometer. The flow of time was measured with a digital stop watch capable of registering time

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accurate to ± 0.1 s. An average of three or four sets of flow of times for each solution was taken for the purpose of calculation of viscosity. The accuracy of the viscosity measurements was ± 0.5 %. Accuracy in experimental temperature was maintained at ± 0.1K by means of thermostatic water bath. These basic parameter u, η, ρ were measured at 303.15K and at various concentrations (0.00M to 0.043M). The acoustical parameters were calculated from u, η, ρ value using standard formulae.

Results

From the measured values ultrasonic velocity(u), density(ρ) and viscosity (η) various acoustical parameters such as the adiabatic compressibility(β_a),acoustic impedance (z), intermolecular free length (L_f) and relative association (R_A) were calculated by using the following relations[12,13,14]

Ultrasonic velocity	$(u) = n\times\lambda$	(1)
Adiabatic compressibility	$(\beta_a) = 1/u^2\rho$	(2)
Acoustic impedance	$(z) = u.\rho$	(3)
Intermolecular free length	$(L_f) = K / u.\rho^{1/2}$	(4)
Relative association	$(R_A) = (\rho /\rho_o).(u_o / u)^{1/3}$	(5)

Where, K is the temperature dependant Jacobson constant.

Temp (T)	303	308	313
Kx10⁴	207.556 x 10^{-8}	209.431 x 10^{-8}	211.306 x 10^{-8}

Where, T is the absolute temperature,ρ_0, ρ and u_0, u are the density and ultrasonic velocity of solvent and solution respectively.

The experimentally measured values of ultrasonic velocity (u), density (ρ) and viscosity (η) of the solutions and calculated values of acoustical parameters such as adiabatic compressibility (β_a),acoustic impedance (z), intermolecular free length (L_f) and relative association (R_A) are reported in Table -1 for the binary mixtures of valine with water at 30.3.15K,

Table-1: Ultrasonic velocities, densities, viscosities, adiabatic compressibility's, acoustic impedances, intermolecular free lengths, relative association for valine +water at different temperatures with constant frequency 2MHz.

Water +Valine

m **mol kg^{-1}**	**u** **ms^{-1}**	**ρ** **Kg m^{-3}**	**η** **Nm^{-2}s**	**βx10^{-10}** **m^{2}N^{-1}**	**)$^{-6}$** **$^{-2}$**	**L_f** **A^0**	**R_A**
303.15K							
0.000	1508.80	997.2	0.9941	4.4051	1.50458	0.43562	1.00167
0.008	1510.18	1000	1.0098	4.3847	1.51018	0.43462	1.00418
0.017	1511.84	1002	1.0175	4.3664	1.51486	0.43371	1.00582
0.026	1516.16	1003	1.0277	4.3544	1.51770	0.43311	1.00653
0.034	1514.68	1004	1.0388	4.3413	1.52074	0.43246	1.00720
0.043	1516.30	1006	1.0510	4.3235	1.52540	0.43157	1.00885

Where m, mole fraction; ρ, density of the solution ; η,viscosity of solution; u, ultrasonic velocity;β, adiabatic compressibility; z, acoustic impedance; L_f, intermolecular free length; R_A, relative association.

Discussion

The increase in **density** with molal concentration suggest a solute-solvent interaction exist between the electrolytes and water .In other words the increase in density may be interpreted to the structure maker of the solvent due to H-bonding. Similarly, the decrease in density with concentration indicator structure-breaker of the solvent. It may be also true that solvent-solvent interactions bring about a bonding, probably H-bonding between them. So, size of the resultant molecule increases and hence there will be decrease in density.

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The **viscosity** is an important parameter in understanding the structure as well as molecular interaction occurring in the solutions. From above tables, it is observed that viscosity of the solutions shows a non-linear behavior in both the systems [13]. The increase in viscosity with concentration in all the systems suggests that the extent of complexation increase with increase in concentration.
The ultrasonic velocity (u) in aqueous amino acids at $2MH_z$ frequency, for different temperatures and various concentrations (m) have been determined using Eq. (1) and experimental values of u have been presented in Tables 1 (for the system water + valine). From the tables we observe the trends of all acoustical parameters with variation in concentration and temperature. The ultrasonic velocity increases with molal concentration of solute as well as rise in temperature.

In the binary liquid system of valine in water, the variation of ultrasonic velocity, adiabatic compressibility(βa) and acoustic impedance (Z) shows non linear variation with increase in molar concentration of valine This may be attributes to molecular association and complex formation .The complex formation and molecular association may be brought about through a hydrogen bonding possible between the molecules [15], which describe the structure making and breaking effect of the valine This also indicates the hydrophilic and hydrophobic nature of valine in water.
Ultrasonic velocity and acoustic impedance and relative association shows increasing trend with concentration,
whereas the **adiabatic compressibility** and **intermolecular free length** shows decreasing trend to the corresponding concentration. This shows the complex formation and molecular dissociation. It also indicates weakening of hydrogen bond at this molar concentration [16].This is because as the concentrations of solute increases, a larger portion of water molecules are electrostatic and the amount of bulk water decreases causing the compressibility to decrease[17]. The compressibility of a solvent is higher than that of a solution and it decreases with increase in concentrations.

Specific acoustic impedance is defined as impedance offered to the sound wave by the components of mixture. Mathematically it is directly proportional to ultrasonic velocity and inversely proportional to that of adiabatic compressibility and shows similar behavior to that of ultrasonic velocity and opposite to adiabatic compressibility. The non-linearly decrease impedance with molar concentration shows that molecular interaction in aqueous valine solution is dissociative [18].

Decreasing trend of **intermolecular free length** with concentration and temperature concluded that there is significant interaction between solute and solvent molecules due to which the structural arrangement is also affected. Thus it is clear from the above parameters that there is a strong association between water and amino acid molecules showing hydrophilic nature [19].

Relative Association (R_A) in aqueous amino acids at $2MH_z$ frequency, for different temperatures and various concentrations (m) have been determined using Eq. (5) the property which can be studied to understand the molecular interaction is the relative association (R_A). It is influenced by two factors: (i) Breaking up of the associated solvent molecules on addition of solute in it and (ii) The salvation of solute molecule[19]. The former leads to the decreases and later increases in concentrations From Tables 1(for the system water+ serine) it is observed that, R_A increases with increase in the solute concentrations and decrease with temperature. The graph for (R_A) versus mole fraction (m) of this systems were plotted as shown in Fig.5 This is due to salvation of solute molecules which also indicates the presence of molecular association between solute and solvent.

Conclusions

The nonlinear variation of ultrasonic velocity and other thermo acoustical parameters with molar concentration of valine in water provides useful information about the observed complex formation in the binary liquid mixture may be due to the formation of hydrogen bonding and the tendency of solute-solvent interaction.

Acknowledgement

One of the authors is thankful to the Head of the Dep't of Physics, Dr. BAMU, Aurangabad for providing necessary facilities, and Ms.Kalyani Bhate for helpful discussion.

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ISSN: 2277-9655
Scientific Journal Impact Factor: 3.449
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