iJRASET
International Journal For Research in Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 9 **Issue:** III **Month of publication:** March 2021

DOI: https://doi.org/10.22214/ijraset.2021.33182

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International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 9 Issue III Mar 2021- Available at www.ijraset.com

Ultrasonic Characterization of Ternery Liquid Mixtures of Sodium - 4-Amino- 2-Hydroxy Benzoic Acid in 50% Ethanol at Different Temperatures

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Abstract: ***Ultrasonic wave propagation in liquid has been the subjects of exhaustive research which has been carried out theoretically and practically. There are many approaches and spectroscopic techniques used to determine the structure-function relation of molecules. All these methods are very useful in studying the structures of the compound as well as physicochemical characters. Among the techniques used, ultrasonic velocity measurements through liquid medium gain much more importance in assessing the nature of molecular interactions. In the present investigation, experimental and theoretical study is carried out about the results of ultrasonic velocity (v), density (ρ) and viscosity (η), surface tension (σ) along with estimated parameters like hydration number, apparent molar volume (Φ_v) for the ternary liquid mixture of sodium salt of 4-amino, 2-hydroxy benzoic acid in 50% ethanol at 0.1M, 0.01M and 0.001M concentration range. The temperatures at which the study is carried out are 298.15K, 303.15K and 308.15K. The obtained results are used to discuss behavior of solute and molecular interactions in the solutions.***

Keywords: Ultrasonic velocity, Density, ultrasound velocity, surface tension, Molar cohesive energy and molar hydration number.

I. INTRODUCTION

There has been large number of studies done on the molecular interaction in liquid system. There are many approaches and spectroscopic techniques used to determine the structure-function relation of molecules. All these methods are very useful in studying the structures of the compound as well as physicochemical characters. Interactions between atoms, group of atoms, ions and molecules vary widely with respect to their bond strength to differentiate these classes known as bond types. These classes are well suited for the understanding and description of the majority of molecular systems. Therefore it is highly desirable to understand the molecular interactions involved in the formation of molecular complexes. Among the techniques used, ultrasonic velocity measurement through liquid medium is much more important to understand the nature of molecular interactions [1-5]. The number of researcher reported that [6-7] viscometric and ultrasonic sound velocity data furnish wealth of information about the interactions like solute-solute, solute-solvent etc. The number of water molecules that are in interaction with solute molecule is termed as hydration number[8]. The study apparent molar volume, molar cohesive energy and hydration number furnish a good data to study the liquid mixtures. Barnartt[9] and Passyanski A[10] have derived relations for the estimation of molar hydration number.

Among the number of techniques used to derive hydration number, a new method is introduced by Kalyansundaram S., Bhawanth R. and others [11-13]. Sodium-4-amino-2-hydroxy benzoic acid dihydrate is also called as para-amino salicylic acid (PAS) which was primarily used as an antibiotic to treat tuberculosis [14]. Its potency is less than that of the current five first line drug (Isoanizes, Rifampicine, Ethanbutol, Pyrazinamide and Streptomycin) for treating tuberculosis and its cost is higher, but it is still useful in the treatment of multidrug-resistant tuberculosis [15]. Due to insolubility of free acid, its sodium salt which is soluble in water is used in the present investigation. The main aim of the present study is to explore the molecular interactions exists between solute – solvent in ternaery liquid mixtures. For the present study, liquid mixture of Sodium-4-amino-2-hydroxy benzoic acid dihydrate in 50% ethanol as a solvent is selected. The measurements of ultrasonic velocity and density [16-17] and their derived acoustic and thermodynamic parameters like, apparent molar volume, surface tension, molar cohesive energy, hydration number [18-19] are useful and have wide applications in studying the physico-chemical behavior of solution mixture. All the measurements are taken at 298.15K, 303.15K and 308.15K temperatures.

ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
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II. EXPERIMENTAL SECTION

A. Materials

A.R. grade Sodium-4-amino-2-hydroxy benzoic acid dihydrate was used for investigation. All the solutions were prepared in distilled water. Weights have been taken on digital electronic balance. (Model-CB/CA/AT-Series).

III. METHODS

The ultrasonic velocity of different liquid mixture were measured by using ultrasonic interferometer (Model-M-83). Mittal Enterprises, New Delhi). The frequency was set at 4MHz frequency and the instrument work with an accuracy of ±2m/s. The measurements of densities (ρ) were carried out by using digital densitometer (Model - DMA-35, Anton Paar). The constant temperature was maintained by using thermostat with continuous circulation of water .

IV. RESULTS AND DISCUSSIONS

The measured values of ultrasonic velocity (v), density (ρ) are used to calculate molar hydration number, apparent molar volume , surface tension by using standard formulae [20] and are given in **Table No. 1**

Apparent Molar Volume

$$\phi_v = [1000(d_o-d_s)/C.d_o]+(M/d_o) \quad \text{--------- 1}$$

Where do – Density of solvent

Do – Density of solution, C- Molar concentration

Molar Hydration Number $h = n_w/n_s[1-(\beta_s/\beta_o)]$ ---------2

n_w – Number of moles of water, n_s – Number of moles of solute.

β_s – Adiabatic compressibility of solution.

β_o - Adiabatic compressibility of solvent.

Surface Tension $\sigma = 6.3 \times 10^{-4} \times V_s^{3/2} \times d_s$ ----------3

Molar Cohesive Energy $= \pi_i \times V_m$ ----------4

Table .1 : Apparent molar volume (ϕ_v), Molar hydration number, Surface Tension (σ) and Molar Cohesive Energy of sodium salt of 4-amino, 2-hydroxy benzoic acid

Sr. No.	Temperature(^{0}K)	Concentration (M)	Apparent molar volume (ϕ_v) (m^3/mole)	Molar hydration number (h)	Surface Tension (σ) Dynes/cm	Molar Cohesive Energy ($\pi i \times Vm$)/T Lit.atm/mole
1	298.15	0.1	4.53E+00	1.19E+01	5.63E+02	1.85E+05
2		0.01	2.47E+02	1.04E+02	4.03E+02	2.02E+05
3		0.001	-2.15E+03	1.04E+03	3.99E+02	2.10E+05
4	303.15	0.1	2.39E+00	1.32E+01	5.73E-04	1.50E+05
5		0.01	-4.08E+02	8.78E+01	2.97E+02	2.11E+05
6		0.001	-2.80E+03	1.10E+03	4.21E+02	1.93E+05
7	308.15	0.1	-1.06E+01	1.14E+01	4.36E+02	1.77E+05
8		0.01	-4.55E+02	1.11E+02	4.15E+02	1.82E+05
9		0.001	-3.36E+03	1.06E+03	3.69E+02	1.90E+05

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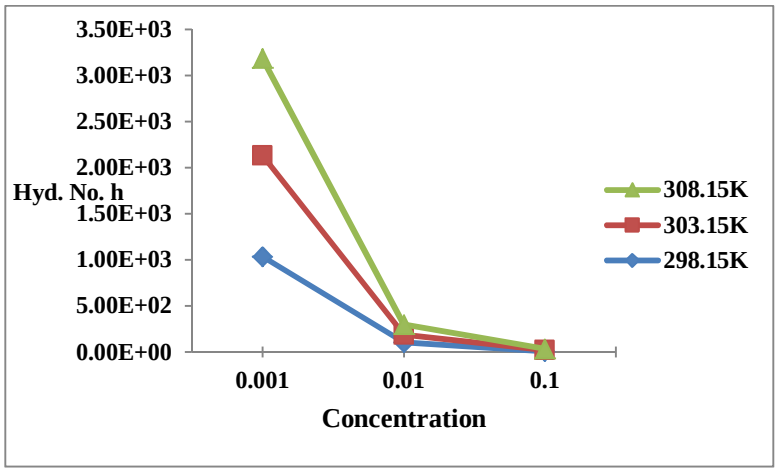

Fig.-1: Molar hydration number (h) Vs Concentration (sodium salt of 4-amino, 2-hydroxy benzoic acid)

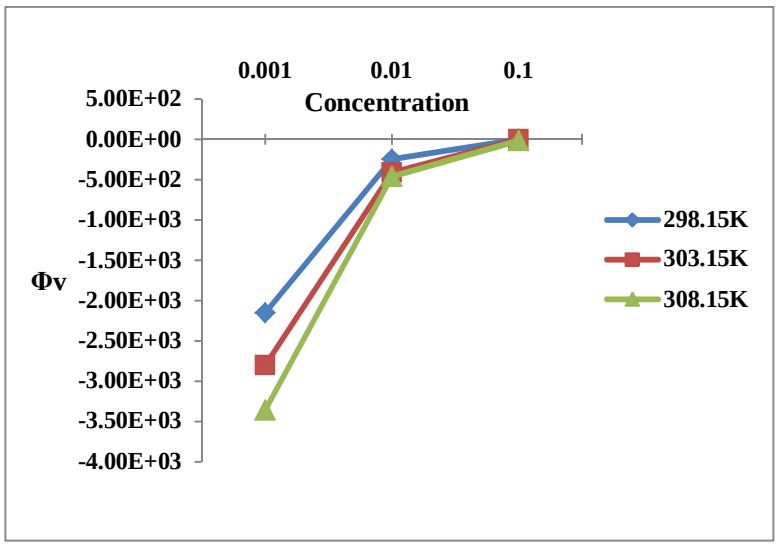

Fig.-2: Apparent molar volume (ϕ_v)Vs Concentration (sodium salt of 4-amino, 2-hydroxy benzoic acid)

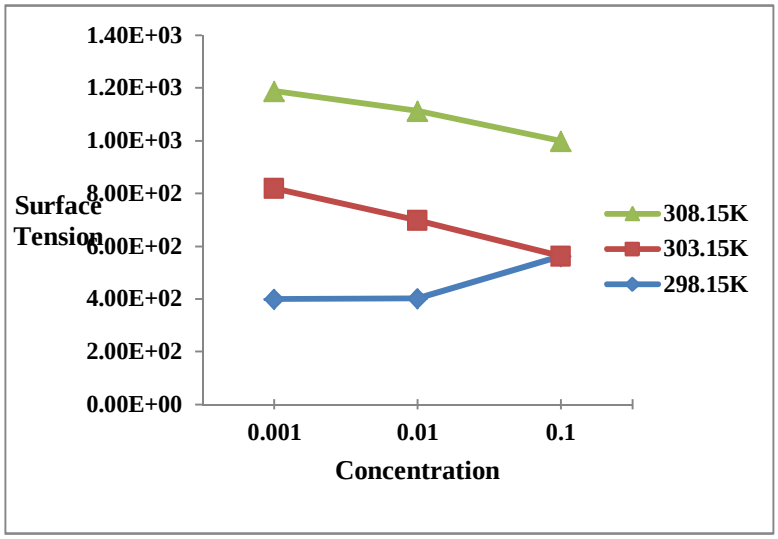

Fig.-3: Surface Tension (σ) Vs Concentration (sodium salt of 4-amino, 2-hydroxy benzoic acid)

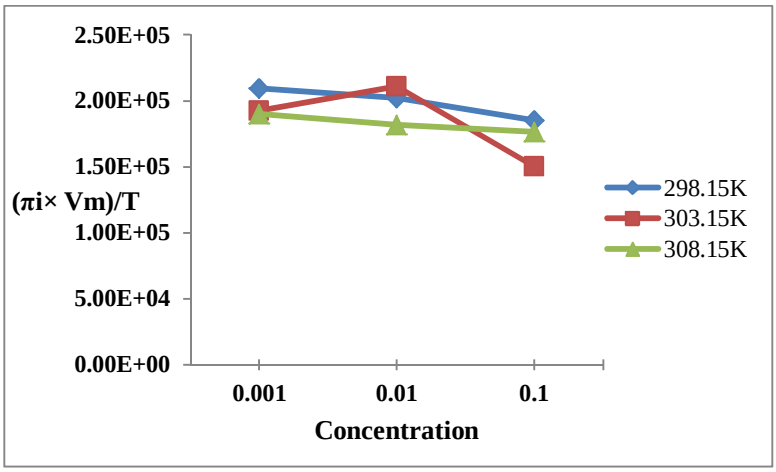

Fig.-4 : Molar Cohesive Energy Vs Concentration (sodium salt of 4-amino, 2-hydroxy benzoic acid)

The experimentally determined and calculated values of molar hydration number, apparent molar volumes, surface tension and molar cohesive energy are shown in Table – 1 and fig. 1, 2, 3 and 4. Molar hydration number shows linear variation with concentration. It decreases with increase in concentration (Fig.1). Molar hydration number shows positive values at all temperatures 298.15 K, 303.15K and 308.15K. The decrease in the values of molar hydration number with rise in concentration indicates that association of solute decreases with water[21]. It may be due to the presence of other polar solvent molecules of ethanol. There may be effect of ethanol molecules on the solvation process which is shown by the variation in the values of hydration number. The values of molar hydration number shows linear variation with temperature may be due to interaction of water and ethanol both molecules with solute molecules.

A linear variation of negative values of ϕ_v with respect to the solute concentration in all the liquid mixtures studied which indicates an existence of strong solute – solvent interaction[13]. The magnitude of ϕ_v, suggests that, strong molecular interaction are present in liquid mixtures. The calculated values of surface tension (σ) and molar cohesive energy barrier ($\pi_i V_m$) are plotted against the concentration shown in fig. 3 and 4. The linear relationship in the values of surface tension and molar cohesive energy is found at 308.15K. It is clear from our study that the quantitative relationship between surface tension and molar cohesive energy holds good for the liquid mixture at 303.15K. It may be said that molar cohesive energy of a liquid system (pure, binary or ternery) conditions surface tension and temperature characterize a liquid system fully[22-23]**.** It can be explained from above discussion that interactions of solute species takes place through destructive overlap of their hydration sphere[24] .

V. CONCLUSION

Sodium salt of 4-amino, 2-hydroxy benzoic acid molecule contains -NH2, - OH and – COOH groups which are hydrophilic groups. So, interaction between solute, water molecules and ethanol molecules complete through hydrophilic hydration. The interaction of hydrophilic hydration co-spheres releases some water molecules from the hydration sphere to the bulk results of an increase in volume with an increase in the concentration of 4-amino, 2-hydroxy benzoic acid. So all these variations focus towards the fact that molecular binding between solute ions and solvent molecules gets loosened with increase in concentration and liquid mixture is of structure breaking nature.

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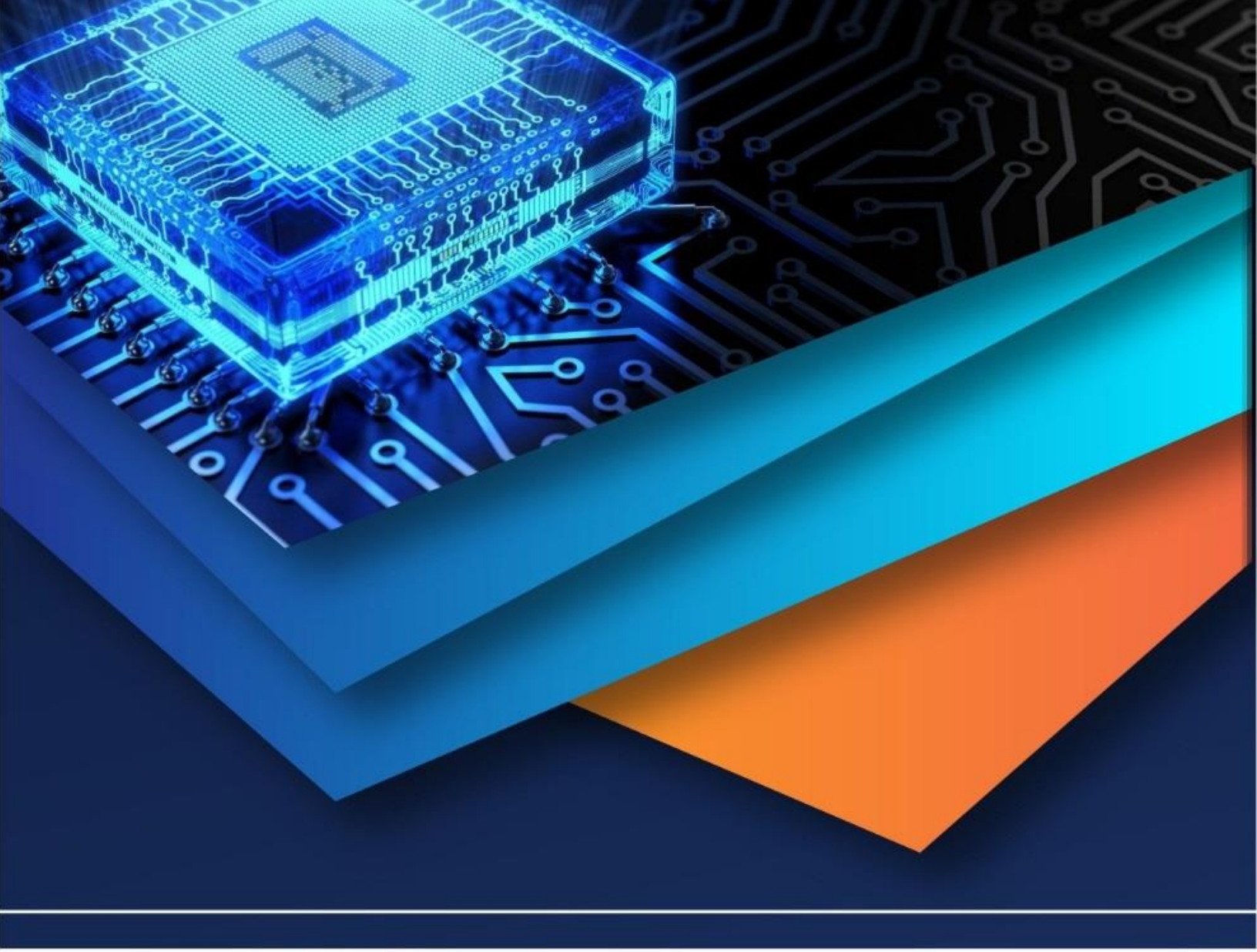

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