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Analysis of Thermodynamic Behaviour of Molecular Interaction in Protein (L-Histidine) and K_2SO_4 Solution at 283 & 293 K Temperatures Through Ultrasonic Tactic

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Abstract

It is very helpful to be able to predict different kinds of intermolecular interaction and the strength of the connection between the solute and solvent with thermo-acoustical and volumetric data. Protein and salts are two types of nutrients that are abundant in the human body. This study has examined a number of volumetric and thermo-acoustical properties of $C_6H_9N_3O_2$+H_2O and $C_6H_9N_3O_2$+H_2O+K_2SO_4 systems' attributes. With ultrasonic velocities (U) and densities (ρ) of 0.02 – 0.2 mol-kg^{-1} concentration of protein ($C_6H_9N_3O_2$) in water and 0.1 mol-kg^{-1} concentration of aqueous potassium salt. The novelty of this tactic is that it exhibits biological and technical applications by observing the pattern of interaction between the protein and salt molecules, which will assist to build more effective future solutions.

Keywords: Potassium sulphate; Velocity; Density; Thermo-acoustical characteristics; Protein.

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1. Introduction

Several investigations have used ultrasonography to investigate the amino acids' thermos-acoustical properties [1-8]. Ultrasonic approach is a versatile, non-destructive technology that anticipates the intermolecular interaction in the binary mixture and acts as a potent probe to access the acoustic characteristics [9,10]. Measurements of the ultrasonic velocity of an aqueous solution of amino acids including electrolyte and non-electrolyte are beneficial in revealing the behavior of the liquid system, intermolecular interaction, complex formation, and related structural alterations [11]. Studying amino acids is a useful method since these are the components that make up proteins. [12] belong to a large biomolecule family. The human body uses amino acids to make protein, which is necessary for a number of other biological functions. Amino acids can be classified as essential, non-essential, or conditional. Human bodies produce conditional and non-essential amino acids; they do not come from diet. But the body is unable to synthesize vital amino acids, thus one must get them from diet. Just nine of the 22 distinct types of amino acids are thought to be

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essential [12]. In this study, we additionally provide L-Histidine, one of the most crucial amino acids that is necessary. It contributes to variety of metabolic processes in the body. Its absence results in a drop in blood pressure. The human body has to have a healthy amount of histidine in order to maintain a rigid blood pressure level. Numerous vital minerals- which are classified into two groups: major minerals (such as Na, K, etc.) and micro minerals (such as Fe, Si, etc.) – are needed by human body. Compared to the former, the latter is needed in less quantities. K is an extremely vital mineral for the body that is necessary for electrical and cellular function. It is one of the primary "electrolytes" in blood [13]. The treatment of hypokalemia or sustaining the body's optimal potassium levels can be achieved by using the binary mixture of L-histidine and potassium salt potassium sulphate (K_2SO_4) as an ionic solvent in this study. Potassium is an essential mineral that is vital to controlling the heart's beating. However, deficiencies in potassium can result in hypokalemia.

In an attempt to lower the risk of hypokalaemia and maintain blood pressure levels in the body, the current study aims to perform a physicochemical evaluation of the interactional behaviour of L-histidine amino acid with aqueous potassium solvent (K_2SO_4) solutions at concentrations of 0.02-0.2 mol/kg and temperatures of 283 and 293 K. Modifying these characteristics at a molar concentration could be helpful for the pharmaceutical and food industries to offer a variety of therapeutic doses, solutions, tablets, capsules, gels, and injections in solution form [13]. The results of the experiment have led to the calculation of several parameters that are relevant to thermo-acoustics: surface tension, adiabatic compressibility, non-linearity parameter, specific heat ratio, relaxation strength, and acoustic impedance [14]. The results and concentration effect of additions are expected to give details about how potassium salt affects the stability of amino acids [14]. Examining the combined properties of both systems (L-histidine + water and L-histidine + water + potassium sulphate) is essential due to their diverse range of applications. A survey of the literature suggests that no such studies have been done up to this point. As a result, this study found that two of the most important tools for analysing the volumetric and acoustic features of the solute–solvent interaction inside a liquid system are the mixed mixture's density and sound speed [15]. These volumetric and thermoacoustic properties exhibit concentration-dependent change, which strongly implies the presence of molecular connections in all systems. L-histidine, an amino acid, interacts more strongly with potassium sulphate, while at greater concentrations, it has orders of magnitude more molecular interactions in both solvents. Thus, it appears that L-histidine molecules attach to K_2SO_4 molecules more readily than they do to water molecules [16]. At higher temperatures, there is a correlation between bigger mass fractions and increased solute and solvent interaction.

After all of these aspects were investigated in relation to solute-solvent and solute-solute interactions amongst the different ionic liquid components, the amino acid ($C_6H_9N_3O_2$) was investigated in these experiments. Variation in the different parameter for the different mixtures is indicative of the nature of interaction between the component in the liquid mixture. Understanding the biochemical process's nature and the structural

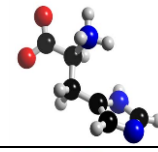
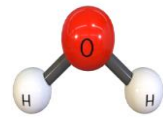
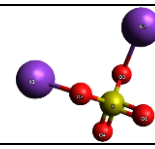
consequences of the biophysical traits inside the body system is largely dependent on this research [17].

2. Components and Procedure

2.1. *Components*

The compounds shown in the Table 1 are AR grade compounds with a purity mass fraction of 99.8 %. They were purchased from Himedia Pvt. Ltd. in Mumbai and used in the current study without any further raffination.

Table 1. Everything related to material.

Sr. No.	Compound	Solute and solvent	Salts and amino acids	Chemical formula	Molecular mass (g/mol)	C.A.S number	Structure
01	L-Histidine	Solute	Crucial amino acid	$C_6H_9N_3O_2$	155.16	71-00-1	
02	Water	1st Solvent	All-purpose solvent	H_2O	18.015	_____	
03	Potassium Sulphate	2nd Solvent	Ionized salt	K_2SO_4	74.120	7778-80-5	

2.1. *Method*

In this work, a solute and solvent were utilized to produce the solution, and an average concentrations of 0.02, 0.04, 0.06, 0.08, 0.1, 0.12, 0.14, 0.16, 0.18 and 0.2 mol/kg^{-1} were reported at two distinct temperatures of 283 K and 293 K, controlled via a digital water bath with an accuracy of ±1 K. The weight was determined with an accuracy of ±0.0001 g utilizing a computerized weighing device. For determining the ultrasonic velocity, we can use a digital ultrasonic interferometer operating at a frequency of 2 MHz, which is from Vi Microsystems Private Limited, Chennai whose overall operating accuracy is 0.0001m/s. The cell used for ultrasonic wave in the quartz crystal is generated by a radio frequency oscillator. In order to determine the densities of solutions, the 10ml specific gravity bottle was used whose accuracy is ±2×10^{-3} Kg/m^3. Using the gathered data of ultrasonic velocity and density, various Thermo-acoustical metrics have been calculated using following defining relations.

2.3. *Defining relations*

Using density and ultrasonic velocity data in conjunction with a formula, the aforementioned volumetric and thermal acoustical parameters were calculated.

1. Adiabatic compressibility (β): $\beta = \frac{1}{\rho * U^2}$ ----------[18]
2. Acoustic impedance (Z): $Z = \rho U$ ----------[18]
3. Relaxation strength (r): $r = 1-(\frac{U}{U_\infty})^2$ ----------[19]
4. Surface tension (σ): $\sigma = (6.3*10^{-4})\rho U^{3/2}$ ----------[19]
5. The Non-linearity parameter(B/A_1): $(B/A_1) = \{2+[\frac{0.98*10^4}{U}]\}$-----[20]
6. Specific heat ratio (γ): $\gamma = \frac{17.1}{T^{\frac{4}{9}} * \rho^{1/3}}$ ----------[20]

3. Procuring and Discussion

The empirically estimated density and ultrasonic velocity of distilled water at various temperatures are shown in Table 2. It compares favorably with published/literature data and observational data.

Table 2. Freshly distilled water at 283 and 293 K ultrasonic velocities and densities.

(T) K	Gathered information		Data from the literature	
	U. Velocity	Density	U. Velocity	Density
283	1447.427	999.700	1448.16 [21]	999.891 [21]
293	1481.496	998.200	1482.63 [22]	998.202 [22]

3.1. *Ultrasonic velocity (U)*

A key physical metric with structural relationships is ultrasonic velocity. The ultrasonic velocity of the necessary amino acid histidine varies with concentration, ranging from 0.02-0.2 mol/kg. In the current experiment, K_2SO_4 0.1 M solutions of the electrolyte salt solvents were examined at different temperatures (i.e., 283 and 293 K). Fig. 1 and Table 3 display the acquired data, which demonstrate that ultrasonic velocity rises when temperature and concentration both rises. The concentration and temperature of the system have an impact on the ultrasonic velocity. The expansion of the particle association among the medium's constituents with increasing ultrasonic velocity is seen, and is attributed to molecular contact. [23,11].

3.2. *Density (ρ)*

Density is one significant physicochemical property that depends on temperature and pressure. The concentration-dependent increase in density, which indicates a rise in solute-solvent interaction while a drop in density indicates a fall in solute-solvent interaction, may also be used to explain the density of a solute-solvent contact metric. The volume

contraction brought on by the presence of solute molecules is what causes the density to increase with concentration. According to one interpretation of the data in Fig. 2 [24], the solvent is becoming more structured as a result of the solute addition, as indicated by the growing density value in the current investigation.

3.3. *Adiabatic compressibility (β)*

The solute's β may be determined by squeezing the quantity of hydration surrounding its molecule. The molar concentration of the amino acid ($C_6H_9N_3O_2$) and the amount of aqueous K_2SO_4 (solvent) are found to decrease with an increase in the value of adiabatic compressibility (β), as seen in Table 3. As Fig. 3 illustrates, the observed decrease in the solvent's adiabatic compressibility might potentially be attributed to the weakening of the hydrogen bond within the solution. Certain solvent molecules become attached to an ion during the solute's dissolution in the solvent. This is known as the ion-solvent interaction. [11,25].

3.4. *Acoustic impedance (Z)*

The acoustic impedance rises as the amount of $C_6H_9N_3O_2$ solution, as seen in Fig. 4. This is because the complex that develops in its solution (($C_6H_9N_3O_2$) + water + K_2SO_4) alters the acoustic impedance value by causing the relative velocity of the particle to increase and fall. Therefore, an increase within certain ranges in any type of solution indicates a stronger bond between the constituent elements of the combination. Table 3 [26] shows that particles move more thermally at higher temperatures, which also causes an increase in their acoustic impedance value.

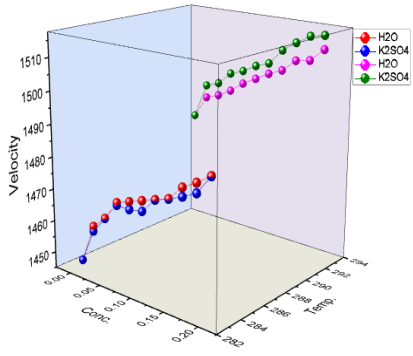


Fig. 1. Variation of velocity with concentration and temperature

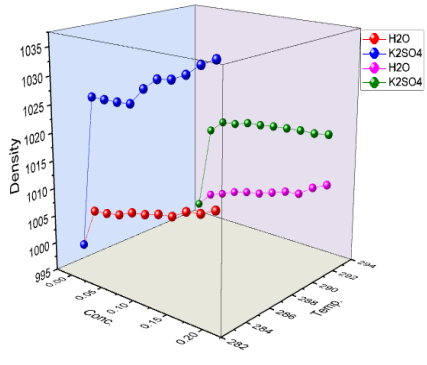


Fig. 2. Variation of density with concentration and temperature.

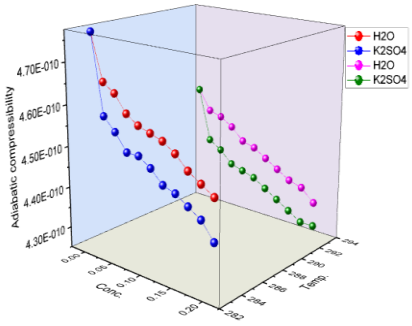


Fig. 3. Variation of adiabatic compressibility with concentration and temperature.

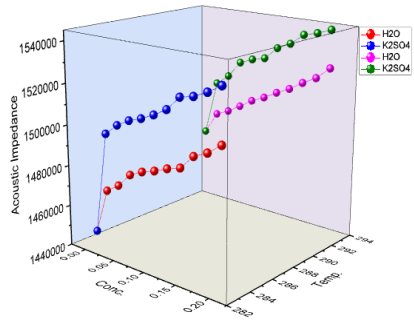


Fig. 4. Variation of acoustic impedance with concentration and temperature.

3.5. *Relaxation strength (r)*

The strength of relaxation diminishes as concentration and temperature rise shown in Fig. 5. L-Histidine + potassium sulphate + water has more benefits than L-Histidine + water on its own. The more thorough finding suggests that compared to the aqueous systems, the molecular bonds between L-histidine, potassium sulphate, and water are stronger [27].

3.6. *Surface tension (σ)*

This measure is used to analyze the surface composition of the mixture's aqueous solution. These factors were used to gauge the strength of the solution's intermolecular interactions. The surface tension in the solution depicted in Fig. 6 rises in a pattern that suggests a strong correlation when the solute is added to the experimental solvent [28].

3.7. *Non-linearity parameter (B/A)*1

A closer look at Fig. 7 also shows that there is a little rise in Balizar's non-linear parameter (B/A) 1 for the two systems under consideration: L-Histidine + water and L-Histidine + water + potassium sulphate. Anharmonicity and the intermolecular mode of vibration of the study system are demonstrated to be less common, and a growth in the value of the Balizar non-linear parameter, as presented in Table 4, further indicates the existence of weak contact forces and associating tendencies [27].

3.8. *Specific heat ratio (γ)*

Based on the liquid's specific heat, heat is required for every degree of temperature increase. Fig. 8 illustrates how the specific heat ratio varies for various amino acid weight fractions (0.02-0.2mol-kg-1). The temperature is increasing and the heat capacity ratio (ɗz) is decreasing when amino acids are introduced to both clean water and an aqueous salt

solution. These results for the specific heat ratio offer compelling evidence that an increase in L-Histidine concentration corresponds to an increase in density [28].

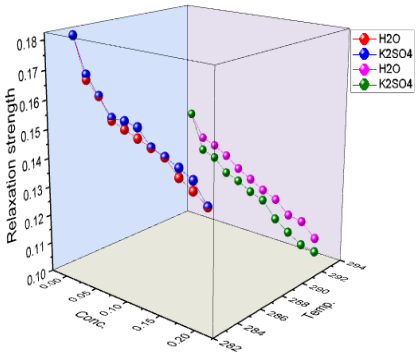


Fig. 5. Variation of relaxation strength with concentration and temperature.

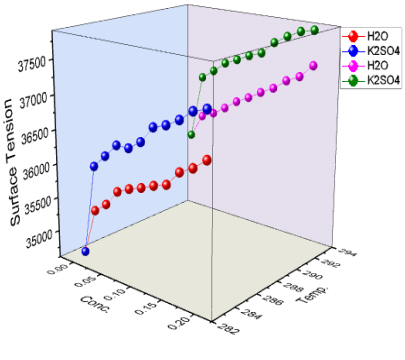


Fig. 6. Variation of surface tension with concentration and temperature.

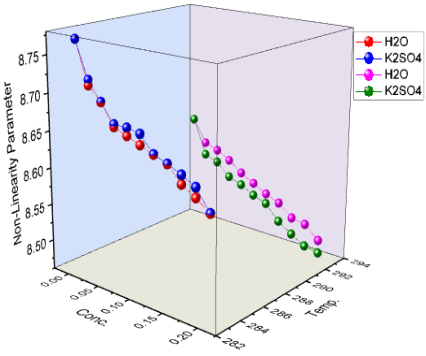


Fig. 7. Variation of non-linearity parameter with concentration and temperature.

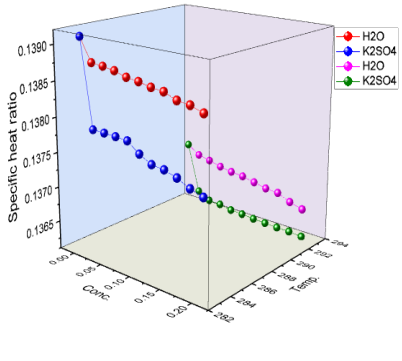


Fig. 8. Variation of specific heat ratio with concentration and temperature.

4. Conclusion

The L-Histidine – K_2SO_4 interaction in aqueous solution is sufficiently covered by the current work on amino acid–salt interaction. Future biological and technical applications will benefit from studying the pattern of interaction between the amino acid and salt molecules, which will assist to build more effective future solutions. When the binary combination (L-Histidine + water + K_2SO_4) is at temperature (283 and 293 K) and concentration (0.02-0.2 mol/kg), density and ultrasonic velocity define different thermos-acoustic characteristics. The aqueous liquid mixture also exhibits substantial intermolecular interaction. The system including potassium salt and aqueous amino acid exhibits high intermolecular H-bonding, as demonstrated by the experimental results. Higher concentrations have an extremely strong H-bonding interaction, as seen by the acoustical

parameter. Despite the fact that the solute-solvent interaction is larger than the solvent-solvent interaction, the observed and computed acoustical parameters interactions between the solvent and the solute are expected. The intensity of the intermolecular contact is shown to grow as L-histidine concentration rises, indicating a solute-solvent interaction. It follows that measuring the ultrasonic velocity in the specified media is a useful tool for determining the physico-chemical characteristics of the medium.

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