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Thermo-acoustic analysis of Molecular Interaction in L-Histidine and K_2SO_4 Solution at 283 & 293K Temperatures Using Ultrasonic Studies

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ABSTRACT

Predicting various types of intermolecular interactions and the strength of the bond between the solute and solvent using thermos-acoustical and volumetric data is highly useful. Salts and amino acids are two types of nutrients that are plentiful in the human body. Several properties of histidine+H_2O and histidine+H_2O+K_2SO_4 systems, both volumetric and thermos-acoustical, have been investigated in this work. Thermodynamic L-histidine ($C_6H_9N_3O_2$) studies have been conducted in an ionic salt (K_2SO_4) solution at two different temperatures. $C_6H_9N_3O_2$ has been examined at several mass fraction ranges in water and aqueous potassium salt solution (K_2SO_4), with ultrasonic velocities and densities of 0.1 mol/kg (i.e., 0.02 – 0.2 mol/kg). Utilizing ultrasonic velocity and density data, various thermos-acoustical features have been identified, including surface tension, adiabatic compressibility, non-linearity parameter, specific heat ratio, relaxation strength, and acoustic impedance. A study has been carried out to investigate the physicochemical behavior and nature of the interaction of L-Histidine in potassium salt (K_2SO_4) water-based solutions at two different temperatures (283 and 293 K). Numerous intermolecular interactions between various component mixes at various mass fractions have been interpreted in the current investigation of the binary system (potassium sulphate + histidine). Based on the whole scenario, we can also infer that higher mass fractions at higher temperatures are associated with greater interactions between the solute and solvent. Consequently, figuring out the medium's physical and chemical properties (as depicted in Fig. a) can be accomplished by measuring the ultrasonic velocity in the designated media.

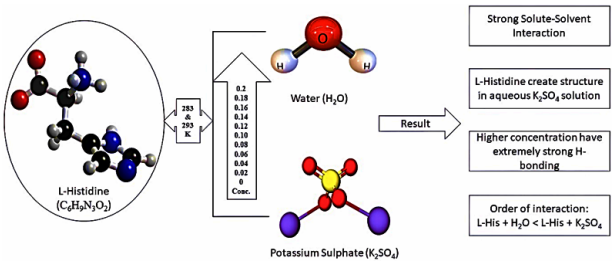


Fig. (a) Graphical Abstract

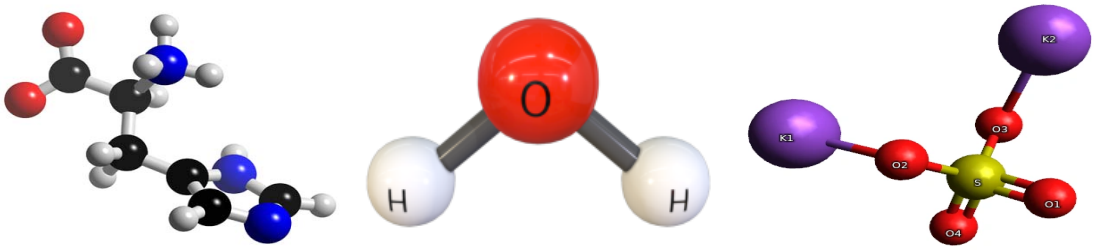
Keyword: Potassium sulphate, Velocity, Density, Thermos-acoustical characteristics, Ionic salts, and L-histidine

INTRODUCTION

Ultrasonography has been utilized in several studies to examine the thermos-acoustical characteristics of amino acids[1–8]. The ultrasonic technique is a flexible, non-destructive technology that serves as a strong probe to access the acoustic properties and predicts the intermolecular interaction in the binary mixture[9,10]. An aqueous solution of amino acids, containing both electrolyte and non-electrolyte, can be subjected to ultrasonic velocity measurements to learn more about the behavior of the liquid system, intermolecular interactions, complex formation, and associated structural modifications[11]. Since they constitute the components of proteins, studying amino acids is a helpful approach.[12] Belonging to a broad family of biomolecules. The body uses amino acids to make protein, which is essential for many other biological processes. It is possible to categorize amino acids as conditional, non-essential, or essential. Conditional and non-essential amino acids are produced by the human body; they are not obtained from diet. However, necessary AA must be obtained from the diet because the body is unable to manufacture them. Of the 22 distinct forms of AA, only nine are considered essential[13]. We also include L-histidine in our study, which is one of the most important amino acids. It supports a range of bodily metabolic functions. Blood pressure drops when it is absent. A healthy level of histidine is necessary for the human body to sustain a stable blood pressure level. The binary combination of L-histidine and potassium salt potassium sulphate (K_2SO_4) as an ionic solvent in this study can be used to treat hypokalaemia or maintain the body's appropriate potassium levels. One necessary component for regulating the heart's rhythm is potassium. However, hypokalaemia can be brought on by potassium deficits. A physicochemical assessment of the interactional behavior 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 is the goal of the current study. This will help to maintain blood pressure levels in the body and reduce the risk of hypokalaemia. For the pharmaceutical and food sectors to provide a range of therapeutic dosages, solutions, tablets, capsules, gels, and injections in solution form, it could be beneficial to modify these properties at a molar concentration[14]. The experiment findings have prompted the computation of several thermo-acoustically significant parameters, including relaxation strength, specific heat ratio, adiabatic compressibility, surface tension, non-linearity parameters, and acoustic impedance[15].

It should be possible to learn more about how potassium salt impacts the stability of amino acids from the findings and the concentration effect of additions. In[16]. Given the wide range of applications for both systems (L-histidine + Water & L-histidine + Water + Potassium Sulphate), it is imperative to investigate their combined characteristics. A review of the literature indicates that there haven't been any of these investigations completed yet. Thus, the density and sound speed of the mixed mixture are two of the most crucial parameters to analyze when examining the volumetric and acoustic aspects of the solute–solvent interaction inside a liquid system[17]. There is a concentration-dependent shift in these volumetric and thermoacoustic characteristics, which strongly suggests that these systems have molecular linkages. At higher concentrations, L-histidine exhibits orders of magnitude more molecular interactions in both solvents and interacts more strongly with potassium sulphate. Hence, it seems that K_2SO_4 molecules are more likely to bind to L-histidine molecules than they are to water molecules[18]. Greater solute and solvent interaction are correlated with larger mass fractions at higher temperatures. Following the examination of these factors concerning interactions between the various components of ionic liquids, both solute-solvent and solute-solute, the amino acid ($C_6H_9N_3O_2$) was examined in these tests. The biochemical process's nature and its structural ramifications of the biophysical characteristics inside the body system are mostly dependent on this study.[19]

EXPERIMENTAL AND MATERIALS



(a) L-Histidine (b) Water (c) Potassium Sulphate

Fig. (b). Structural 3D diagram of L-Histidine, water and potassium sulphate

Table 1(a): Attributes of Chemicals

Chemicals	CAS No.	Origin	Mol. Wt.	Mass Fraction Purity
Solute: L-Histidine	71-00-1	Hi. Media. Pvt. Limited	155.16	≥0.099 %
Solvent.1- Water	----------		18.015	
Solvent.2- Potassium sulphate	7778-80-5		74.120	

Synthesis

For the preparation of following systems:

System 1: H_2O + L-Histidine

System 2: H_2O + L-Histidine + Potassium Sulphate

We used, the mass fraction method. According to the mass fraction formula weight of corresponding substance can be easily determined.

$$\text{Weight of Substance} = \frac{\text{Molecular Weight} \times \text{Molality} \times \text{Volume}}{1000} \quad (1)$$

The following amount of weight obtained in grams for different concentrations of materials which we had to be synthesized as described in Table 1(b).

Table 1(b): Calculated amount of substance as per formula(1)

Substance/Chemicals	Molecular Weight (mol/kg)	Volume (mL)	Molality (mole)	Weight of Substance (g)
Solute (L-Histidine)	155.16	50 mL	0.02	0.1551
			0.10	0.7758
			0.20	1.5516
Solvent (Potassium Sulphate)	74.120	550 mL	0.10	4.0766

After weighing the amount of solute and solvent, a stock solution of solvent is prepared by adding 4.0766 g of Potassium Sulphate in 550 mL of double distilled water. Later different solute concentrations (0.02-0.2 mol/kg) of solution synthesised using 50-50 mL of stock solution by adding various amount of solute. And then this solution characterized by using ultrasonic interferometer.

Apparatus

- **Ultrasonic Digital Interferometer:** Operating at 2 MHz frequency.
- **Computerized Water Bath:** To maintain temperatures of 283K and 293K with an accuracy of ±1K.
- **Automated Scale:** For precise weight measurements (±0.0001 g).
- **10 mL Density Container:** To measure solution density (±2 × 10^{-2} kg/m^{-3}).

Procedure

Preparation of Solutions

(a) Prepare a series of solutions with molal 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.

(b) Accurately weigh the solute using the automated scale to ensure precision in molality.

Temperature Regulation

(a) Set the computerized water bath to 283 K and allow the solutions to equilibrate at this temperature.

(b) Repeat the process for 293 K, ensuring that each temperature is stable before conducting measurements.

Density Measurement

(a) Use the 10 mL container to measure the density of each solution. Fill the container with

the prepared solution and record the mass to calculate density.

Ultrasonic Velocity Measurement

(a) Place the solution in the ultrasonic digital interferometer.

(b) Measure the ultrasonic velocity with a precision of ±0.0001 m/s at both temperatures for each concentration.

(c) Ensure that the quartz crystal in the interferometer is properly calibrated and functioning.

Data Collection

(a) Record the ultrasonic velocity, temperature, and calculated density for each concentration at both temperatures.

Thermo-Acoustical Calculations

(a) Utilize the collected data along with pre-existing relations to compute additional thermos-acoustical parameters, such as adiabatic compressibility and other relevant properties.

Data Analysis

- Analysed the relationship between ultrasonic velocity, concentration, and temperature.
- Plot graphs to visualize trends and derive any correlations.

Defining relations

The previously described volumetric and thermal acoustical characteristics were computed using density and ultrasonic velocity data together with a formula that has been identified in the literature.

Relative association (RA): = $\{(\frac{\rho}{\rho_0})(\frac{U_0}{U})^{1/3}\}$[20]

Intermolecular free-length (L_f): = K $(\beta)^{1/2}$ [21]

Isothermal compressibility (kT_1) = $\frac{1.33*10^{-8}}{(6.4*10^{-4}*U^{\frac{3}{2}}\rho)^{3/2}}$[22]

Isothermal compressibility (kT_2): = $\frac{17.1*10^{-4}}{T^{4/9}*U^2*\rho^{1/3}}$ [23]

RESULTS AND DISCUSSION

The following data table displays the ultrasonic velocity and density of distilled water at different temperatures, which are calculated empirically. It performs well in comparison to observational and published/literature data.

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

Temperature (T)K	Gathered information		Data from the literature	
	U. Velocity	Density	U. Velocity	Density
283	1447.427	999.700	1448.16[24]	999.891[24]
293	1481.496	998.200	1482.63[25]	998.202[25]

Ultrasonic velocity (U)

Ultrasonic velocity is an important physical measure having structural links. The required amino acid histidine's ultrasonic velocity ranges from 0.02-0.2 mol/kg depending on concentration. K_2SO_4 0.1M solutions of the electrolyte salt solvents were investigated in the current experiment at two distinct temperatures (283 and 293K). The obtained results are shown in Fig. 1, which show that ultrasonic velocity increases as temperature and concentration grow. The ultrasonic velocity is dependent on the concentration and temperature of the system. Molecule interaction is responsible for the observed expansion of the particle association among the medium's constituents with increased ultrasonic velocity[26,11].

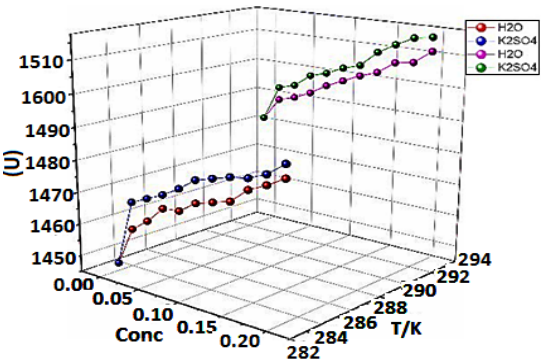


Fig. 1. Variation of Velocity with Concentration

Density (ρ)

One important physicochemical property that is dependent on both pressure and temperature is density. The density of a solute-solvent contact metric can instead be explained by the concentration-dependent increase in density, which denotes a rise in solute-solvent interaction and a decline in solute-solvent interaction, respectively. Concentration-related increases in density are caused by the volume contraction that solute molecules produce. The increasing density value in the current experiment suggests that the solvent is getting more structured as a result of the solute addition, which is consistent with one interpretation of the data in Figure 2[27].

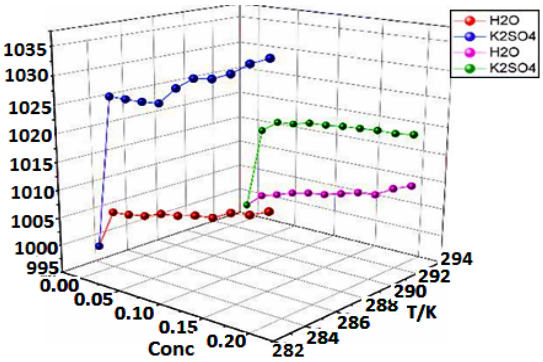


Fig. 2. Variation of Density with Concentration

Relative Association

Another important property that may be investigated to understand the interactions between a solution and its solute is relative association (RA). It is influenced by two factors: (i) the solvation of the solute molecules and (ii) the dissolution of the associated solvent molecules with the addition of a solute. The latter results in an increase in RA, whilst the former produces a decrease in RA. According to Fig. 3 from the current experiment, at 283K and 293K, RA reduces linearly with increasing solute concentration, suggesting that molecule-to-molecule dissociation occurs in all solvent systems following solute addition[28].

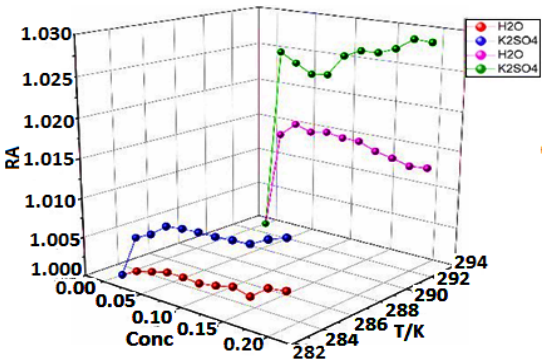


Fig. 3. Variation of Relative Association with Concentration

The free length between molecules (L_f)

There is no linearity in the adiabatic compressibility values due to the intermolecular free length. This indicates that there are some interactions between electrolyte salt solutions and niacin[29]. In the present binary combination, the intermolecular free length increases with increasing temperature Fig. 4. The possibility that this is because thermal energy rises with temperature suggests that related molecules in the liquid mixture might break their bonds and migrate apart, decreasing contact and perhaps weakening cohesive forces. Furthermore, when heat energy increases, molecules go further apart and the entropy of their structural arrangement increases as well, both of which tend to lessen intermolecular interactions[30].

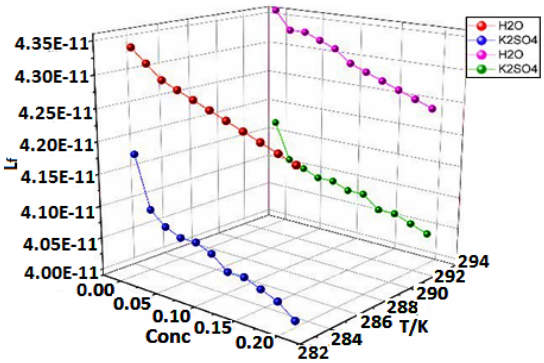


Fig. 4. Variation of Intermolecular Free Length with Concentration

Isothermal compressibility (kT)

The whole isothermal compressibility (kT) pattern ($C_6H_9N_3O_2$) is displayed using the results of the isothermal compressibility technique developed by MC Gowan (kT1) in Fig. 5 and Pandey *et al.,* Fig. 6 illustrate the kT2 approach. The concentration and temperature of water and potassium salts cause a decrease in L-histidine (0.1 mol/kg). This declining trend indicates that the free volume has dropped[31]. The behavior of L-histidine as its concentration ($C_6H_9N_3O_2$) increases at two different temperatures is depicted visually in Fig. 5-6. The patterns of this parameter indicate that the value falls as the amino-acid content increases. This demonstrates how the fluidity of the solution has decreased due to increased contact between the molecules of the solute and the solvent[32].

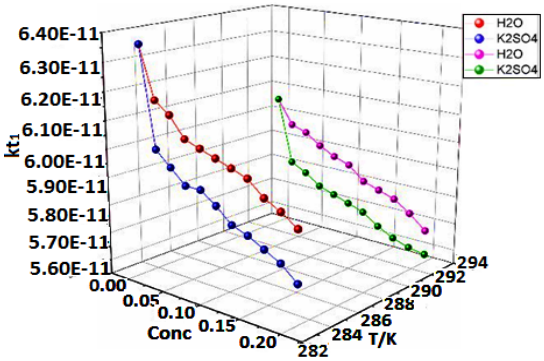


Fig. 5. Variation of Isothermal compressibility (kT1) with Concentration

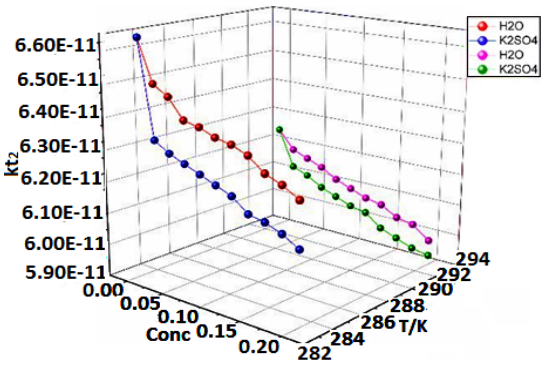


Fig. 6. Variation of Isothermal compressibility (kT_2) with Concentration

CONCLUSION

The present research on the interaction between amino acids and salts adequately covers the L-Histidine –K_2SO_4 in aqueous solution. Studying the pattern of interaction between the salt and amino acid molecules can help to develop more efficient future solutions, which will be beneficial for biological and technology applications in the future. Different thermos-acoustic properties are defined by density and ultrasonic velocity when the binary combination (L-Histidine + water + K_2SO_4) is at temperature (283 & 293K) and concentration (0.02-0.2 mol/kg). Significant intermolecular interaction is also seen in the aqueous-liquid combination. The experimental results show that the combination including potassium salt and aqueous amino acid has significant intermolecular H-bonding. The acoustical parameter indicates that the H-bonding interaction is highly strong at higher concentrations. The observed and computed acoustical parameters interactions between the solvent and the solute are predicted, even though the solute-solvent interaction is greater than the solvent-solvent interaction. As the concentration of L-histidine increases, the strength of the intermolecular contact increases, suggesting a solute-solvent interaction. Consequently, figuring out the physicochemical properties of the medium may be done with the help of monitoring the ultrasonic velocity in the designated media.

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Conflicts of interest

None of writers have any conflict of interest.

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