A Study to Exhibits Physico-chemical Behavior of L-Histidine in Aqueous Saccharide Solutions: A Thermo-acoustical Approach

Pooja R. Sonune*, Urvashi P. Manik, and Paritosh L. Mishra
*S. P.College, Chandrapur, Maharashtra, India.

Abstract

Maintaining a healthy B.P. (Blood Pressure) and B.G. (Blood Glucose) level in the human body requires amino acid (L-Histidine) and Saccharides (Glucose and Fructose). In view of this scenario, an attempt has been done to investigate the nature of interaction and physicochemical behavior of L-Histidine in aqueous solutions of Saccharide at the temperature of 288 and 298K. The density and ultrasonic velocity of an L-Histidine of concentrations (0.02, 0.04, 0.06, 0.08, 0.1, 0.12, 0.14, 0.16, 0.18 & 0.2M) in 0.1M saccharide solution (glucose and fructose) at different temperatures were measured experimentally. From the aforementioned experimental results, the various thermo-acoustic parameters (viz. adiabatic compressibility, acoustic impedance, relative association, relaxation strength, isothermal compressibility, surface tension, non-linearity parameter & specific heat ratio) have been explored. Additionally, these parameters allow for interactions between solutes, solvents, and ions. The current investigation of the binary system (L-histidine + glucose/fructose) interpreted many types of intermolecular interactions between various mixtures of components at various mass fractions of components. And based on the overall scenario, we may infer that higher mass fractions at higher temperatures are associated with stronger solute and solvent interactions.

Keywords: Amino acid, density, intermolecular interactions, saccharide, thermo-acoustical parameter, ultrasonic velocity.

Introduction

Due to the fact that binary mixtures have numerous applications in a variety of pharmaceutical, medicinal, industrial, and technological processes [1], the ultrasonic method is a flexible non-destructive technique that functions like a powerful probe to access the acoustic properties and predicts the intermolecular interaction in the binary mixture [2,3].Volumetric and thermos-acoustical properties are examples of thermodynamic parameters that offer important insights into solute-solvent and solvent-solvent interactions [4].The behavior of the liquid system, intermolecular interaction, complex formation, and associated structural changes are all usefully revealed by ultrasonic velocity measurements of an aqueous solution of amino acid with electrolyte and non-electrolyte [5].Volumetric and ultrasonic velocity measurements have been used in numerous studies over the past 20 years to look into how hydrated proteins are [6–8].Amino acids are frequently viewed as the best model compound for analyzing proteins because they are the fundamental structural components of proteins [9–

Corresponding authors: E-mail: *[a]poojasonune28@gmail.com)

11].Proteins are present throughout the body and serve a huge range of purposes [12].As a result of their significant contribution to the energy of protein denaturation, the study of this solute-solvent and solute-solute interaction is crucial. Protein solutions are known to change in structure and configuration when salts or solvents are added [13].The genetic code only recognizes 22 essential and non-essential -amino acids out of the hundreds of significant amino acids found in nature. The current article makes an attempt at the hydrolysis of proteins to yield g L-histidine, an essential amino acid that is heavily utilizedby the body. A decrease in blood pressure is brought on by its absence. In order to maintain a rigid blood pressure level, it is important to maintain a healthy level of histidine in the human body.

It is also widely notable that saccharides are a common type of non-electrolyte with a number of hydroxyl groups, and that these poly-hydroxyl compounds aid in stabilizing the globular protein's native conformation [14–17].The behavior of some carbohydrates and amino acids in an aqueous medium has been studied by numerous researchers using an ultrasonic technique [18, 19].The unit structure of carbohydrates is called a saccharide. Saccharides are sugars or carbohydrates that are the primary energy source for a variety of biochemical reactions.The quantity or arrangement of hydroxyl groups throughout saccharides affects how they hydrate [20,21].Various types of saccharides, including monomer, di, oligo, and poly, are found in nature. However, for the purposes of the study, we selected monomer, the most basic form of sugar from which all other forms of carbohydrates are derived [22,23]. These include glucose and fructose; the monosaccharide glucose is essential for metabolism, where the chemical energy is taken via glycolysis and the citric acid cycle to supply energy to living things.

Let's go over some of the fundamentals of blood sugar. All of the cells in your body receive their major energy from the glucose and fructose in your blood, which may be maintained when your blood sugar is normally between 70 and 120 mg/dl.If the level drops too low, your body may produce catecholamine chemicals to cause a rise in blood glucose levels. Your body will produce insulin and other hormones if your blood glucose levels rise too high in order to bring them down to a healthy range. Maintaining normal blood pressure levels involves using an identical set of procedures. In many respects, maintaining healthy blood pressure is more important than maintaining a healthy blood sugar level. What links these two systems together? An unfortunate connection exists between the production of nitric oxide in blood vessels and insulin, which is involved in controlling blood sugar levels. Nitric oxide is crucial for healthy blood vessels since it is one of the few substances that may increase blood vessel size while reducing blood pressure [24]. Knowing the different ways that bioactive chemicals work and how the biochemical processes in the body behave thermodynamicallyin a live creature depends in large part on the interaction of saccharides with model molecules of proteins and the temperature dependency of this interaction [25].

Numerous physicochemical investigations of amino acids in aqueous carbohydrate solutions have been conducted, and this research explores the volumetric and viscometrical characteristics of L-histidine in an aqueous disaccharide maltose solution [26]. We investigated L-Histidine in an aqueous monosaccharide (glucose, fructose) solution as a result of this thought. The interaction of a monosaccharide (glucose, fructose) and an amino acid (L-histidine) in water has been investigated in the current paper. Thus, aqueous mono-saccharide solution (glucose &fructose) and L-Histidine amino acid are needed to maintain a healthy B.P. and B.G. level. The goal of this work is to present a picture of the molecular interactions. That took place in the solution for keeping B.P.

and B.G. at the proper level under ambient temperature conditions in order to get around this problem. Information on the impact of saccharides on the stability of amino acids is anticipated to be revealed by the outcome and concentration effect of additives [26].

Experimental Details

Materials- Without further raffination, the following substances were used in the current investigation after being purchased from Himedia Pvt. Ltd. in Mumbai. Every single one of them is an AR-grade chemical. The mole fraction of amino acids in the saccharide solution, which is present in this research at a concentration of 0.1 mol/kg, fluctuates in concentration from 0.02 to 0.2 mol/kg.

Table.1 Chemicals used in paper

Chemicals	CAS No.	Mass Purity	Molecular Formula	Molecular Weight
L-Histidine	71-00-1	≥0.99	$C_6H_9N_3O_2$	155.16 g/mol
Glucose	50-99-7	≥0.99	$C_6H_{12}O_6$	180.16 g/mol
Fructose	57-48-7	≥0.99	$C_6H_{12}O_6$	180.16 g/mol

Table.2 Abbreviations used in paper

No.	Symbol	Abbreviation
1	M	Molal concentration in mol/kg
2	CAS	Chemical Abstract Service
3	MHz	Mega-Hertz
4	U_∞	The infinite value of ultrasonic velocity
5	ρ_o	Density of water
6	U_o	The ultrasonic velocity of water
7	T	Temperature

Method

1. 1.This experiment was run at four distinct temperatures (i.e., 283 & 298K), which were maintained through a digital water bath with accuracy ±1K.
2. A digital weighing machine with a ±0.0001g precision was used to measure the weight.
3. A digital ultrasonic interferometer havinga 2MHz frequency and a 0.0001m/sprecision was used to measure ultrasonic velocity.
4. Utilizing a 10 ml bottle with a specific gravity density, it was possible to calculate the density of the solutions with $\pm 2*10^{-2}kg/m^{-3}$ accuracy.
5. Other thermos-acoustical metrics have been estimated using established relations utilizing the collected data.

Defining relations

The aforementioned volumetric and thermal acoustical propertieswere computed using density and ultrasonic velocity measurements, together with a formula that has been accepted in the literature.

1. Adiabatic compressibility (β):

$$\beta = \frac{1}{\rho * U^2} \text{ ----------------------[27]}$$

2. Acoustic impedance (Z):

$$Z = \rho U \text{ ------------------------[28]}$$

3. Relative association (R_A):

$$R_A = \left(\frac{\rho}{\rho_0}\right)\left(\frac{U_0}{U}\right)^{1/3} \text{ ---------------[29]}$$

4. Relaxation strength (r):

$$r = 1-\left(\frac{U}{U_\infty}\right)^2 \text{---------------------[30]}$$

5. Isothermalcompressibility(k_T):

$$k_T = \{1.33*10^{-8}/(6.4*10^{-4}U^{3/2}\rho)^{3/2}\} \text{--[31]}$$

6. Surface tension (σ):

$$\sigma = (6.3*10^{-4})\rho U^{3/2} \text{-----------[32]}$$

7. non-linearity parameter(B/A):

$$(B/A) = \{2+[0.98*10^4/U]\} \text{----[33]}$$

8. Specific heat ratio (γ):

$$\gamma = \frac{17.1}{T^{\frac{4}{9}} * \rho^{1/3}} \text{---------------------[33]}$$

Result and discussion

Following a comparison with observed and published data, the following table of data presents thedistilled water's density and ultrasonic speed at various temperatures, as measured experimentally.

Table.3 Densities and ultrasonic velocities of newly distilled water at various temperatures. (i.e., 288 & 298K).

mperature (T) K	DataObtained		iterary Evidence	
	. Speed (U)	ensity (ρ)	Speed (U)	ensity (ρ)
288	ɫ66.032	)9.103	ɫ66.25 [34]	)9.100 [34]
298	ɫ98.101	)7.051	ɫ97.06 [35]	)7.025 [35]

Ultrasonic Velocity (U) - In Table 4, the three systems' ultrasonic velocities and densities are presented. The value of ultrasonic speed is found to increase as temperature and solute concentrations rise. The intermolecular interaction may have increased, which would explain this increase interaction between L-Histidine and aqueous saccharide solutions, which could be brought on by a general increase in cohesion generated by solute-solvent and solute-solute interaction in solution, as seen in Fig. 1.

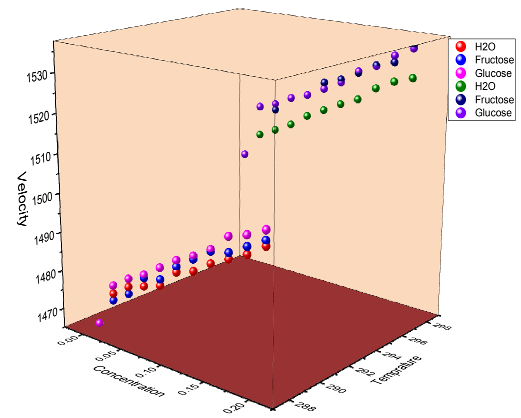

Fig. 1 Ultrasonic Velocity Variation with Concentration

Density (ρ) - Additionally, a rise in density with concentration may be attributed to the density, a measurement of solute-solvent interaction., indicating an increase in solute-solvent contact, as opposed to a drop in density, demonstrating a solute-solvent interaction with a lesser magnitude. As can be shown in Tables 4 & Fig. 2 [36], the volume shrinks with concentration, which is caused by the presence of solute molecules.

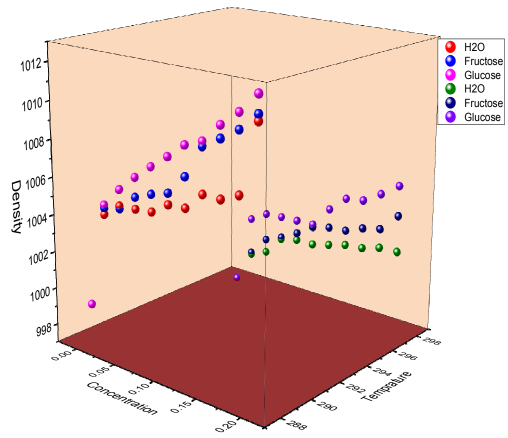

Fig. 2 Variation of Density with Concentration

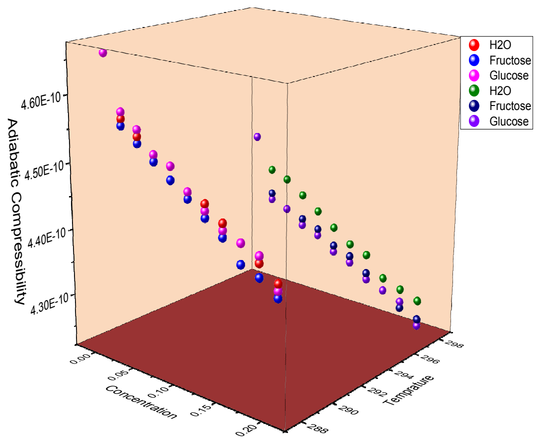

Fig. 3Adiabatic compressibility varies with concentration

Adiabatic Compressibility (β) – It is possible to determine the kind of interaction present in a liquid mixture using adiabatic compressibility, which is dependent on the volume and is much more sensitive to different forms of contact. As the concentration of amino acids, increases in the three systems, the value of adiabatic compressibility (Fig. 3) drops. The effect of the surrounding solvent molecule's electrostatic field, also known as electrostriction, is thought to be responsible for the decline in adiabatic

Relaxation strength(r)- In order to understand the molecular connection that exists in the systems, relaxation strength is a crucial feature. The relationship between relaxation strength and adiabatic compressibility is direct, and the creation of the complex by the solvent molecule surrounding the solute molecule is the reason why relaxation strength decreases with concentration at a constant temperature, as illustrated in Fig. 6 [41].compressibility. L-Histidine + glucose + water has a greater magnitude of value than L-Histidine + fructose + water and L-Histidine + water. The bigger result indicates that L-Histidine + glucose + water exhibits stronger molecular interaction than the other two systems [37].

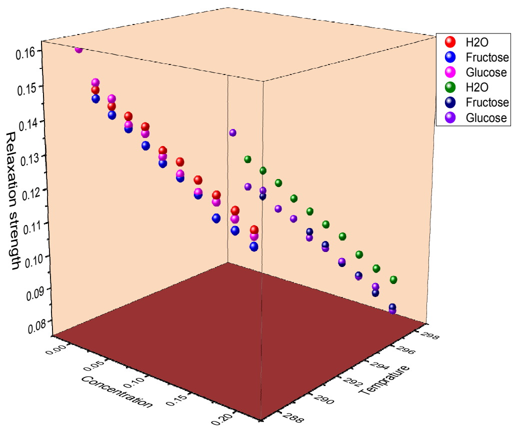

Fig. 6 Variation of Relaxation strengthwith Concentration

Acoustic impedance(Z) -The ratio of sound pressure (P) to particle velocity (U) at a specific frequency is known as acoustic impedance. represented in "rayals" [38]. The system's acoustic impedance is shown to rise when amino acid concentrations in both saccharide solutions rise. Figure 4 displays a sample plot of Z v/s conc. for L-Histidine in a solution of 0.1% glucose and 0.1% fructose at various temperatures shown in Fig. 4 & Table 5. This is in line with the theoretical requirement since U and both rises as the solute concentration rise. Effective solute-solute interaction is responsible for this rise in Z value with solute concentration [39].

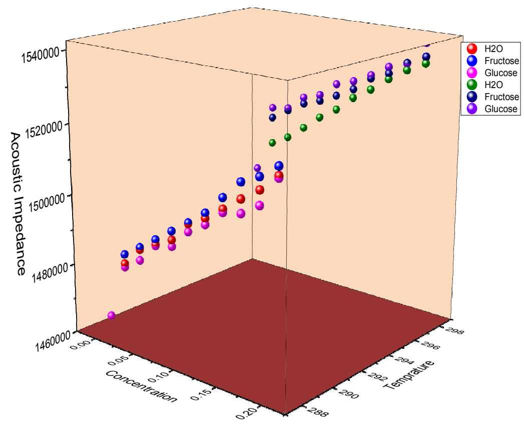

Fig. 4Acoustic impedance varies with Concentration

Relative Association (R_A)–The association relative parameter called R_A is utilized to access an association in any solution in relation to an association that exits in water or a solvent at zero degrees Celsius. The latter causes the relative connection to rise while the former causes it to diminish. In the current investigation, in Table 5, the value of R_A increases as the concentration of solutes rises, indicating a strong ion-solvent interaction that does so as well [39, 40].

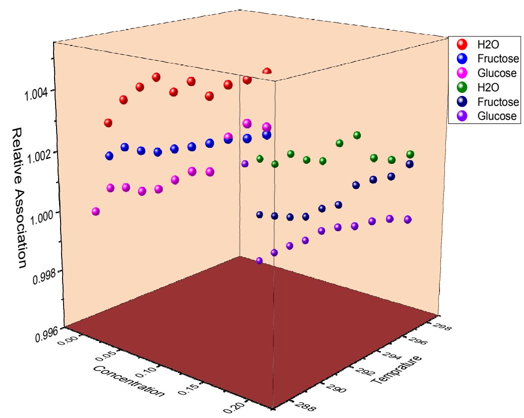

Fig. 5 Variation of Relative Association with Concentration

Isothermal compressibility (K_T) –The Mc'Gowan approach employs isothermal compressibility (K_T), as seen by the Fig. 7 trend. With higher concentration, it gets smaller. the relationship between K_T value and concentration. Relationship between average kinetic energy and the decline in free volume of the component solute-solvent molecule in the saccharide's solution and the change in K_T value with an increase in amino acid concentration appears to be causal [42].

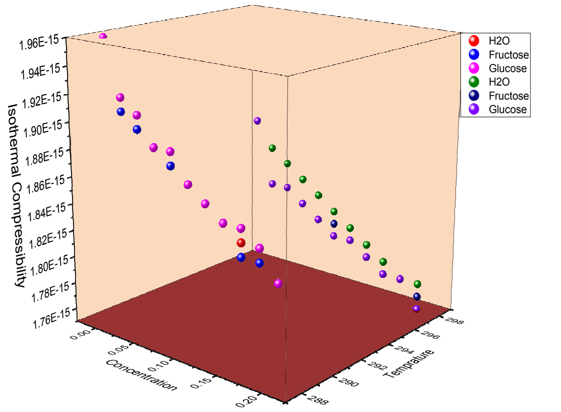

Fig. 7 Variation of Isothermal compressibilitywith Concentration

Surface Tension(σ)–This parameter is used to investigate the surface makeup of the mixture's aqueous solution. These variables were applied to determine how strong the intermolecular interactions were in the solution. As the solute is added to the experimental solvent, the surface tension increases in a trend that indicates a significant association in the solution shown in Fig. 8 [43].

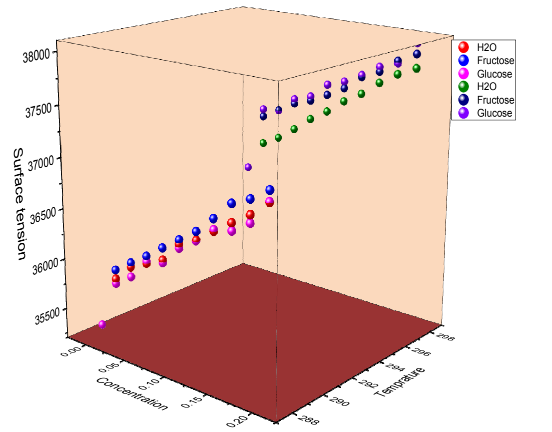

Fig. 8 Variation of Surface tensionwith Concentration

Non-linearity parameter(B/A) – The examination of this table also reveals that Balizar's non-linear parameter (B/A), for both the system, L-Histidine+glucose and L-Histidine+fructose under consideration, exhibits a little rise. The research system's intermolecular mode of vibration and anharmonicity are shown to be less prevalent, and the presence of associating tendencies and weak contact forces is also shown by an increase in the value of the Balizar non-linear parameter shown in Table 7 [44].

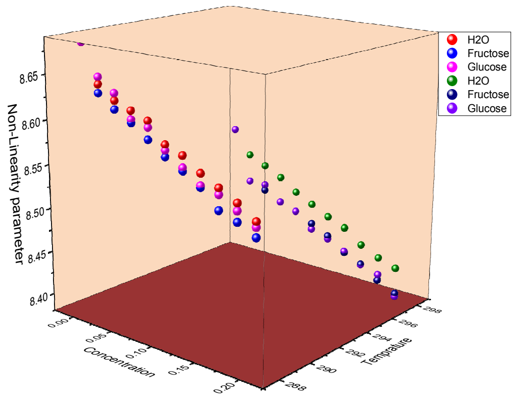

Fig. 9 Variation of Non-linearity parameterwith Concentration

Specific heat ratio (ɣ) – The amount of heat needed for each degree of temperature rise is based on the specific heat of the liquid. The variation of the specific heat ratio for different weight fractions of amino acids (0.02-0.2mol-kg^{-1}) is shown in Fig. 10. With the temperature rising and amino acids being added to both pure water and an aqueous saccharide solution, the heat capacity ratio (ɣ) is declining. These specific heat ratio results provide strong evidence that increasing L-Histidine concentration leads to an increase in density.

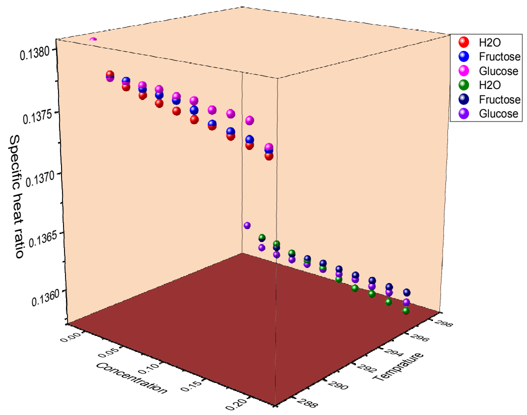

Fig. 10 Variation of Specific heat ratiowith Concentration

Conclusion

Saccharides' interactions with proteins have attracted a lot of attention because they are used in a variety of biochemical processes, including those in immunology, biosynthesis, medicine, and pharmacology. Based on the analysis of experimental and computational results for all parameters, we can say that interactions between solute and solvent molecules take place. The interaction of L-histidine amino acid with a monosaccharide solution may be further investigated with the use of this study's crucial foundational facts and theoretical underpinnings.According to the results, there is a significant solute-solvent interaction in this system, and this interaction strengthens as the concentration of the solute (L-histidine) rises. It was determined by the results that L-histidine creates structures in an aqueous monosaccharide solvent.It is also deduced from the acoustical and volumetric parameters that the strength of the H-bonding interaction increases with concentration. The L-Histidine amino acid interacted in the order (L-Histidine + glucose + water) > (L-Histidine + fructose + water) > (L-Histidine + water) in all three solvents (water, glucose, and fructose).According to the entire scenario, higher mass fractions at higher temperatures are linked to stronger solute and solvent interaction for sustaining a normal B.P. and B.G. level.

Contribution Authorship Statement with Credit:

Sonune Pooja R.: Research, software, data collection, methodology, and first draught writing. Formal analysis, software, and writing the first draught, according to Mishra Paritosh L. Conceptualization, Methodology, Supervision, Writing - Review & Editing: Manik Urvashi P.

Conflict of Interest Statement:

The author attests having no known financial conflicts of interest or intimate relationships that would have appeared to have an impact on the work presented in this publication.

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