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On the Thermal properties of Aspartic acid using Ultrasonic Technique

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Abstract: Generally, Ultrasonic studies are extensively used in the conformational analysis of organic molecules. In the present work, attempts have been made to investigate the thermal properties of aqueous solution of aspartic acid at various concentrations using Ultrasonic technique. The results reveal that the present method can also be used as an additional tool for further use of future applications, as these are rarely reported in literature.

Keywords: Amino acids, Ultrasonic, Thermal Diffusivity, Thermal Conductivity.

1. Introduction:

Amino acids, the monomer units of protein molecule plays an important role in all biological species [1, 2]. Moreover, the use of bio-based products to replace those made from increasingly costly imported petroleum has gained momentum [3, 4]. For example, there is considerable interest in replacing some kind of amino acid, a petroleum-based, water soluble polymer, with a bio-based alternative. Among them, aspartic acid acting a vital role as general acids in enzyme active centers, as well as in maintaining the solubility and ionic character of proteins [5]. For the past two decades, a significant study has been carried out to investigate the hydration of proteins through volumetric and ultrasonic measurements, since these properties are sensitive to the degree and nature of hydration [6, 7]. Due to the complex molecular structure of proteins, direct study is somewhat difficult. Hence, in recent years the useful approach, ultrasonic technique has become a powerful tool in providing information regarding the molecular behavior of liquids owing to its ability of characterizing physiochemical behavior of the medium.

Ultrasonic measurements are extensively used to study the molecular interactions in pure liquids, liquid mixtures and ionic interactions in solutions comprising of either single or mixed solutes [8]. The present investigation deals with the study of molecular interaction in aspartic acid. Most of the work on binary mixtures is channelized towards the estimation of thermodynamic parameters like adiabatic compressibility, free length, etc., and their excess values so as to relate them towards explaining the molecular interactions taking place between the components of the binary mixtures [9-11]. Other than this work, studies on aspartic acid in literature are sparse particularly on the thermal diffusivity and thermal conductivity. So here it is planned to study this aspartic acid by ultrasonics specifically for the thermal properties. Recently Bama *et al* [12] have studied the thermal properties of D-Mannitol by using ultrasonic technique. To the best of our knowledge, no reports are available on thermal properties of aspartic acid by using ultrasonic technique. Since thermal properties are important in order to understand the sample properties in depth.

2. Sample Preparation and Methods:

The solutions of aspartic acid were prepared by dissolving in distilled water (the solvent). The molar solutions of aspartic acid (0.005, 0.01, 0.02, 0.03 and 0.04 M) were prepared by standard procedure. Measurement of ultrasonic velocity is generally made either by continuous wave method or by pulse methods. In the present study, continuous wave variable path interferometer is used. The accuracy of ultrasonic velocity determination in non–aqueous solutions is 0.001%. The ultrasonic measurements is carried out on these solutions for various acoustical parameters at different temperatures (35°C, 45°C, 55°C) and different concentrations.

3. Results and Discussion

3.1. Ultrasonic measurements

The ultrasonic studies of amino acid + water systems are useful to understand several biochemical processes such as protein hydration, denaturation, aggregation etc. Lagemann and Dunbar [13] were the first to point out qualitative determination of the degree of association in liquids from sound velocity. Now, a lot of reports are available in the literature for such ultrasonic studies in liquids and liquid mixtures [14,15]. Here ultrasonic measurements are carried out in aqueous solution of aspartic acid for different concentration using the ultrasonic interferometer (of fixed frequency 2 MHz). From the knowledge of ultrasonic velocity and density of a liquid, various acoustical parameters such as adiabatic compressibility, free lengh etc. can be obtained. The measured values are listed in Table 1. From Fig. 1 it is observed that the the increase in ultrasonic velocity at higher concentrations may be due to polymer-polymer interaction and decrease in velocity with increase in temperature may be due to the weakening of intermolecular forces between the molecules.

The variation of ultrasonic velocity in liquids depends upon the increase or decrease of intermolecular free length [18,19]. Figure 2 describes the variation of free length for different value of temperature and concentration. Since the free length L_f is proportional to the adiabatic compressibility (β_{ad}) the same trend of variation similar to the variation of free length has repeated in Fig. 3. However, the decrease in β_{ad} and L_f mat also be attributed to the internal interaction between the π electrons which is concluded by Anbananthan [20].

Here the main aim of this present work is to find the thermal properties of aspartic acid using ultrasonic technique. In 2010, Bama *et al* [21] have reported the thermal properties of jatrophal oil using ultrasonic technique by schaaff's theory. No reports are available on the thermal properties of aspartic acid using ultrasonic technique. Hence thermal conductivity can be computed from the intermolecular distance and this distance is found from the ultrasonic velocity. Since the velocity of sound in liquid (u) is found from ultrasonics, the intermolecular free length can be deduced [22] from the available volume per mole V_a as follows.

According to Schaaff's theory [23], V_a can be expressed as

$$V_a = V \left(1 - \frac{u}{u_\infty} \right) \tag{1}$$

where $u_{\infty} = 1600 \text{ m} \cdot \text{sec}^{-1}$. The intermolecular free length L_f is calculated using the following equation

$$L_f = \frac{2V_a}{Y} \tag{2}$$

where the surface area per mole Y can be written as

$$Y = (36\pi NV_{0})$$
⁽³⁾

The ultrasonic velocity is used to calculate the intermolecular free length, which in turn is used to compute the thermal conductivity. Thermal conductivity in liquids is evaluated from the intermolecular free length L_f if we assume the latter to be the mean free path; thus, the thermal conductivity is

$$k = \frac{1}{3}CL_{f}U\tag{4}$$

Thermal diffusivity (α) is calculated from the following equation

$$\alpha = \frac{k}{\rho C} \tag{3}$$

To calculate the thermal conductivity, the Brownian motion for heat diffusion was assumed, which is a very good approximation. With the mean free length and the velocity of sound in aspartic acid, the thermal conductivity is calculated and given in Table 2 (error in measurements is less than 2%). Thermal diffusivity of aspartic acid for different concentrations were calculated from thermal conductivity. It is found that thermal conductivity decreasing with increasing temperature (Fig.3). This is most expected behavior in most of the fluids which is explained by the fact that at random, the free electrons moving in fluids also collide with the atoms contained in the fluids [24, 25]. Due to these collisions, their kinetic energy is wasted to some extent.

When the temperature of such fluids is increased, their collisions with the containing atoms become more frequent and ultimately more energy is wasted. This obviously reduces their thermal conductivity.

Table : 1 Values of ultrasonic velocity (m/sec) in aspartic acid at various Concentrations in the temperature range 308–328 K

Con/Temp	Ultrasonic Velocity (msec ⁻¹)					
	308K	318K	328K			
0.005	1541.17	1526.41	1512.10			
0.01	1541.60	1526.50	1512.78			
0.02	1544.61	1527.36	1513.60			
0.03	1544.63	1528.66	1513.01			
0.04	1541.96	1529.86	1514.03			



Figure 1:Variation of Ultrasonic Velocity with concentration and temperature

(5)

Con/Temp	Density (ρ)/ Kg m ⁻³			$\begin{array}{c} A diabatic \ Compressibility \ (\beta_{ad}) \\ \times 10^{-10} \ m^2/N \end{array}$			Free Length (L _f)/ ×10 ⁻¹⁰ m		
	308K	318K	328K	308K	318K	328K	308K	318K	328K
0.005	996.8	996.4	999	4.3479	4.2601	4.1806	0.4429	0.4357	0.4363
0.01	999.9	999.9	999.4	4.3671	4.2658	4.1865	0.4434	0.4396	0.4368
0.02	999.9	1001	1001.5	4.3688	4.2859	4.1909	0.4437	0.4399	0.4372
0.03	1003	1003.6	1003	4.3692	4.2946	4.2132	0.4448	0.4414	0.4375
0.04	1005	1005	1004.1	4.3765	4.2992	4.2154	0.4449	0.4416	0.4379

Table : 2 Calculated values of Density, Adiabatic compressibility and Free length in aspartic acid atvarious concentrations in the temperature range 308–328 K



Figure 2: Variation of Adiabatic Compressibility $(\beta_{ad}) \times 10^{-10} \text{ m}^2/\text{N}$ and Free Length $(L_f)/\times 10^{-10}$ m with concentration and temperature

Table : 3 Calculated values of thermal conductivit	y and diffusivity of aspartic acid at various
concentrations in the temperature range 308-328	Κ

	Thermal Conductivity (K) W/m/K			Thermal Diffusivity ×10 ⁻¹⁰ m ² /sec			
Con/Temp	308K	318K	328K	308K	318K	328K	
0.005	0.2711	0.2664	0.2616	0.2270	0.2160	0.2216	
0.01	0.2712	0.2665	0.2621	0.2271	0.2230	0.2189	
0.02	0.2713	0.2668	0.2622	0.2280	0.2240	0.2202	
0.03	0.2714	0.2670	0.2623	0.2290	0.2250	0.2206	
0.04	0.2717	0.2673	0.2626	0.2293	0.2260	0.2207	



Figure 3: Variation of thermal conductivity with concentration and temperature

4. Conclusion

Ultrasonic studies have been carried out in the solutions of aspartic acid at five different temperatures and concentrations. It is concluded that there exist a weak molecular interactions in the liquid mixtures. The trend of increase in adiabatic compressibility and free length with increase of solute concentration further comolecular interaction. This interaction indicates that there is a possibility of some complex formation such as hydrogen bond in the present system. As the temperature increases, the hydrogen bonds are broken up due to thermal agitations and hence the ultrasonic velocity decreases. As the temperature increases, the hydrogen bonds are broken up due to thermal agitations and hence the ultrasonic velocity decreases. The increasing value of acoustical impedance supports the possibility of molecular interactions between the unlike molecules. The study of the solution properties of liquid mixtures consisting of polar as well as non-polar components finds applications in industrial and technological processes. Finally thermal properties of aspartic acid are calculated using the ultrasonic velocity by Schaaff's theory, it is found that as temperature increases thermal conductivity decreases due to the collision between atoms, this apparently reduces their thermal conductivity. Definitely these results will provide an additional information for future applications of aspartic acid.

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