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Acoustic and Viscometric Investigations of Aqueous D-Pantothenic Acid Calcium Hemi-salt

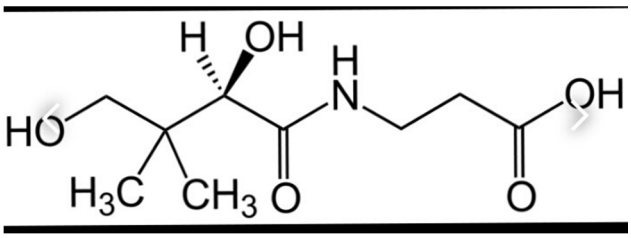
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Abstract: ***Acoustic and viscometric measurements are increasingly being used to investigate the properties of pure components as well as the nature, strength, and order of intermolecular interactions between constituents in solution. The density (ρ), viscosity (n), and ultrasonic velocity (U) of aqueous D-Pantothenic acid hemi-calcium salt at 298.15K and 300.15K were measured. Various thermo -acoustic parameters such as adiabatic compressibility, free length (L_f), free volume (V_f), internal pressure, acoustic impedance (Z), Gibb's free energy (G), and molar sound velocity (R) have been calculated using experimentally measured data.***

Acoustic parameters are useful in understanding molecular interactions in binary liquid mixtures.

Keywords: Ultrasonic velocity, Free length, acoustical parameters, Acoustic impedance.

Graphical Abstract



Fig; D-pantothenic acid hemi-calcium salt.

I. INTRODUCTION

Understanding the nature of molecular interactions requires an ultrasonic study of liquids and liquid mixtures. Thermo-acoustic features of liquid mixtures have been widely employed to investigate the elapse of an actual liquid mixture's behaviours from ideality [1]. The calculated acoustical parameters and ultrasonic velocity provide crucial information about molecular interactions.

Through ultrasonic investigation of liquid mixtures containing polar and non-polar components, it is possible to understand the molecular interactions and structural behaviours of molecules and their mixtures. The structural arrangement as well as the form of the molecules are influenced by intermolecular interactions [2]. At various temperatures, ultrasonic velocities, as well as density and viscosity, are monitored at various temperatures to gain a better knowledge of the physico-chemical properties and molecular interactions between the contributing components of these mixes [3]

Ultrasonic velocity is a temperature dependent quantity in most of the solutions. It also depends on the concentration of the solute used. The measurements of density, viscosity, and related thermodynamic parameters are used to explain the nature, strength, and order of the molecular interaction. Studies of molecular interactions can be carried out by spectroscopic methods [4].

Ultrasonic technique is widely used over these methods because of low cost, easy to use, less time consuming and it gives more precise results. In the present work, an attempt has been made to examine the variety of thermodynamic properties of aqueous [5-7]. variation in temperature, size, shape, and nature of the mixture from the graphical and analytic perspectives in order to understand its nature.

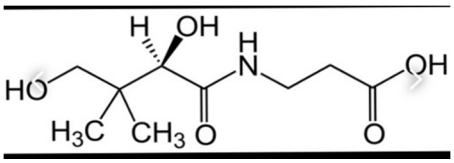
II. MATERIALS AND METHODS

Hemi-calcium salt of aqueous D-pantothenic acid Pantothenic acid is the amide of pantoic acid and - alanine, and it is a 99 percent analytical reagent. Pantothenic acid, often known as vitamin B5, is a water-soluble vitamin that is an essential nutrient. It is usually found as a calcium and as its alcohol analogue, the pro-vitamin panthenol (pantothenol). Pantothenic acid is required for the synthesis and metabolism of proteins, carbohydrates, and lipids in animals. Pantothenic is the name of the anion.

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D-pantothenic acid has a molecular weight of 238.27, according to LOBA Chemie in India.
This chemical (methanol) has an almost white crystalline appearance and is hydroscopic. It is light and air stable, and its aqueous solution is slightly alkaline. It has a melting point of 195-196°C and is water and glycerol soluble.

The molecular structure of this compound is as follow



A digital ultrasonic pulse echo velocity meter was used to measure the ultrasonic velocities of the solution under investigation (VCT-70A). The digital ultrasonic pulse echo velocity meter is a simple and unique direct reading digital technology that can accurately detect the velocity of ultrasonic waves as well as monitor echoes for attenuation measurements. To create and receive ultrasonic echo waves via the solution under observation, one piezo-electric transducer is installed at the end of the liquid cell. The temperature in and surrounding the cell was controlled by circulating water from an Acculab scales thermostat (model- i-therm, AI-7982). The water was allowed to circulate through the double-walled measuring cell, allowing the desired temperature to be achieved. To determine the viscosity of the solutions, an Ostwald's type viscometer is used. The viscometer was set with fresh water immersed in the water bath which was kept at the experimental temperature. The flow time was measured by using a digital stop watch having high accuracy. The temperature the viscometer was maintained by using the same temperature controller.

A. Mathematical Formulation

1) Acoustic Impedance (Z): The specific acoustic impedance is given by

$$Z = U\rho_s \ (Kgm^{-2}s^{-1})$$

ρ_s = Density of solution
U = ultrasonic velocity of solution

2) Adiabatic Compressibility (β)

$$\beta_{ad} = 1/U^2\rho_s \ (N^{-1}m^2)$$

3) Free Length (L_f)

$$L_f = K_T \beta^{1/2} \ (m)$$

Where, K_T is temperature dependent constant $(93.875+0.375T)\ 10^{-8}$

4) Free Volume (V_f)

$$V_f = (M_{eff}\ U/k\eta)^{3/2} \ (m^3mol^{-1})$$

Where, M_{eff} = Molecular weight
K is the temperature independent constant (4.28×10^9)

5) Internal Pressure (π_i)

$$\pi_i = bRT(k\eta/U)^{1/2} \ (\rho^{2/3}/M_{eff}^{7/6}) \ (pa)$$

b = 2 for all liquids
R = Gas constant (8.314)
T is temperature in Kelvin
K is the temperature independent constant (4.28×10^9)

6) *Molar volume (V_m)*

$$V_m = M_{eff}/\rho \ (m^3.mol^{-1})$$

7) *Molar sound velocity*

$$R = M_{eff}/\rho \ (U)^{1/3} \ (m^5N^{-1})$$

8) *Relaxation Time (τ)*

$$\tau = 4/3\eta\beta \ (sec)$$

9) *Gibb's Free Energy:* The Gibb's free energy can be estimated from the following relation.

$$\Delta G = - kT \log[h/\tau KT] \ (Jmol^{-1})$$

III. RESULTS AND DISCUSSION

The observed values of densities, viscosities and ultrasonic velocities of aqueous D-Pantothenic Acid Calcium Hemi-salt for different concentrations from 0.01 to 0.5 mol kg^{-1} at 298.15 K and 303.15K are presented in table 1. For systematic understanding the effect of concentration and temperature on these parameters, the graphs have been plotted and they are shown in fig. 1(a-c).

Table 1. Experimental data of density, viscosity and ultrasonic velocity of aqueous D-Pantothenic Acid Calcium Hemi-salt at 298.15 K and 303.15K

At temperature 298.15K

Concentration (mol kg^{-1})	Density $\rho\ 10^3$ ($kg.m^{-3}$)	Viscosity $\eta\ 10^{-3}$ (Pa-s)	Ultrasonic velocity, u ($m.s^{-1}$)
0.01	996.393	0.000900	1492.94
0.02	995.942	0.000905	1493.94
0.03	996.443	0.000916	1492.94
0.04	996.643	0.000906	1493.54
0.05	989.629	0.000910	1493.54
0.06	995.741	0.000921	1494.14
0.07	996.543	0.000873	1494.14
0.08	997.044	0.000906	1494.14
0.09	995.691	0.000894	1494.73
0.1	998.046	0.000923	1494.73
0.2	996.793	0.000917	1495.331
0.3	998.647	0.000924	1497.127
0.4	999.048	0.000930	1498.927
0.5	999.850	0.000941	1500.129

At temperature 303.15K

Concentration (mol kg^{-1})	Density ρ 10^3 ($kg.m^{-3}$)	Viscosity, η 10^{-3} (Pa-s)	Ultrasonic velocity, u ($m.s^{-1}$)
0.01	1016.852	0.000827	1503.75
0.02	1016.852	0.000840	1503.75
0.03	1016.187	0.000834	1503.75
0.04	1016.852	0.000840	1503.35
0.05	1016.801	0.000840	1504.35
0.06	1017.773	0.000843	1466.02
0.07	1018.285	0.000807	1503.75
0.08	1017.824	0.000866	1504.96
0.09	1018.490	0.000854	1504.96
0.1	1017.415	0.000858	1504.96
0.2	1018.541	0.000849	1506.171
0.3	1018.183	0.000854	1506.778
0.4	1018.643	0.000841	1507.993
0.5	1019.359	0.000829	1509.819

Fig. 1 (a) This shows the density variation of an aqueous D-Pantothenic Acid Calcium Hemi-salt solution, which increases with increasing concentration and decreases with increasing temperature, as expected. As the concentration of solute particles in the solution increases, so does the density.

Density increases with concentration, indicating that solute-solvent and solvent-solvent interactions are of lesser magnitude. The increase in density with concentration is caused by a decrease in volume, which is caused by the presence of solute molecules. In other words, the increase in density caused by the added solute can be attributed to the solvent's structure-maker. Similarly, the decrease in density with concentration indicates that the solvent is a structure-breaker. It's also possible that solvent-solvent interactions result in bonding, most likely H-bonding [8-10].

Viscosity is an important parameter in understanding the structure as well as molecular interactions occurring in the solution. Viscosity (η) is defined as the resistance per unit area of a fluid to flow.

Fig.1 (b) The viscosity of the solution increases with concentration and decreases with temperature. Intermolecular attractive forces prevent molecules from freely flowing in a liquid. At lower temperatures, viscosity is found to be greater due to intermolecular forces caused by an increase in solute, which causes attraction between the solvent and solute, demonstrating the solute's structure-making capability [11]. As the temperature rises, the cohesive forces weaken, resulting in a decrease in viscosity.

As shown in fig. 1(c)the ultrasonic velocity of an unstudied aqueous solution increases with concentration and temperature. The ultrasonic velocity (u) is proportional to the intermolecular free length. Intermolecular free length is a significant factor because it determines sound velocity in a fluid state.

The presence of an ion causes the intermolecular free length to change. As a result, the ultrasonic velocity of a solution differs from that of the solvent. The ultrasonic velocity must increase as the free length decreases due to the increase in concentrations [12]. As a result of the structural properties of the solutes, the system's ultrasonic velocity increases. The solute that boosts ultrasonic velocity is of the structure maker type (SM). At higher temperatures, the increase in velocity indicates a weakening of solute-solvent interactions [13]. The compressibility of the solution decreases as the density and viscosity increase.

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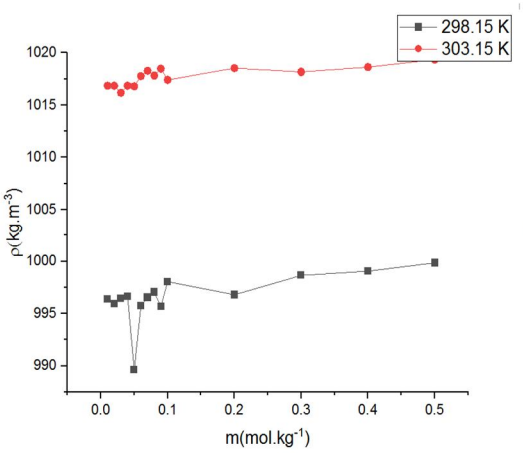


Fig. (a)

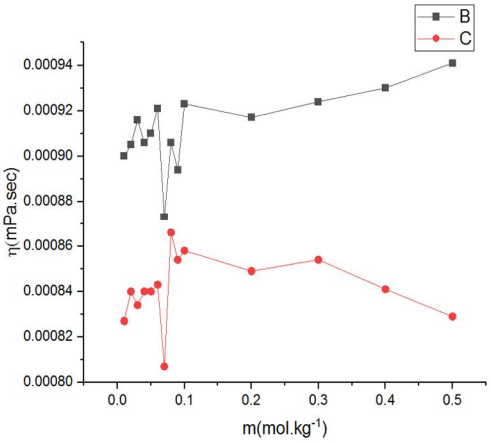


Fig. (b)

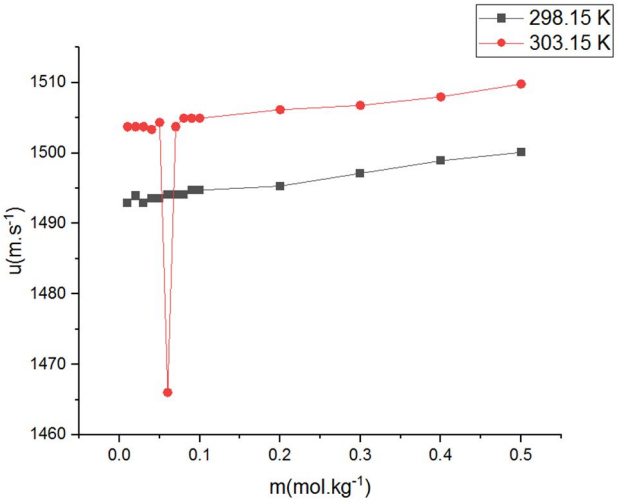
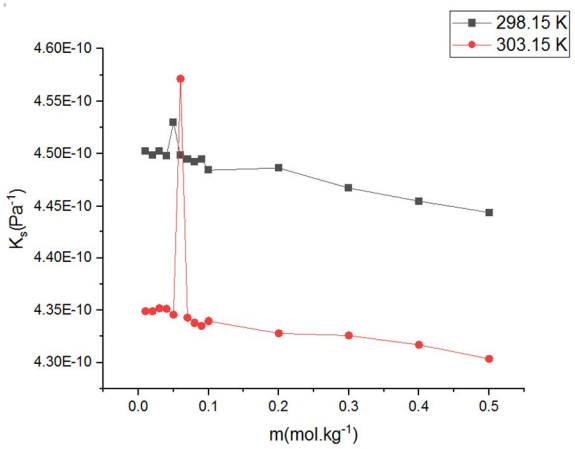
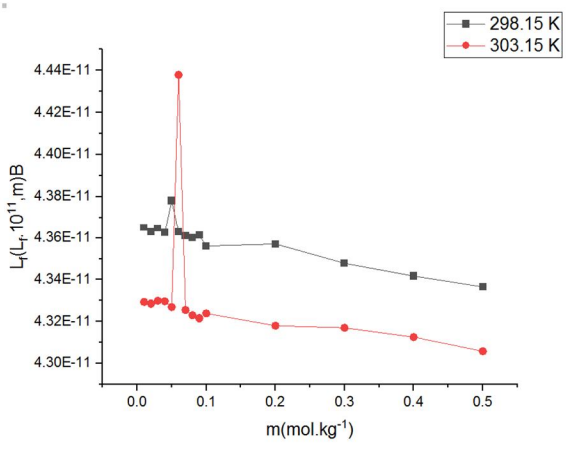


Fig.(c)

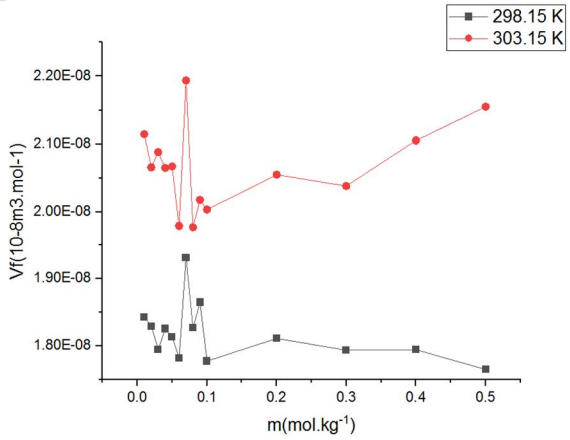
Figure 1. Effect of concentration and Temperature on (a) Density (b) Viscosity (c) Ultrasonic velocity of aqueous D-Pantothenic Acid Calcium Hemi-salt.



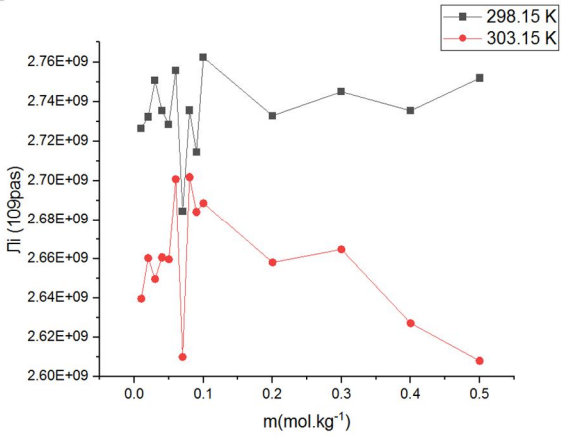
(a)



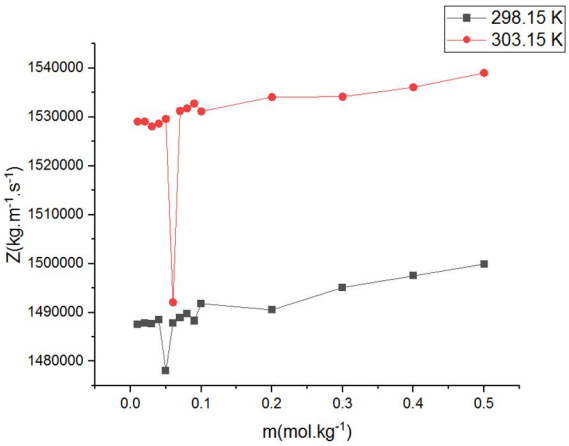
(b)



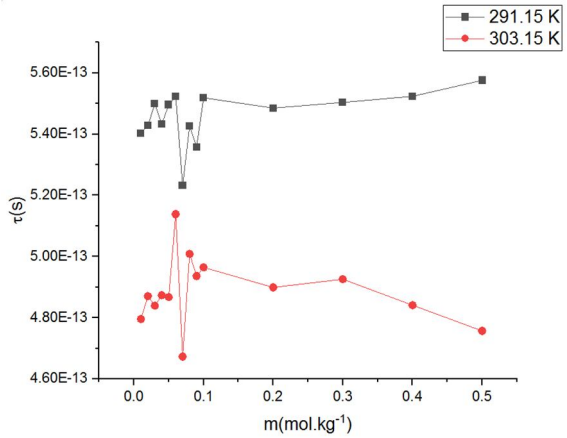
(c)



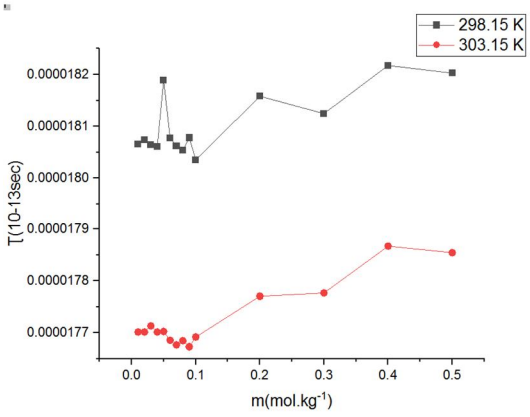
(d)



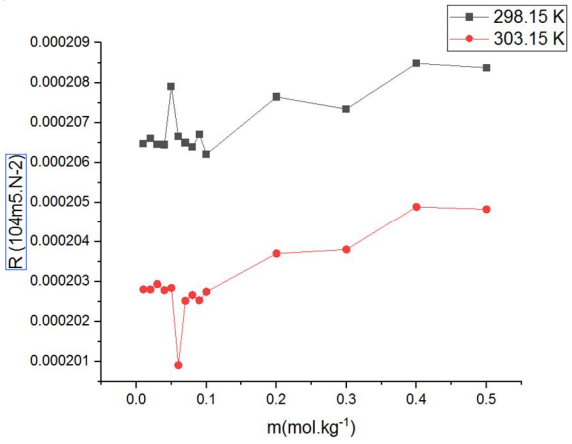
(e)



(f)

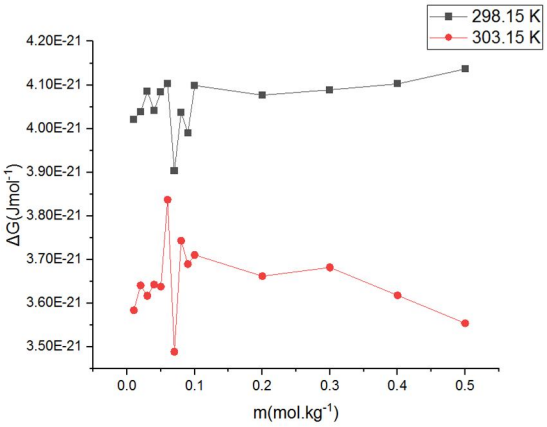


(g)



(h)

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(i)

Figure 2. Effect of Adiabatic compressibility, Free length, Free volume, Internal pressure, Acoustic impedance, Relaxation time, Molar volume, Rao constant, Gibbs free energy, of aqueous D-Pantothenic Acid Calcium Hemi-salt.

Because of compressibility, the hydrogen bonding between like or unlike components in a solution either increases or decreases. As the concentration of aqueous D-Pantothenic Acid Calcium Hemi-salt solution increases, so do the values of adiabatic compressibility [Fig 2(a)]. The decrease in adiabatic compressibility supports the existence of a strong solute-solvent interaction, which could be due to strong intermolecular hydrogen bonding between aqueous D-Pantothenic Acid Calcium Hemi-salt and water molecules.

The intermolecular free length gradually decreases [Fig. 2(b)]. The decrease in the value of intermolecular free length supports the existence of strong solute-solvent interaction, which could be attributed to the presence of strong intermolecular hydrogen bonding between Calcium Hemi-salt and water molecules.

The decrease in free volume with concentration could be due to increased hydrogen bonding between the solute and solvent molecules, resulting in less space between them. Figure 2(c) depicts the changes in free volume as concentration and temperature rise [14].

Internal pressure is a crucial metric in understanding the intermolecular interactions that occur in D-Pantothenic Acid aqueous solution. As shown in Fig. 2(d), internal pressure rises with increasing concentration but decreases with increasing temperature, as shown in Fig. 2(d). The strengthening of the cohesive force between the molecules could be causing the increase in internal pressure.

The thermal energy of molecules increases as the temperature rises, causing the thermal agitation of ions to rise [15].

The product of density and ultrasonic velocity is acoustic impedance. As seen in [Fig. 2(e)], the acoustic impedance increases as the concentration of solute and temperature increase. Strong interactions between the solute-solvent molecules may cause an increase in the value of acoustical impedance as temperature rises, whereas weak molecular interactions between the solute-solvent molecules cause a nonlinear trend in the value of acoustical impedance [16].

In order to analyze molecular aggregation in solution, relaxation time is a crucial metric to consider. The relaxation time increases with the concentration of the solute but decreases as the temperature rises, indicating greater interactions between the solute and the solvent [Fig.2(f)].

Molar volume is a valuable measure for studying a solution's intermolecular interactions. At a certain temperature and pressure, it is the volume occupied by one mole of a substance. Figure 2(g) indicates that molar volume increases with concentration and temperature, showing that strong solute-solvent interactions exist in D-Pantothenic Acid aqueous solution [17]. Figure 2(h) Rao's constant increases linearly with concentration and temperature. The fact that Rao's constant rises indicates that there are strong intermolecular interactions in the existing system [18]. Due to the H-bonding of unlike molecules in the solution, Gibb's free energy exposes the molecules' tighter packing. The strong hydrogen bonding between the molecules in the solution is indicated by the increase in Gibb's free energy with concentration, as illustrated in Figure 2(i). With increasing temperature, Gibb's free energy decreases, implying that the molecules in the solution have less time to reorganize themselves.

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Table 2. Adiabatic compressibility, free length and free volume of aqueous D-Pantothenic Acid Calcium Hemi-salt at 298.15K and 303.15K

Conc. (mol/kg)	Adiabatic compressibility (β) 10^{-10} ($N^{-1}m^2$)		free length (L_f) 10^{-11} (m)		free volume (V_f) 10^{-8} (m^3mol^{-1})	
	298.15K	303.15K	298.15K	303.15K	298.15K	303.15K
0.01	4.503	4.349	4.365	4.329	1.84	2.115
0.02	4.499	4.349	4.363	4.329	1.83	2.1
0.03	4.503	4.352	4.365	4.330	1.79	2.088
0.04	4.498	4.351	4.363	4.330	1.83	2.065
0.05	4.530	4.346	4.378	4.327	1.81	2.067
0.06	4.499	4.572	4.363	4.438	1.78	1.978
0.07	4.495	4.343	4.361	4.325	1.93	2.194
0.08	4.493	4.338	4.360	4.323	1.83	1.976
0.09	4.495	4.335	4.361	4.322	1.86	2.018
0.1	4.485	4.340	4.356	4.324	1.78	2.004
0.2	4.487	4.328	4.357	4.318	1.81	2.055
0.3	4.468	4.326	4.348	4.317	1.79	2.038
0.4	4.455	4.317	4.342	4.313	1.79	2.105
0.5	4.444	4.304	4.336	4.306	1.77	2.155

Table 3. Internal Pressure, Acoustic Impedance and Relaxation Time of D-Pantothenic Acid Calcium Hemi-salt at 298.15K and 303.15K

Conc. (mol/kg)	Internal Pressure (π_i) 10^9 (Pa)		Acoustic Impedance (Z) 10^6 ($Kg.m^{-2}.s^{-1}$)		Relaxation Time (τ) 10^{-13} (s)	
	298.15K	303.15K	298.15K	303.15K	298.15K	303.15K
0.01	2.726	2.640	1.488	1.529	5.403	4.796
0.02	2.732	2.660	1.488	1.529	5.429	4.871
0.03	2.751	2.650	1.488	1.528	5.499	4.839
0.04	2.735	2.661	1.489	1.529	5.434	4.873
0.05	2.729	2.660	1.478	1.530	5.496	4.867
0.06	2.756	2.701	1.488	1.492	5.524	5.138
0.07	2.684	2.610	1.489	1.531	5.232	4.673
0.08	2.736	2.702	1.490	1.532	5.427	5.009
0.09	2.714	2.684	1.488	1.533	5.358	4.936
0.1	2.762	2.689	1.492	1.531	5.519	4.965
0.2	2.733	2.658	1.491	1.534	5.486	4.899
0.3	2.745	2.665	1.495	1.534	5.504	4.926
0.4	2.735	2.627	1.498	1.536	5.524	4.841
0.5	2.752	2.608	1.500	1.539	5.576	4.757

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Table 4. Molar Volume, Rao's Constant and Gibb's Free Energy of D-Pantothenic Acid Calcium Hemi-salt at 298.15K and 303.15K

Conc. (Mol/kg)	Molar Volume (Vm) 10^{-5} (m^3/mol)		Rao's Constant (R) 10^{-4} (m^5N^{-1})		Gibb's Free Energy (ΔG) 10^{-21} (J mol^{-1})	
	298.15K	303.15K	298.15K	303.15K	298.15K	303.15K
0.01	1.807	1.770	2.06	2.03	4.021	3.584
0.02	1.807	1.770	2.07	2.03	4.038	3.641
0.03	1.806	1.771	2.06	2.03	4.086	3.617
0.04	1.806	1.770	2.06	2.03	4.042	3.643
0.05	1.819	1.770	2.08	2.03	4.084	3.638
0.06	1.808	1.769	2.07	2.01	4.103	3.837
0.07	1.806	1.768	2.06	2.03	3.903	3.489
0.08	1.805	1.768	2.06	2.03	4.037	3.743
0.09	1.808	1.767	2.07	2.03	3.991	3.690
0.1	1.804	1.769	2.06	2.03	4.099	3.711
0.2	1.816	1.777	2.08	2.04	4.077	3.662
0.3	1.812	1.778	2.07	2.04	4.089	3.682
0.4	1.822	1.787	2.08	2.05	4.103	3.618
0.5	1.820	1.785	2.08	2.05	4.137	3.554

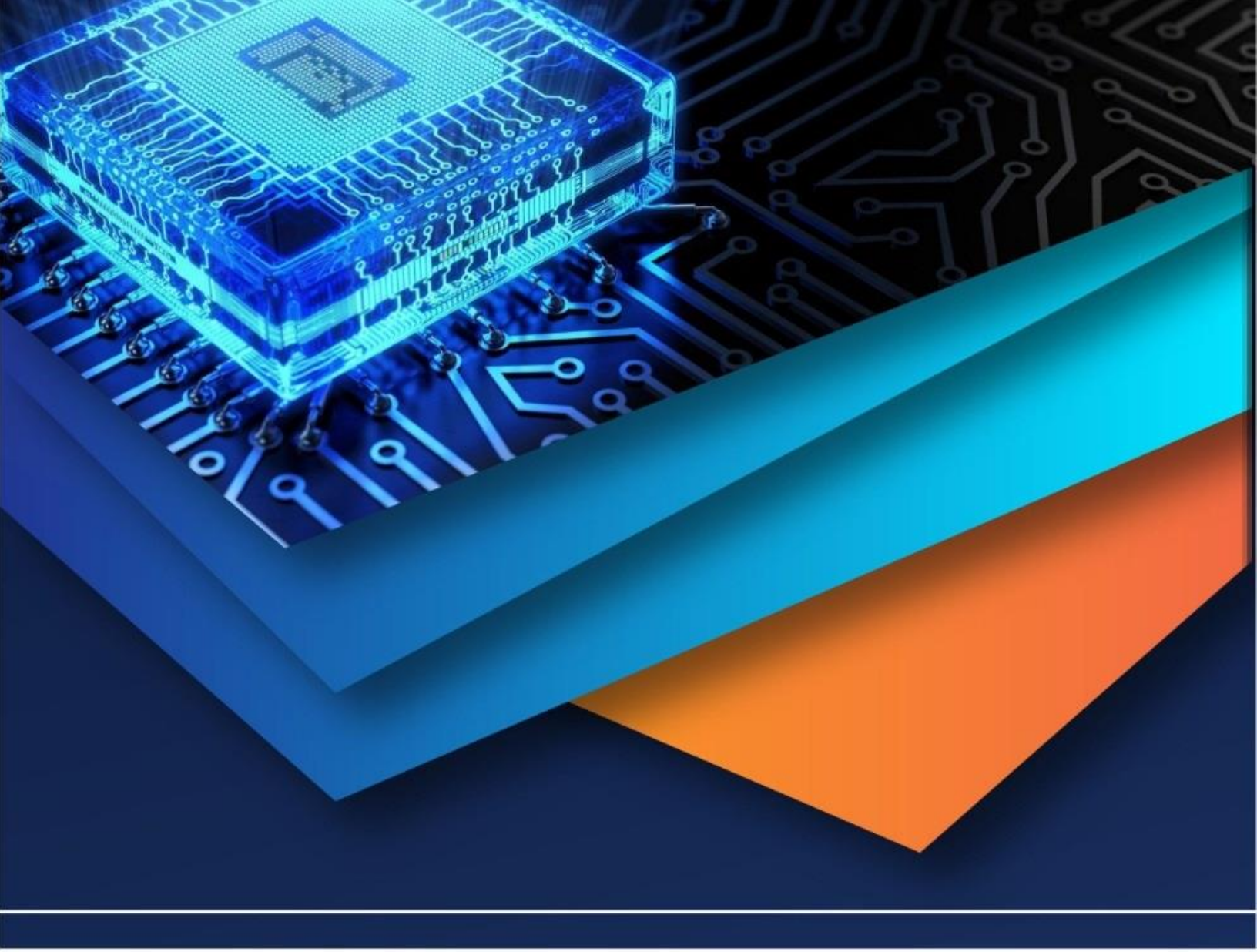
IV. CONCLUSION

The density, viscosity, ultrasonic velocity, and other acoustical parameters of an aqueous solution of D-Pantothenic Acid Calcium Hemi-salt were measured in this study at different concentrations (0.01-0.5) mol kg-1 at 298.15K and 303.15K. The existence of molecular interactions has been demonstrated by variations in basic and physical parameters. As a result, the nature of the solute and solvent, as well as their concentration, play an important role in determining the interactions that occur in the aqueous solution.

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