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Acoustic and Viscometric Investigation of Pyridoxine Hydrochloride (B6) At Temperatures of 298.15k and 303.15k

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ABSTRACT

In the present study ultrasonic velocity(u), density(ρ) and viscosity(η) have been measured at frequency 2 MHz in the binary mixtures of pyridoxine hydrochloride with water in the concentration range (0.001 to 0.09) at 298.15k and 303.15k using multifrequency ultrasonic interferometer. 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 (η), and ultrasonic velocity (U) of aqueous Pyridoxine Hydrochloride (B6) at 298.15K and 303.15K were measured. Various thermo -acoustic parameters such as adiabatic compressibility, free length (Lf), free volume (Vf), internal pressure(πi), acoustic impedance (Z), Gibb's free energy (ΔG), 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

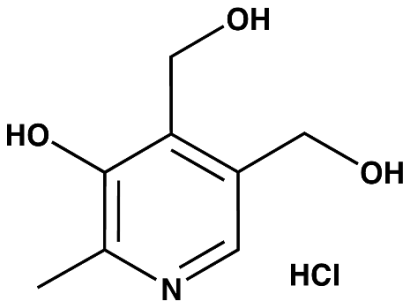

Fig. pyridoxine hydrochloride B6 (2D Structure)

I. INTRODUCTION

Ultrasonic velocity measurements have become popular in recent years for detecting molecular interactions in binary mixtures. This research is non-destructive and has been proven to be useful in a variety of fields, including medicinal, agricultural, industrial, and polymer chemistry.

In the sphere of agriculture, ultra-sound waves have been widely used in chemical additives (fertilizers and plant protection preparations) to increase food production yield. Ultrasound waves have been used in materials chemistry to prepare biomaterials, protein microspheres, and modify polymers and polymer surfaces, among other things

Researchers use ultrasonic velocity to determine thermodynamic parameters and anticipate intermolecular interactions between the hydrochloride salt and the solvent [1-2].

The ultrasonic study of liquids and liquid mixtures is required to understand the nature of molecular interactions. Thermo-acoustic properties of liquid mixtures have been frequently used to investigate how much a real liquid combination deviates from ideal behaviour. The ultrasonic velocity and acoustical characteristics calculated provide essential information about molecular interactions. It is possible to study the molecular interactions and structural behaviours of molecules and their mixtures using the ultrasonic investigation of liquid mixtures combining polar and non-polar components. Intermolecular interactions affect the structural arrangement as well as the shape of the molecules [3]. Ultrasonic velocities, as well as density and viscosity, are measured at different temperatures to learn more about the physico-chemical properties and molecular interactions between the contributing components [4].

Ultrasonic velocities (U), viscosity (η), and density (ρ) measurements are commonly used to characterize the physico-chemical behaviour of liquid mixtures [5]. These features are widely utilized to predict intermolecular interactions and estimate thermodynamic properties. In most solutions, ultrasonic velocity is a temperature-dependent variable. It also relies on the solute concentration used. Ultrasonic velocity is used to determine the amount of adsorbent added to milk, fuels, fruit juices, and drinks because it is useful in determining solute-solvent interactions [6–7]. The type, strength, and order of the molecular interaction are explained using density, viscosity, and related thermodynamic characteristics. Spectroscopic studies of molecular interactions are possible.

Ultrasonic technology is preferred over conventional approaches because it is less expensive, easier to use, takes less time, and produces more precise results. The purpose of this study is to investigate the various thermodynamic properties of aqueous solutions [8]. To comprehend the nature of the combination, graphical and analytic perspectives on temperature, size, form, and nature are used [9-10].

II. MATERIALS AND METHODS

In 1934, Paul Glory, a Hungarian physician, found a chemical that might treat a skin ailment in rats. (Dermatitis acrodynia). Samuel Lepkovsky discovered vitamin B6 from rice bran in 1938 and termed the molecule vitamin B6. In 1938, Harris and Folkers discovered the structure of pyridoxine, and Snell discovered the two forms of vitamin B6, pyridoxal and pyridoxamine, in 1945. Because of its structural

similarity to pyridine, vitamin B6 was given the name pyridoxine.

Pyridoxine Hydrochloride is a water-soluble vitamin B that comes in a hydrochloride salt form. The active form of pyridoxine hydrochloride is formed. Phosphatidyl pyridoxal 5'-phosphate (PLP) is a key component in a variety of enzymatic reactions, including the synthesis of amino acids, neurotransmitters, and sphingolipids. This vitamin is necessary for the proper functioning of red blood cells, the neurological system, and the immune system, as well as the maintenance of appropriate blood glucose levels. Pyridoxine hydrochloride is a form of the vitamin pyridoxine. It comes from the amino acid pyridoxine. Vitamin B is a group of water-soluble vitamins that are typically found together in foods and are all required for optimal growth and metabolism.

According to LOBA Chemie in India, the molecular weight of Pyridoxine Hydrochloride is 205.64gm/mol. It has a melting point of 207°C and is soluble in water.

A digital ultrasonic pulse-echo velocity metre was used to measure the ultrasonic velocities of the solution under discussion (VCT-70A). The digital ultrasonic pulse-echo velocity metre is a one-of-a-kind direct-reading digital instrument that can accurately detect ultrasonic wave velocity and monitor echoes for attenuation measurements. One piezoelectric transducer is placed at the liquid cell's end to generate and receive ultrasonic echo waves via the solution under study. The temperature in and around the cell was maintained by circulating water from an Acculab scale thermostat (model-i-therm, AI-7982).

The required temperature was achieved by allowing water to pass through the double-walled measurement cell. The viscosity of the solutions is measured using an Ostwald-type viscometer. To set the viscometer, fresh water was immersed in the water bath, which was kept at the experimental temperature. The flow time was measured using a highly accurate digital stopwatch. The viscometer was kept at the same temperature by using the same temperature controller.

Mathematical Formulation

Acoustic Impedance (Z):

The specific acoustic impedance is given by

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

ρ_s= Density of solution

U = ultrasonic velocity of solution

Adiabatic Compressibility (βad):

The adiabatic compressibility is defined as the fractional decrease of volume per unit increases of pressure and it is given by,

$\beta ad = 1/U2\ \rho$ ($N^{-1}m^2$)

Free Length (L_f):

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

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

Free Volume (V_f):

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

Where, Meff = Molecular weight

K is the temperature independent constant (4.28×10^9)

Internal Pressure (π_i):

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

Molar volume (Vm):

$Vm = Meff/\rho$ ($m^3.mol^{-1}$)

Molar sound velocity (R):

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

Relaxation Time (τ):

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

Gibb's Free Energy (ΔG):

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

Table 1. shows the observed densities, viscosities, and ultrasonic velocities of Pyridoxine Hydrochloride at 298.15 K and 303.15 K at different concentrations ranging from (0.001 to 0.09) mol kg^{-1}

The graphs in Fig. 1 have been drawn to help understand the effect of concentration and temperature on these parameters in a systematic way (a-c).

Table 1. Experimental data of ultrasonic velocity, density and viscosity of Pyridoxine Hydrochloride at 298.15K and 303.15K

Compositions M (mol/kg)	298.15k			303.15k		
	Velocity(U) (m/s)	Density(ρ) (kg/m^3)	Viscosity(η) (Pa.sec)	Velocity(U) (m/s)	Density(ρ) (kg/m^3)	Viscosity(η) (Pa. sec)
0.001	1494.733	994.839	0.000891	1503.144	1016.085	0.000821
0.002	1494.136	994.689	0.000891	1502.540	1002.321	0.000812
0.003	1494.136	995.140	0.000907	1503.144	1017.620	0.000830
0.004	1456.319	994.990	0.000899	1503.144	1016.852	0.000840
0.005	1495.136	995.040	0.000902	1503.748	995.107	0.000819
0.006	1494.136	995.140	0.000910	1503.748	1017.517	0.000827
0.007	1495.733	995.391	0.000910	1503.748	1016.443	0.000819
0.008	1494.733	995.441	0.000864	1503.144	1016.699	0.000819
0.009	1494.733	993.787	0.000901	1503.748	1016.494	0.000821
0.01	1494.733	994.940	0.000910	1503.748	1017.415	0.000837
0.02	1495.331	996.894	0.000920	1504.353	1017.210	0.000850
0.03	1496.528	997.946	0.000915	1505.564	1017.569	0.000835
0.04	1497.127	998.447	0.000929	1505.750	1013.834	0.000832
0.05	1498.326	1001.152	0.000896	1506.778	1019.155	0.000823
0.06	1498.870	1000.351	0.000928	1507.993	1020.434	0.000837
0.07	1498.927	1000.000	0.000912	1508.601	1020.332	0.000827
0.08	1500.129	999.995	0.000906	1509.819	1021.815	0.000831

Table No.2 Adiabatic compressibility, free length and free volume of Pyridoxine Hydrochloride at 298.15K and 303.15K

Compositions M (mol/kg)	298.15K			303.15K		
	Adiabatic Compressibility (β_a) 10^{-10} ($N^{-1}m^2$)	free length (L_f) 10^{-11} (m)	Free volume (V_f) 10^{-8} (m^3mol^{-1})	Adiabatic Compressibility (β_a) 10^{-10} ($N^{-1}m^2$)	free length (L_f) 10^{-11} (m)	Free volume (V_f) 10^{-8} (m^3mol^{-1})
0.001	4.499	4.363	1.87	4.356	4.333	2.137
0.002	4.503	4.365	1.87	4.419	4.363	2.2
0.003	4.501	4.364	1.84	4.349	4.329	2.12
0.004	4.739	4.478	1.79	4.353	4.330	2.082
0.005	4.496	4.361	1.86	4.444	4.376	2.164
0.006	4.501	4.364	1.83	4.346	4.327	2.132
0.007	4.491	4.359	1.85	4.351	4.329	2.182
0.008	4.496	4.362	2.00	4.353	4.331	2.18
0.009	4.504	4.365	1.87	4.351	4.329	2.174
0.01	4.499	4.363	1.85	4.347	4.327	2.112
0.02	4.486	4.357	1.86	4.344	4.326	2.116
0.03	4.474	4.351	1.91	4.335	4.322	2.211
0.04	4.468	4.348	1.90	4.350	4.329	2.259
0.05	4.449	4.339	2.05	4.322	4.315	2.354
0.06	4.450	4.339	1.95	4.309	4.309	2.298
0.07	4.451	4.340	2.03	4.306	4.307	2.378
0.08	4.444	4.336	2.06	4.293	4.301	2.363
0.09	4.427	4.328	2.04	4.292	4.300	2.406

Table No.3 Internal pressure, Acoustic impedance and Relaxation Time of Pyridoxine Hydrochloride at 298.15K and 303.15K

Compositions M (mol/kg)	298.15K			303.15K		
	Internal pressure $(\pi i)10^9$Pascal	Acoustic impedance (Z) 10^6Kg.m^{-2}s^{-1}	Relaxation Time (τ) 10^{-13} Sec	Internal pressure $(\pi i)10^9$Pascal	Acoustic impedance (Z) 10^6Kg.m^{-2}s^{-1}	Relaxation Time (τ) 10^{-13} Sec
0.001	2.708	1.487	5.345	2.629	1.527	4.768
0.002	2.709	1.486	5.350	2.592	1.506	4.784
0.003	2.716	1.487	5.444	2.629	1.530	4.813
0.004	2.739	1.449	5.680	2.644	1.528	4.875
0.005	2.707	1.488	5.407	2.573	1.496	4.853
0.006	2.720	1.487	5.462	2.624	1.530	4.792
0.007	2.702	1.489	5.449	2.592	1.528	4.751
0.008	2.634	1.488	5.180	2.593	1.528	4.754
0.009	2.687	1.485	5.411	2.596	1.529	4.762
0.01	2.702	1.487	5.458	2.622	1.530	4.851
0.02	2.669	1.491	5.503	2.592	1.530	4.923
0.03	2.629	1.493	5.459	2.537	1.532	4.827
0.04	2.617	1.495	5.535	2.494	1.527	4.826
0.05	2.527	1.500	5.315	2.443	1.536	4.742
0.06	2.569	1.499	5.506	2.465	1.539	4.809
0.07	2.516	1.499	5.412	2.420	1.539	4.748
0.08	2.507	1.500	5.368	2.428	1.543	4.757
0.09	2.501	1.504	5.443	2.396	1.543	4.749

Table No.4 Molar volume, Rao's Constant and Gibb's Free energy of Pyridoxine Hydrochloride at 298.15K and 303.15K

Compositions M (mol/kg)	298.15K			303.15K		
	Molar volume (Vm)10^{-5} (m^3/mol)	Rao's Const.(R) $10^{-4}(m^5N^{-1})$	Gibb's Free Energy (ΔG) $10^{-21}(J.mol^{-1})$	Molar volume (Vm)10^{-5} (m^3/mol)	Rao's Const.(R) $10^{-4}(m^5N^{-1})$	Gibb's Free Energy (ΔG) $10^{-21}(J.mol^{-1})$
0.001	1.809	2.07	3.981	1.772	2.03	3.563
0.002	1.810	2.07	3.985	1.796	2.06	3.575
0.003	1.819	2.08	4.049	1.779	2.04	3.597
0.004	1.819	2.06	4.205	1.780	2.04	3.644
0.005	1.819	2.08	4.024	1.819	2.08	3.627
0.006	1.819	2.08	4.061	1.779	2.04	3.581
0.007	1.828	2.09	4.052	1.791	2.05	3.549
0.008	1.828	2.09	3.866	1.790	2.05	3.551
0.009	1.831	2.09	4.026	1.790	2.05	3.558
0.01	1.829	2.09	4.058	1.789	2.05	3.626
0.02	1.856	2.12	4.088	1.819	2.08	3.680
0.03	1.874	2.14	4.059	1.838	2.11	3.608
0.04	1.893	2.17	4.110	1.864	2.14	3.607
0.05	1.918	2.19	3.961	1.884	2.16	3.543
0.06	1.919	2.20	4.090	1.882	2.16	3.594
0.07	1.940	2.22	4.027	1.901	2.18	3.547
0.08	1.940	2.22	3.997	1.899	2.18	3.554
0.09	1.956	2.24	4.048	1.919	2.20	3.548

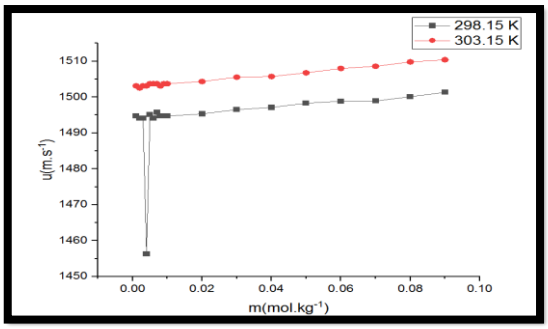

Fig.(a)

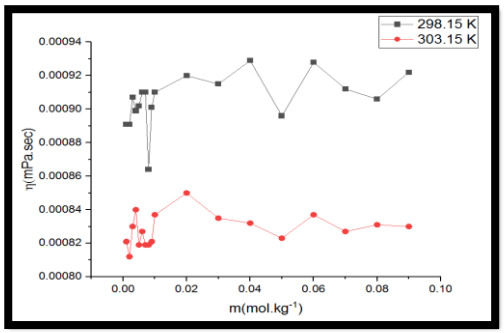

Fig.(b)

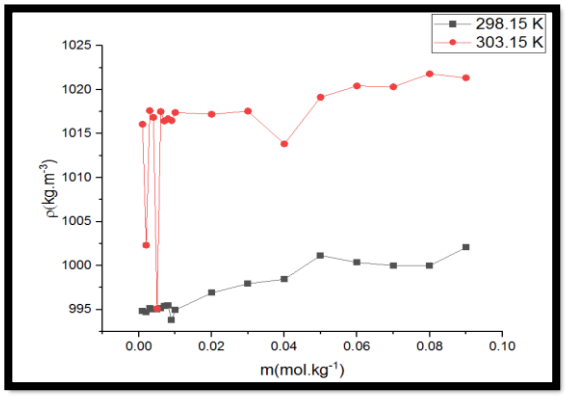

Fig.(c)

Figure 1. Effect of concentration and Temperature on (a) velocity (b) viscosity (c) density of Pyridoxine Hydrochloride at 298.15K and 303.15K

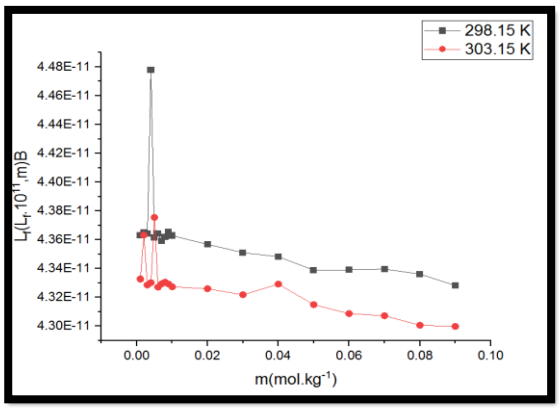

Fig.(a)

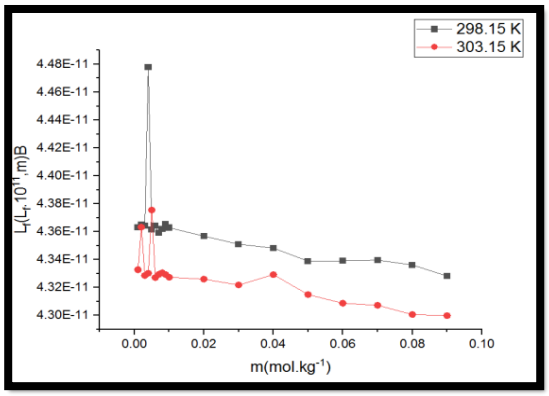

Fig.(b)

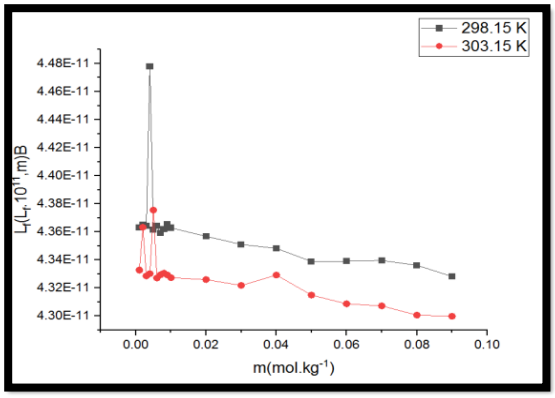

Fig.(c)

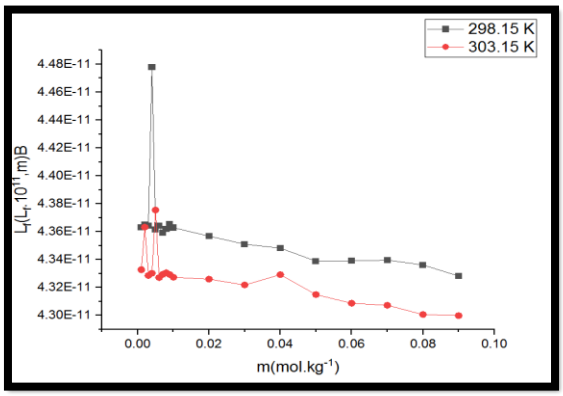

Fig.(d)

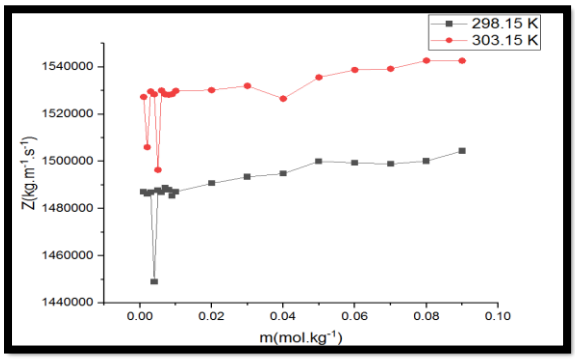

Fig.(e)

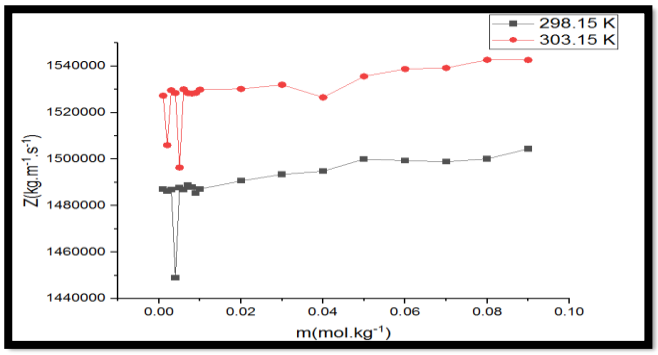

fig.(f)

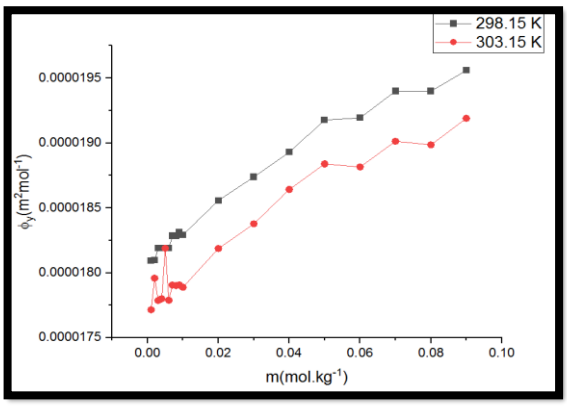

Fig.(g)

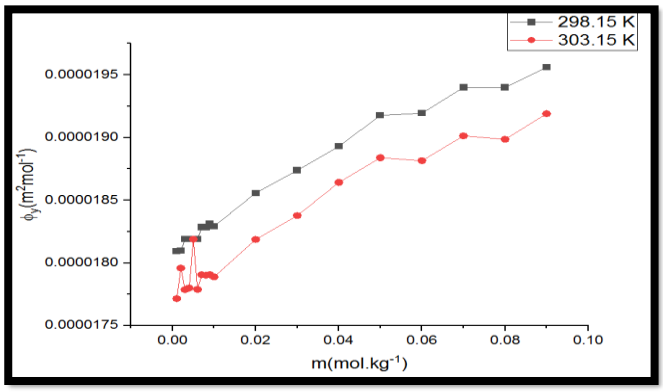

fig.(h)

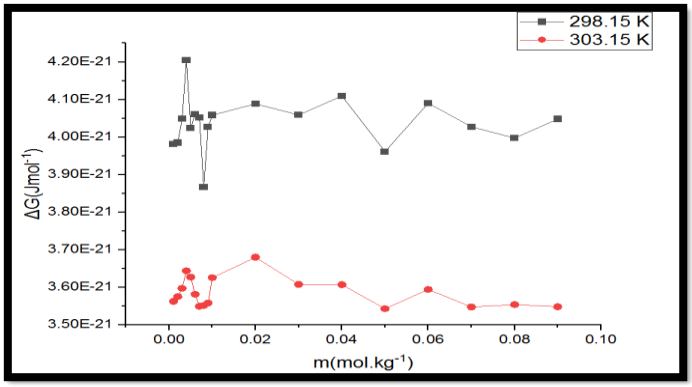

Fig.(I)

Figure 2. Effect of Adiabatic compressibility, Free length, Free volume, Internal pressure, Acoustic impedance, Relaxation time, Molar volume, Rao constant, Gibbs free energy, of Pyridoxine Hydrochloride at 298.15K and 303.15K

IV. CONCLUSION

Figure 1(a) illustrates how temperature and concentration affect an unstudied aqueous solution's ultrasonic velocity. The intermolecular free length is inversely correlated with the ultrasonic velocity (u). Intermolecular free length is important because it affects the speed of sound in a fluid condition.

The intermolecular free length varies when an ion is present. As a result, a solution's ultrasonic velocity is different from the solvents. Due to the rise in concentrations, the ultrasonic velocity must rise as the free length falls [11-12]. The solutes' structural characteristics cause a rise in the system's ultrasonic velocity. The substance that increases ultrasonic speed is a structure-maker (SM). The rise in velocity at higher temperatures denotes a weakening of the solute-solvent interactions.

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) When a solution is concentrated, its viscosity rises, and when it is heated, it falls. The attraction forces between molecules in a liquid restrict molecules from moving freely. The capacity of the solute to form structures is shown by the fact that at lower temperatures, viscosity is found to be larger because of intermolecular forces brought on by an increase in solute, which attracts the solvent to the solute [13]. The viscosity drops as the temperature rises because the cohesive forces become weaker.

Fig. 1 (c) depicts the density fluctuation of pyridoxine hydrochloride, which, as would be predicted, rises with concentration and falls with temperature. The density of the solution increases together with the concentration of solute particles. Since density rises with concentration, solute-solvent and solvent-solvent interactions are said to be weaker. Due to a reduction in volume brought on by the presence of solute molecules, density increases with concentration. In other words, the solvent's structure-maker is responsible for the solute's increased density. A similar indication that the solvent is a structure-breaker is the reduction in density with increasing concentration. Bonding, most likely H-bonding, may also happen via interactions between solvents [14–15].

As the density and viscosity of the solution increase, so does its compressibility. The hydrogen bonding between like or unlike components in a solution either increases or decreases due to compressibility. The values of adiabatical compressibility increase as the

concentration of pyridoxine hydrochloride solution increases [Fig 2(a)]. The decrease in adiabatic compressibility suggests the presence of a strong solute-solvent interaction, which could be attributed to strong intermolecular hydrogen bonding between pyridoxine hydrochloride and water molecules. The intermolecular free length decreases gradually [Fig. 2(b)]. The decrease in intermolecular free length value supports the presence of strong solute-solvent interaction, which could be attributed to the presence of strong intermolecular hydrogen bonding between pyridoxine hydrochloride and water molecules.

Increased hydrogen bonding between the solute and solvent molecules, resulting in less space between them, could explain the decrease in free volume with concentration. Figure 2(c) shows how free volume changes as concentration and temperature rise [16]. Internal pressure is an important metric for understanding the intermolecular interactions in pyridoxine hydrochloride aqueous solution. Internal pressure increases with increasing concentration but decreases with increasing temperature, as shown in Fig. 2(d) (d). The increase in internal pressure could be caused by the strengthening of the cohesive force between the molecules.

As the temperature rises, the thermal energy of molecules rises, causing the thermal agitation of ions to rise [17]. Acoustic impedance is the product of density and ultrasonic velocity. As shown in Fig. 2(e), the acoustic impedance increases with increasing solute concentration and temperature. Strong interactions between solute-solvent molecules can cause an increase in the value of acoustical impedance as temperature rises, whereas weak molecular interactions cause a nonlinear trend in the value of acoustical impedance [18]. Relaxation time is an important metric to consider when analysing molecular aggregation in solution. The relaxation time increases with solute concentration but decreases with temperature, indicating more interactions between the solute and the solvent fig.(2f)

Molar volume is a useful metric for studying the intermolecular interactions of a solution. It is the volume occupied by one mole of a substance at a given temperature and pressure. Figure 2(g) shows that molar volume increases with concentration and temperature, indicating that pyridoxine hydrochloride aqueous solution has strong solute-solvent interactions [19].

Figure 2 (h) Rao's constant increases linearly with concentration and temperature. Rao's constant rise indicates that there are strong intermolecular interactions in the current system [20]. Because of the H-bonding of unlike molecules in the solution, Gibb's free energy reveals 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 shown 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.

V. CONCLUSION

The ultrasonic velocity, viscosity, density and other acoustical parameters of an aqueous solution of pyridoxine hydrochloride were measured in this study at different concentrations (0.001-0.09) 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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