



## PREDICTION OF MOLECULAR INTERACTION OF L-ALANINE AT ACIDIC, BASIC AND ISOELECTRIC PH BY DENSITY, VISCOSITY, SOUND VELOCITY AND CONDUCTANCE MEASUREMENT

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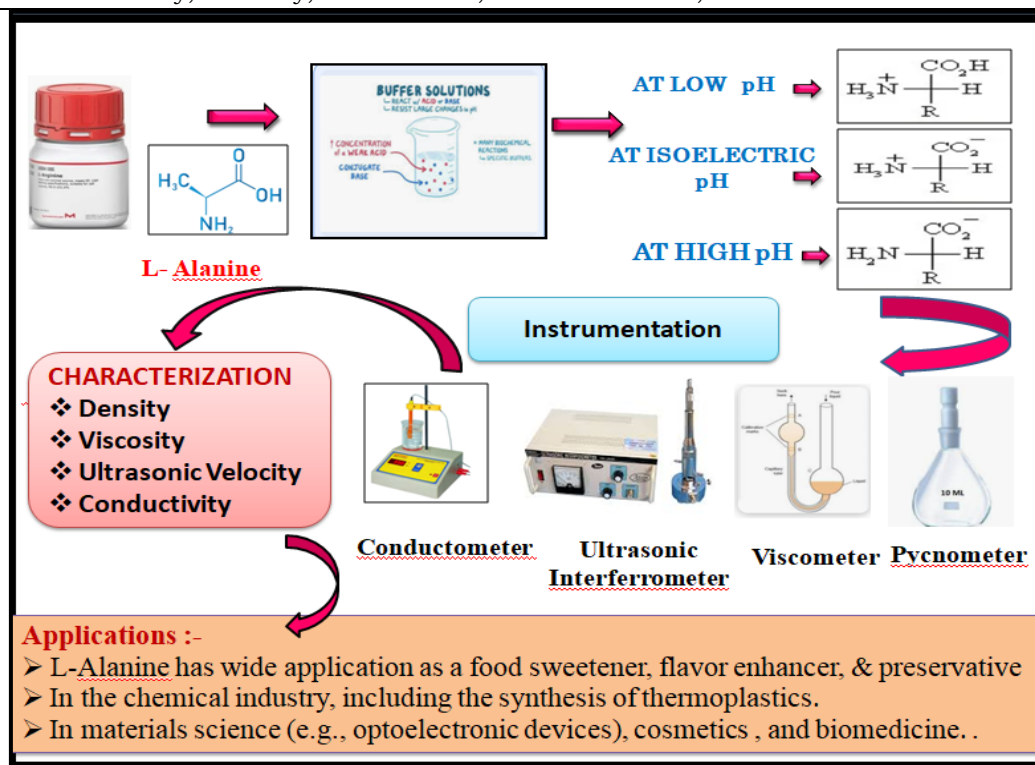
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### ABSTRACT:

Molal conductance depends upon figure of ions exist in the solution. It is openly related with the ions forms on dissolution of solute in solvent. The mobility of ions because of repeated collision among solute ions and solvent molecules since the mean free path of molecules in aqueous medium is very small is suggested by Shcherbakov, V. V., Artemkina, Y. M., Akimova, I. A., & Artemkina, I. M. (2021). Similarly the internal pressure ( $\pi$ ) of the experimental solution is a lone factor which varies due to all the internal exchanges like hydration, ion-solvent exchanges, quantum reflex forces of scattering and dielectric constant effect is explained by Han, M., Li, T. C., Chen, X., & Yang, H. Y. (2024). Therefore solute ion-solvents interaction in investigational solution may be derived by using internal pressure & conductance. The ultrasound velocity and molal conductance are measured for L-Alanine at acidic, basic and isoelectric pH by using buffer solution as a solvent at various molality and hotness. The results are used to discuss the performance of solute ions and solvents molecules in terms of molecular interactions.

**Keywords:** Sound velocity, Viscosity, Conductance, Internal Pressure, Ion-solvent interactions.



## INTRODUCTION:

It is well known that electrolytic conductance is a measure of a material's capability to permit electric current to flow through it. The new trend is to explain electrolytic conductance in terms of molal conductance. It is the capability to conduct electricity by measuring the conductance of all ions created by single mole of an electrolyte in a given solution is explained by Mizuhata, M. (2022). An electrolytic conductance depends on ions present in the certain liquid. The primary factors affecting conductance are molality of experimental solution, nature of solute, temperature, the nature of the solvent (polarity & viscosity), and size of the ions. It is directly linked with the creation of ions of solute in solution is explore in the research of Antonio, M. R., Nyman, M., & Anderson, T. M. (2009) According to Walden's rule for same electrolyte in different solvents system, the product of its molal conductivity at infinite dilution ( $\Lambda^\circ$ ) and the solvent's viscosity ( $\eta$ ) is about a constant Molal conductance also depends on hotness of the solvent system. The revision of internal pressure ( $\pi$ ) in investigational solution gives assets of data about the liquid medium is cleared by Termini, G. (2023). According to Reichardt, C. (2007) It is the essential character accustomed to clarify the thermodynamic character of L-Alanine at low (acidic), isoelectric pH (neutral) and high pH (basic). Both the parameters are affected by rather changes occurring in the solvent medium either due to molecular exchange or hotness change. The intermolecular interactions in solvent system (buffer solution) can be explained by the study of internal pressure. It is designed by measurement of ultrasound velocity showed that internal pressure ( $\pi$ ) and conductance are correlated. Both parameters are affected by number of ions exists in the given system is explore by Rapier, C. E., Shea, K. J., & Lee, A. P. (2021) Hence, these parameters may be interpreted in terms of molecular excha It is well known that electrolytic conductance is a measure of a material's capability to permit electric current to flow through it. The new trend is to explain electrolytic conductance in terms of molal

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## EXPERIMENTAL SECTION:

### MATERIALS:

Analytical reagent L- Alanine is used in the present analysis. All solutions of L-Alanine (at specific pH) were prepared by using double distilled water. Buffer solution is used as solvent. All the readings were taken in the concentration range 0.02, 0.04, 0.06, 0.08 and

0.10 molal and temperature range 293.15K to 313.15 K with the interval of 5K

#### METHODS:-

The densities of the solutions were work out accurately using digital densitometer [Model-Mettler Toledo]. Ostwald's viscometer was employed to measure viscosity of solution which was calibrated by double distilled water at all five temperatures. The measurement of ultrasound velocity was carried out by means of ultrasonic multi frequency interferometer (Mittal Type: M-83 Model ), operating at 2 MHz frequency with an accuracy of  $\pm 2$  m/s. Digital conductivity meter is used to find the conductance of the investigational solution. The temperature of the system was maintained by using thermostat. Buffers solution of expected pH was prepared by using  $\text{CH}_3\text{COOH}$  &

$\text{CH}_3\text{COONa}$  and used as stock solvent. Experimental solution of 0.02 molal to 0.10 molal for L-Alanine were prepared by using stock solvent.

#### RESULTS AND DISCUSSIONS :

The calculated values of molal conductance ( $\lambda_m$ ) and internal pressure ( $\pi_i$ ) from the observed values of ultrasonic velocity ( $v$ ), density ( $\rho$ ), viscosity ( $\eta$ ) and conductance ( $K_c$ ) by using typical relation .

Molal Conductance ( $\lambda_m$ ) =  $K_c [1000/m]$  Where,  $K_c$  - Specific Conductance,

$m$ - molality of solution

Internal Pressure (Pa)

$$(\pi_i) = bRT(k\eta/u)^{1/2} (\rho^{2/3} / M \text{ eff}^{7/6})$$

Where  $b$  is Packing factor,  $R$ - Gas constant,  $T$ - Temperature,  $k$  - Constant =  $4.28 \times 10^{-09}$ ,  $u$  and  $\rho$  are ultrasonic velocity and density.

**Table -1 : Molal Conductance ( $\lambda_m$ ) : L- Alanine**

Sr.No.	Temperature (K)	Concentration Mol/Kg	In aqueous Medium ( $\lambda_m$ )	At Low pH ( $\lambda_m$ ) (pH=4.50)	At isoelectric pH ( $\lambda_m$ ) (pH=6.02)	At High pH ( $\lambda_m$ ) (pH=6.30)
1	293.15K	0.02	1336200	243780	297840	1841100
2		0.04	749700	120870	147390	915450
3		0.06	559300	79900	97240	606900
4		0.08	427125	59032.5	72165	453900
5		0.10	459000	46512	57120	361080
1	298.15K	0.02	1586100	275910	344250	2085900
2		0.04	887400	136935	170595	1035300
3		0.06	668100	90780	112540	686800
4		0.08	515100	67065	83512.5	513825
5		0.10	627300	52836	66096	410040
1	303.15K	0.02	1800300	312630	388620	2361300
2		0.04	1025100	155295	192525	1173000
3		0.06	763300	102850	127160	776900
4		0.08	610725	76627.5	94222.5	578850
5		0.10	790500	60996	74664	461040
1	308.15K	0.02	2029800	348330	421770	2616300
2		0.04	1157700	172890	209355	1297950
3		0.06	889100	114410	138210	860200
4		0.08	731850	84915	102510	638775
5		0.10	977160	67320	81090	506940
1	313.15K	0.02	2249100	385560	474300	2830500
2		0.04	1305600	191760	232815	1410150
3		0.06	1013200	127330	153850	936700

4		0.08	856800	94987.5	114367.5	699975
5		0.10	1144440	75174	90576	557940

**Table No. 2 : Internal Pressure ( $\pi$  i ) : L-Alanine**

Sr.No	Temperature (K)	Concentration Mol/Kg	In aqueous Medium ( $\pi$ i )	At Low pH ( $\pi$ i ) (pH=4.50)	At isoelectric pH( $\pi$ i ) (pH=6.02)	At High pH ( $\pi$ i ) (pH=6.30)
1	293.15K	0.00	2.84E+09	4.41E+08	4.05E+08	4.55E+08
2		0.02	2.86E+09	4.43E+08	4.07E+08	4.57E+08
3		0.04	2.88E+09	4.44E+08	4.09E+08	4.59E+08
4		0.06	2.9E+09	4.46E+08	4.1E+08	4.6E+08
5		0.08	2.92E+09	4.47E+08	4.12E+08	4.62E+08
6		0.10	2.94E+09	4.49E+08	4.14E+08	4.63E+08
1	298.15K	0.00	2.71E+09	4.05E+08	3.76E+08	4.18E+08
2		0.02	2.71E+09	4.07E+08	3.78E+08	4.2E+08
3		0.04	2.71E+09	4.08E+08	3.8E+08	4.21E+08
4		0.06	2.71E+09	4.1E+08	3.81E+08	4.22E+08
5		0.08	2.72E+09	4.12E+08	3.83E+08	4.23E+08
6		0.10	2.72E+09	4.17E+08	3.85E+08	4.25E+08
1	303.15K	0.00	2.59E+09	3.83E+08	3.56E+08	3.93E+08
2		0.02	2.59E+09	3.83E+08	3.57E+08	3.94E+08
3		0.04	2.58E+09	3.83E+08	3.57E+08	3.95E+08
4		0.06	2.58E+09	3.85E+08	3.58E+08	3.96E+08
5		0.08	2.58E+09	3.84E+08	3.6E+08	3.97E+08
6		0.10	2.58E+09	3.84E+08	3.61E+08	3.98E+08
1	308.15K	0.00	2.49E+09	3.63E+08	3.35E+08	3.69E+08
2		0.02	2.49E+09	3.64E+08	3.37E+08	3.7E+08
3		0.04	2.49E+09	3.66E+08	3.39E+08	3.71E+08
4		0.06	2.49E+09	3.67E+08	3.4E+08	3.72E+08
5		0.08	2.5E+09	3.68E+08	3.42E+08	3.73E+08
6		0.10	2.5E+09	3.7E+08	3.44E+08	3.74E+08
1	313.15K	0.00	2.4E+09	3.52E+08	3.25E+08	3.57E+08
2		0.02	2.4E+09	3.53E+08	3.25E+08	3.58E+08
3		0.04	2.4E+09	3.54E+08	3.25E+08	3.59E+08
4		0.06	2.4E+09	3.54E+08	3.27E+08	3.6E+08
5		0.08	2.41E+09	3.55E+08	3.27E+08	3.61E+08
6		0.10	2.41E+09	3.56E+08	3.28E+08	3.62E+08

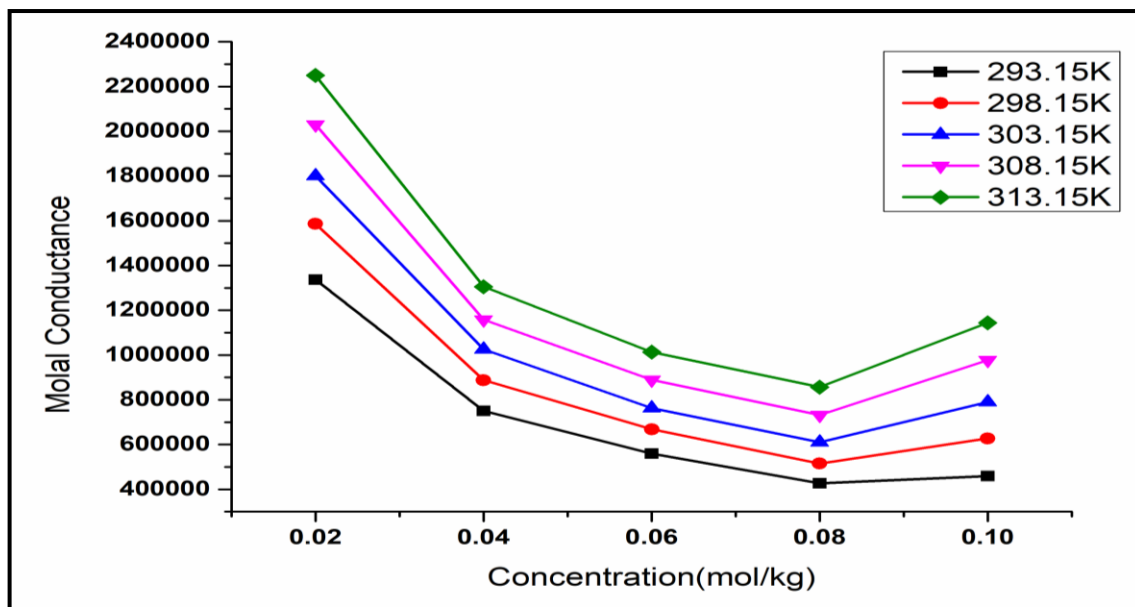


Fig. 1: Molal Conductance ( $\lambda_m$ ) Vs Concentration (Solvent-Water)

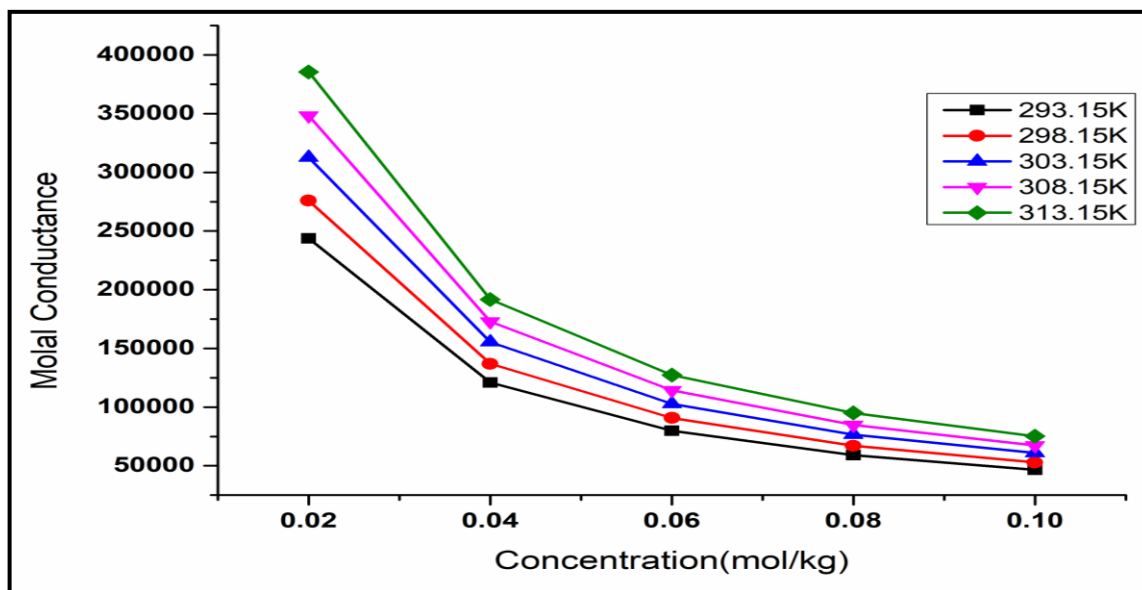
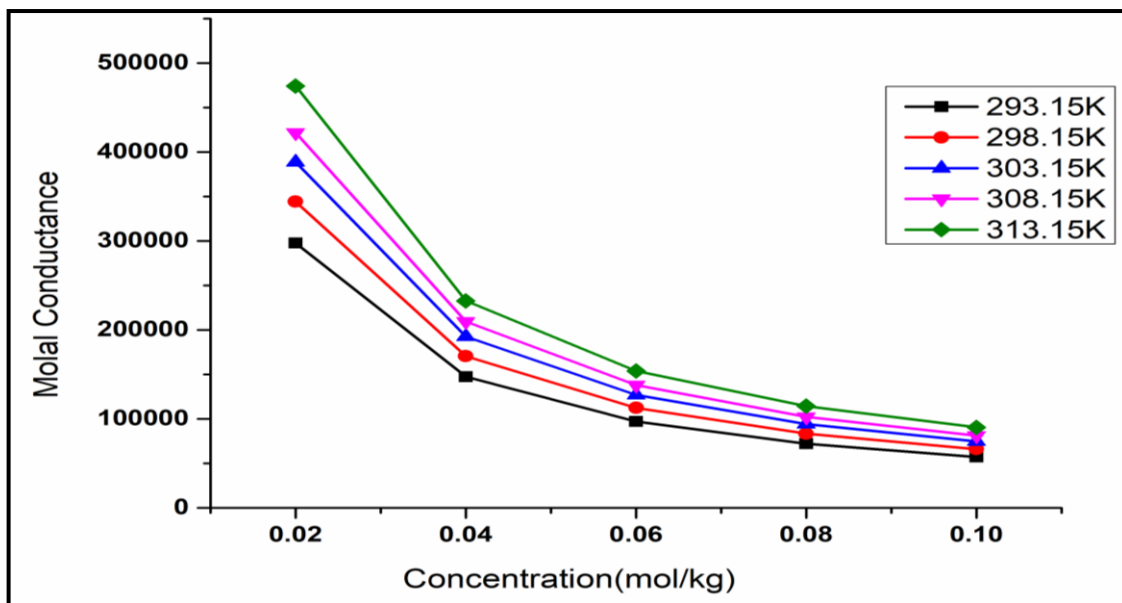
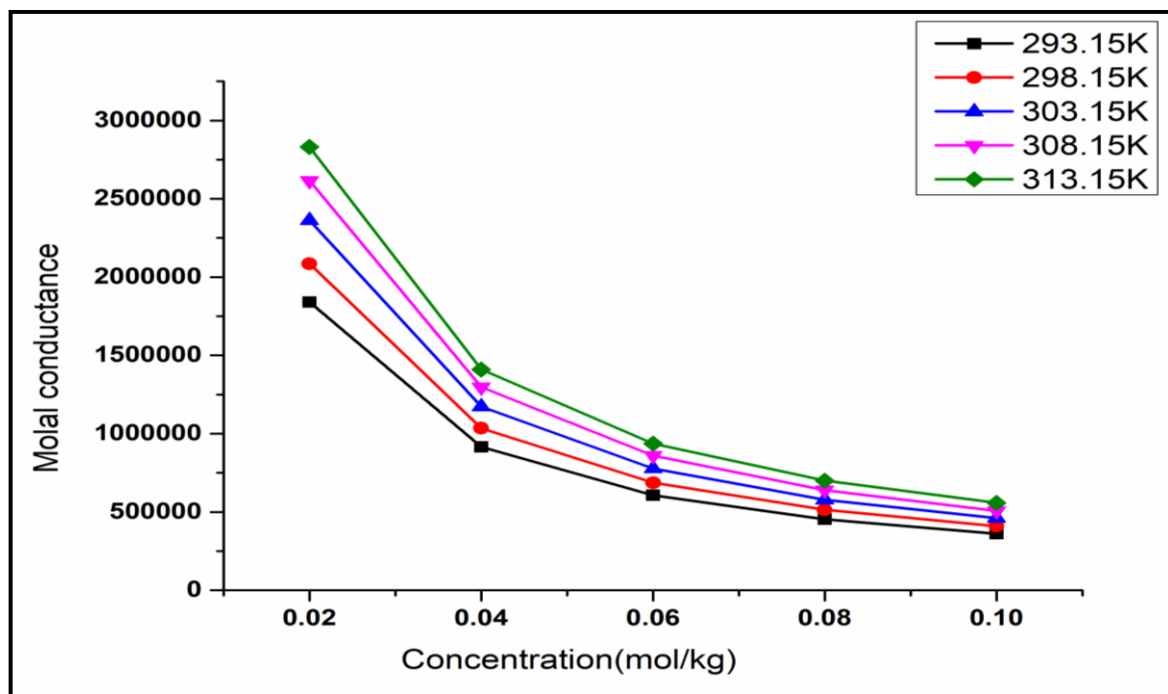


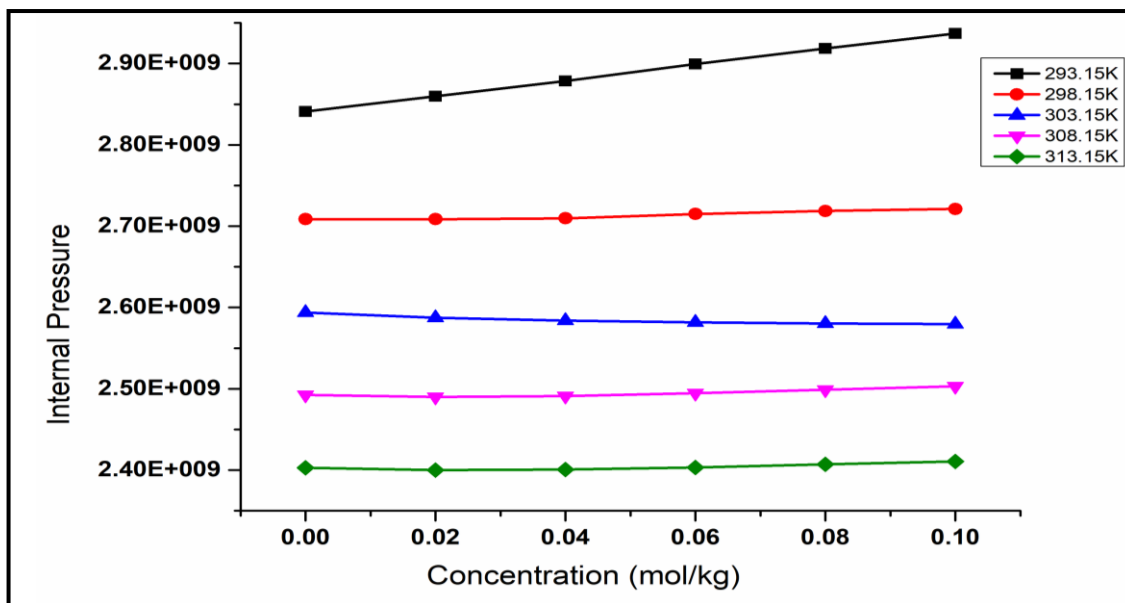
Fig. 2: Molal Conductance ( $\lambda_m$ ) Vs Concentration (Solvent - Buffer solution at low pH)



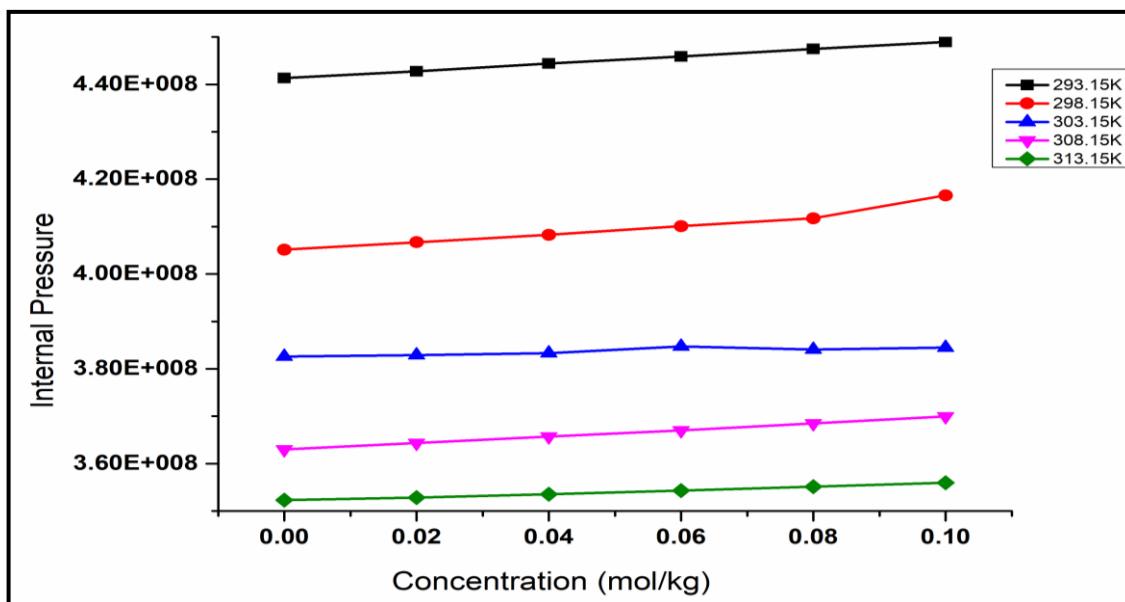
**Fig. 3:** Conductance ( $\lambda m$ ) Vs Concentration (Solvent - Buffer solution at isoelectric pH)



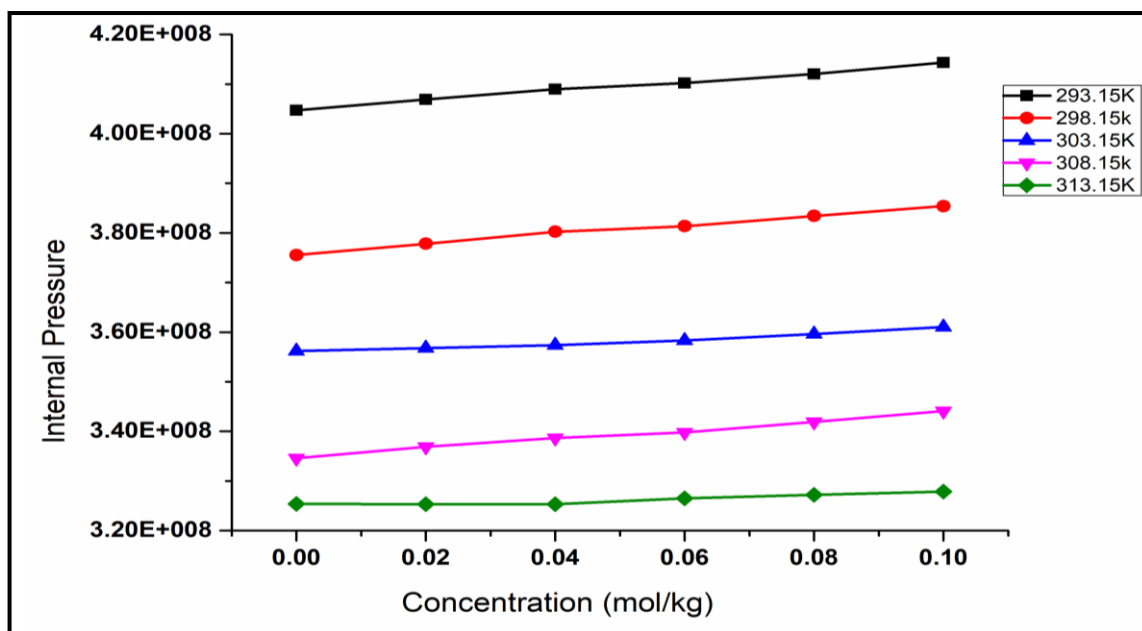
**Fig. 4:** Conductance ( $\lambda m$ ) Vs Concentration (Solvent - Buffer solution at high pH)



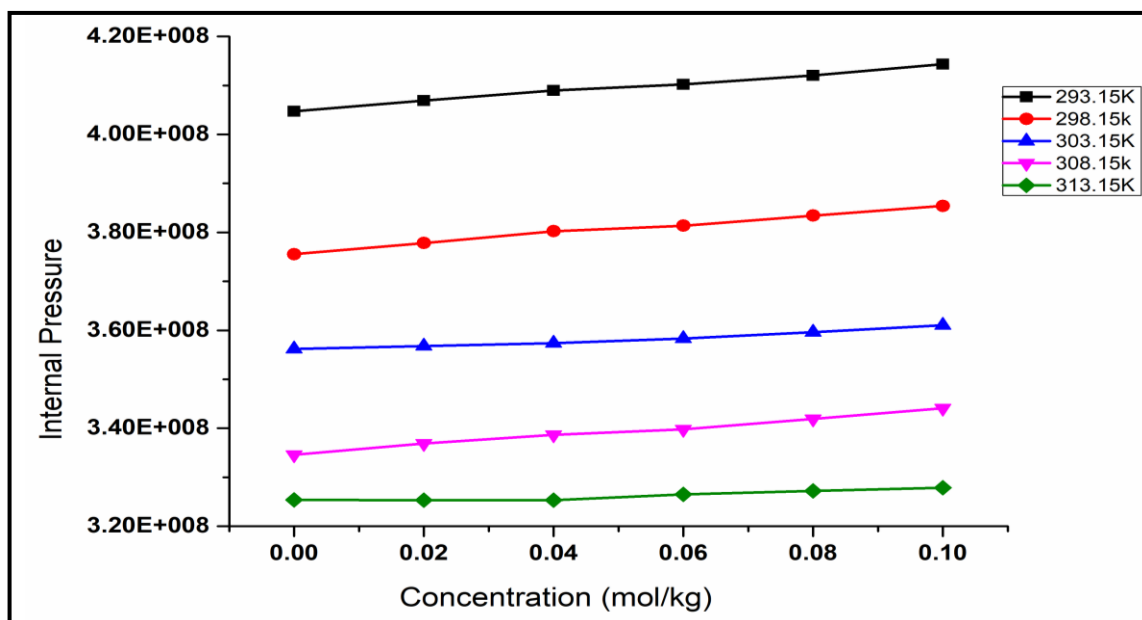
**Fig. 5:** Internal Pressure ( $\pi_i$ ) Vs Concentration (Solvent-Water)



**Fig. 6:** Internal Pressure ( $\pi_i$ ) Vs Concentration (Solvent-Buffer solution at low pH)



**Fig. 7:** Internal Pressure (ri) Vs Concentration (Solvent-Buffer solution at isoelectric pH)



**Fig. 8:** Internal Pressure (ri) Vs Concentration (Solvent-Buffer solution at high pH)

The values of molal conductance ( $\lambda_m$ ) and internal pressure (ri) for the different system of L-Alanine ie, in aqueous medium, at low pH, at isoelectric pH and at high pH are presented in Table - 1 and 2. Fig. 1, 2, 3 and 4 shows the variation in molal conductance of L- Alanine with respect to molal concentration respectively.

Praharaj, M. K., Satapathy, A., & Ahmed, I. (2017) reported that the measurement of molal conductance is extensive and practical techniques for quality manage purposes. It is observed that as molality increases, molal conductance decreases. It resembles with the theoretical aspect of molal conductance. It says

that on dilution, molal conductance increases. At higher molal concentration, ions are closer together. Electrostatic attraction/repulsion and ionic atmosphere effects reduce ionic mobility [Kusova, A. M., Sitnitsky, A. E., & Zuev, Y. F. (2021)]. As concentration growing, the solution becomes more viscous. Higher viscosity slows down ion mobility, further lowering conductance. El Halimi, M. S., Poli, F., Mancuso, N., Olivieri, A., Mattioli, E. J., Calvaresi, M., ... & Soavi, F. (2021) noticed that At higher Molal concentration, some ions associate (especially at low or high pH). This reduces the number of free charge carriers. As hotness rises, solution becomes less viscous. So the ions move more freely i.e, higher ionic mobility hence higher  $\lambda_m$ . Also the hotness favors dissociation of weak electrolytes due to more free ions conductivity gains. So the observations of molal conductance for all four systems are as predictable. The changes in the values of internal pressure ( $\pi_i$ ) of L-Alanine are graphically represented in fig. 5,6,7 and 8. All the four system shows linear variation in the values of internal pressure. It slowly gain with ascend in concentration. It indicates that molecular exchanges are maximum. Reduction in molal conductance with gain in concentration is due to loss in ionic mobility of the ions in the system as shown in fig. 1,2,3 and 4. Shrink in ionic mobility loses its power in doing work against internal pressure ( $\pi_i$ ) [Kreuer, Klaus-Dieter., (2013)]. In other words, when an ion is made to move under a constant electric force in liquids & vacuum, its loss in velocity is a function of the internal pressure of the solution. The values of internal pressure varies linearly with molality for all the system as shown in fig 5,6,7 and 8. Somero, G. N. (2003) reported that In amino acids, internal pressure depends on both molality and pH of buffer solution. Internal pressure generally increases slightly with growing concentration. This is because closer stuffing of ions enhances solute-solvent and solute-solute interactions, leading to stronger consistent forces. In neutral aqueous medium (water pH ~ 6-7), L- Alanine has strong dipole-dipole relations and promotes dense packing of solvent molecules. This results in larger

electrostriction of water and hence superior internal pressure than at low pH, at high pH and at isoelectric pH. At low pH (acidic medium), L-Alanine exist mainly in the cationic form ( $+NH_3^+$ ). According to Ludwig, V., da Costa Ludwig, Z. M., Valverde, D., Georg, H. C., & Canuto, S. (2020), Electrostatic repulsion reduces firmness, but hydration effects gain internal pressure slightly, At high pH (basic medium), they are mostly exist in the anionic form ( $-COO^-$ ). Strong hydration shells also contribute to higher internal pressure. At the isoelectric point (pI), the L-Alanine exists in a zwitterionic form ( $+NH_3^+ - COO^-$ ). In this state, the positive and negative charges balance internally, making the molecule more packed thus net electrostriction of water is less compared to fully cationic or anionic states [Tonti, L., & Floris, F. M. (2021)]. Hence, internal pressure is lower at isoelectric pH than at low pH and high pH.

#### CONCLUSION:

The linear variation of internal pressure with concentration at different temperatures shows the presence of strong, well-defined solute-solvent interactions & absence of any anomalous aggregation in the system. The enlarge in internal pressure and diminish in molal conductance with rise in concentration at all given temperatures indicates compactness of solute and solvent molecules it is also studied by Da Silva, D. A., Messias, A., Fileti, E. E., Pascon, A., Franco, D. V., Da Silva, L. M., & Zanin, H. G. (2022) Thus above results could imply greater ability of strong interaction. The internal pressure of amino acids at different pH values tends to increase slightly with concentration due to enhanced molecular interactions, but the extent of increase depends on whether the amino acid is in cationic, anionic, or zwitter-ionic form. L-Alanine solution at low pH and at high pH exist in ionic form (cationic or anionic). it forms strong hydration shell and contribute higher internal pressure. The internal pressure is minimum at isoelectric pH due to balanced charge distribution and reduced hydration forces. The trend in the variation of values of internal

pressure ( $\pi$ ) is found similar at all temperatures. [Liu, S., Zhang, J., Sun, Z., & Han, D. (2023)]

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