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Exploring Intermolecular Interactions of L-Isoleucine in Aqueous Magnesium Nitrate and Magnesium Sulphate Solutions Across Temperature Variations

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Abstract

Acoustic and volumetric studies were conducted on aqueous solutions of L-isoleucine in the presence of magnesium nitrate and magnesium sulphate solution at temperatures of 288.15K and 298.15K. Ultrasonic sound waves propagating through these experimental solutions demonstrated a direct association between the different molecular interactions among the solution's constituents, both strong and weak. The rising electrostriction of water molecules around the solute and co-solute ions decreased isothermal compressibility (K_T). Significant ion-ion, ion/hydrophilic-hydrophilic, and ion/hydrophobic-hydrophobic interactions happened among various segments of solute and co-solute ions, while ion-solvent interactions dominated. The processes of solvation and ion association brought about the reformation of the water structure. Numerous variables were assessed and highlighted the increased ion-solvent interactions, ion-pair formation, and structure-building capabilities of L-isoleucine in the presence of $MgSO_4$ / $Mg(NO_3)_2$.

Keywords: Amino acid; Electrolytes; Proteins, Interactions; Free length.

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1. Introduction

Over the last two decades, researchers have studied the protein's hydration using acoustical and ultrasonic techniques. These properties are highly responsive to the extent and characteristics of hydration [1-3]. Proteins are difficult to investigate directly because of their complex molecular composition. Thus, a more practical approach would involve examining less complex model substances, including amino acids, that serve as the fundamental constituents of proteins. Amino acid ($-NH_2$) and carboxylic acid ($-COOH$) monomers polymerize to produce proteins. The ($-NH_2$) base and ($-COOH$) acid complicate the chemistry of amino acids. one (H^+) ion is moved from one end of the molecule to another in an aqueous solution to form a zwitterion. Zwitterion molecules have a zero net charge while possessing positive and negative charges [4,5]. The nature of the R-groups is the only difference among most amino acids. Hydrophobic amino acids are those that hate water and

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have non-polar substituents. Amino acids that can establish hydrogen bonds with water and have polar R-groups are known as hydrophilic [6]. The other substituents for amino acids are highly hydrophilic since they have neutral pH and can carry either a positive or negative charge in aqueous solutions [7]. Drugs, carbohydrates, hydro tropes, and physiologically significant substances influence protein stability in a solution. Electrolytes affect protein structure by changing denaturation, solubility, and activity [8,9]. The characteristics related to the movement and energy dynamics of amino acids and peptides within water-based solutions are crucial to pharmaceutical and medicinal chemistry, especially when combined with additives and water [10]. Crucial thermodynamics offer a valuable understanding of non-covalent intermolecular interactions, greatly impacted by the neighbouring solvent and solute molecule [11].

Most research on amino acids has been done in aqueous solutions, either in their pure form or combined with other substances. Still, intermolecular interactions such as ion-solvent, solute-solvent, and ion-dipole interactions between L-isoleucine and aqueous magnesium salt solutions have not been extensively studied, with a notable absence of comprehensive analyses on the thermo-acoustic and volumetric properties of L-isoleucine in such environments [12,13]. The literature [14-18] does not address these properties in detail. This study aims to fill this gap by conducting thorough thermo-acoustical investigations of intermolecular interaction.

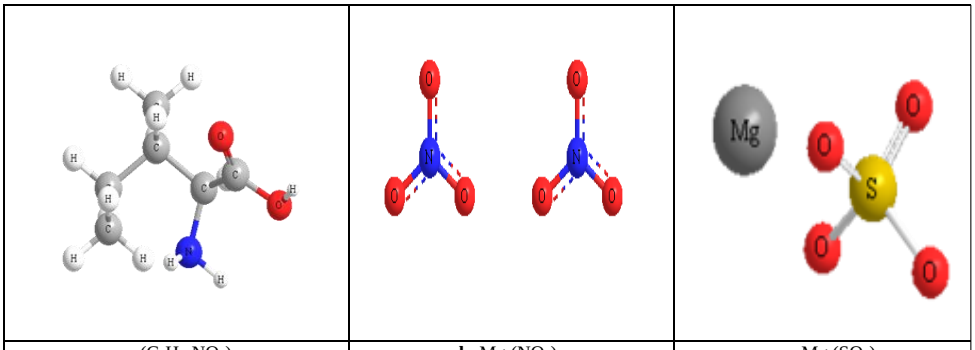
Amino acid studies provide a better understanding of the hydration behaviour of proteins and their interactions with electrolytes. As basic monomer units, amino acids are essential parts of proteins and are involved in many biological processes. L-isoleucine stands out among the essential amino acids because of its branched-chain structure required for haemoglobin creation, blood sugar management, muscle maintenance, energy production, and protein synthesis. The hydrophobic side chain of L-isoleucine is well-known and greatly impacts how it interacts with water and salts. Because of this particular behaviour, L-isoleucine is an essential amino acid for studying the interactions between amino acids and their surroundings, which can help understand the folding and stability of proteins. The special qualities of L-isoleucine and its intricate interactions in aqueous and salt solutions have received little attention. However, studies on amino acids and their interactions with solvents have been conducted extensively. By thoroughly examining these interactions and providing fresh perspectives on the dynamics of L-isoleucine in solution, our work seeks to close this gap [19].

The present study investigated the impact of different concentrations of l-isoleucine in electrolytes on the acoustic characteristics of the solutions. From the experimental values of sound velocity (U) and density (ρ), the various thermo-acoustic parameters, such as Acoustic impedance (Z), specific heat (γ), etc., have been calculated. These inferred parameters elucidate the solute-solvent interactions present in the solutions. The physicochemical characteristics are crucial for comprehending the interactions between ions, undissociated solute molecules, and solvent molecules in the studied binary mixes, including ion-solvent, ion-dipole, and solute-solvent interactions. Moreover, they illustrate the capacity of the components to create structural arrangements in real-world scenarios.

2. Experimental Details

2.1. *Materials*

L-isoleucine (99.9 %), $Mg(NO_3)_2$ (≥ 0.99 %) and $MgSO_4$ (≥ 0.99 %) were purchased form Hi-Media Private Limited, Mumbai, India. 3D structures of L-isoleucine and solvents $Mg(NO_3)_2$ and $Mg(SO_4)_2$ are shown in Fig. 1.



a. ($C_6H_{13}NO_2$) **b.** Mg (NO_3)$_2$ **c.** Mg (SO_4)

Fig. 1. 3D Structural forms of solute L-isoleucine, solvents $Mg(NO_3)_2$ and $MgSO_4$.

2.2. *Method*

The speed of sound was measured using a 2 MHz ultrasonic interferometer crafted by "Mittal Enterprises Ltd.", New Delhi. The instrument boasts a precision level of ±0.1 %. The density determination involved a 10 mL specific gravity density bottle and a digital electronic balance, guaranteeing a high accuracy of ±0.01 Kg/m^3. A digitally controlled constant temperature water bath, under electrical regulation, was employed. It maintained the experimental solution within a double-walled steel measuring compartment at consistent temperatures. The accuracy of temperature readings among themselves was within 0.1K. The precision in measuring the speed of sound and density underwent evaluation by comparing recorded water-based values at different temperatures with corresponding literature values. Discrepancies revealed errors within a range of ±0.2 ms^{-1} for sound density and ±0.0002 g cm^{-3} for velocities.

3. Result and Discussion

Figs. 2 and 3 display the density of L-isoleucine and the sound velocity in water solutions containing magnesium salt. Evidence indicates a positive correlation between the density of a solution and the number of amino acids it contains. Amino acids, in particular, enhance the molecular arrangement of water, increasing density. The data presented in Table 1 shows that increased temperature leads to decreased density. The temperature decrease

signifies that a rise in molecular kinetic energy diminishes the interactions between solute and solvent, reducing density. The study also found that solutions comprising $MgSO_4$ and amino acids have higher densities than aqueous $Mg(NO_3)_2$ solutions. The density of a solution is directly proportional to the concentration of salt in the solution [20-24]. This behavior can be attributed to hydrophilic and hydrophobic constituents in these salt solutions [25,26]. Enhancing the compactness of a structure leads to an increase in its density. This phenomenon is especially noticeable when it comes to carbohydrates. The behavior of ultrasonic waves in solutions is modulated by variables such as temperature and concentration [27]. The observed behavior can be explained by the increased cohesive contacts between l-isoleucine, water, and electrolytes, specifically involving the interactions between the solute and the solvent. Salt in the solution decreases the concentration of readily available amino acids due to heightened intermolecular interactions [28,29].

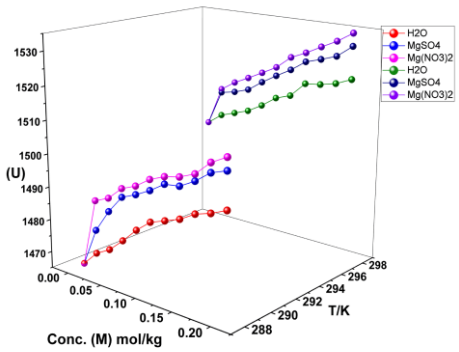


Fig. 2. Plot of velocity across different temperatures and concentrations.

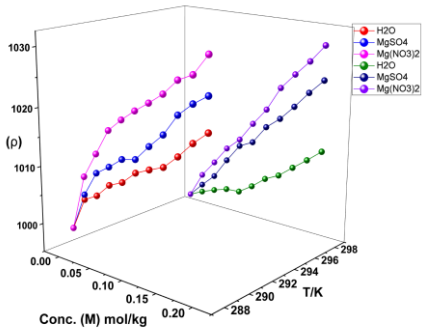


Fig. 3. Plot of density across different temperatures and concentrations.

The pattern shown in Fig. 4 indicates that when the concentration and temperature of L-isoleucine rise, the intermolecular free length value decreases. The strong intermolecular interactions between the molecules of the L-isoleucine and the salts are demonstrated by this diminishing value. As L-isoleucine concentration in solutions rises, the intermolecular free length values fall, indicating a decrease in the distance between the solute and solvent molecules [30,31]. The solution's components form a denser arrangement, which increases the potential energy of contact between them and produces this effect. Lower free length (L_f) values could highlight the development of closely spaced molecules or structural cohesiveness-values of free length calculated by Equation 1.

$$(L_f) = \frac{K\beta}{2} \quad (1)$$

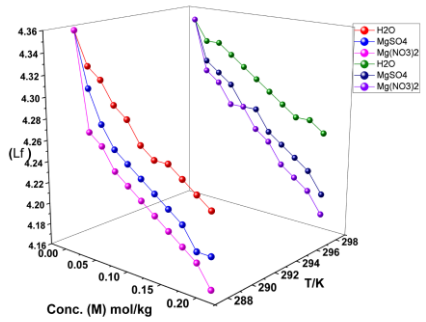


Fig. 4. Plot of free length across different temperatures and concentration.

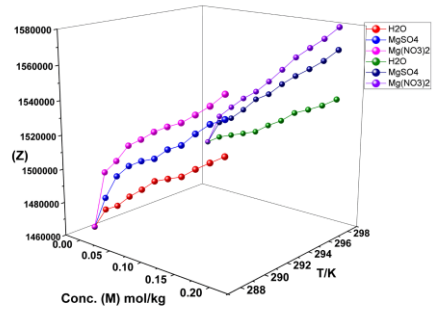


Fig. 5. Plot of Acoustic impedance across different temperatures and concentration.

Acoustic impedance (Z) increases with concentration (Fig. 5), indicating the effectiveness of solute-solvent interactions. Using density and ultrasonic velocity, acoustic impedance is calculated using equation 2. where ρ is density and U is velocity.

$$(Z)= U \times \rho \quad (2)$$

The liquid medium's resistance to sound waves and the strength of its elastic property, which is dependent on structural changes in the solution, is determined by gradually higher acoustic impedance (Z) values in aqueous magnesium nitrate and magnesium sulfate as well as an increase in the proposal that the medium starts to achieve in terms of acoustic impedance for each system when the concentrations of the hydrotropic agent and the solute are equal ionization, molecular connections, and the solute-solvent relationship all affect compressibility, as evidenced by the high solute-solvent interaction in l-isoleucine solutions combined with salts [32].

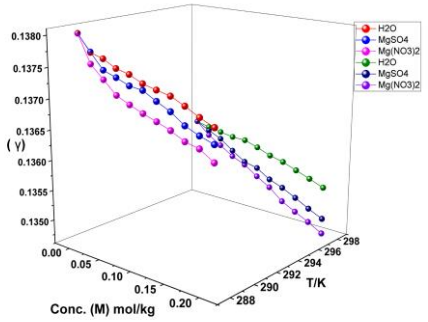


Fig. 6. Plot Specific heat across different temperatures and concentration.

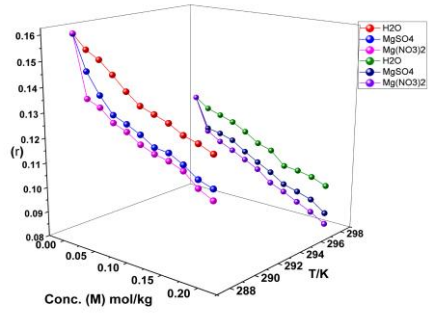


Fig. 7. Plot of Relaxation Strength across different temperatures and concentrations.

The amino acid (L-isoleucine) combination contains water 0.1 M aqueous $Mg(NO_3)_2$ and $MgSO_4$ with weight fractions of 0.02 M to 0.2 M, and the value of specific heat is calculated using Equation 3.

$$(\Upsilon) = \frac{17.1}{T^{\frac{4}{9}} \times \rho^{\frac{1}{3}}} \quad (3)$$

Table 2 shows the calculated values of specific heat, and it is graphically presented in Fig. 6, where the temperature is 288.15K and 298.15K. The specific heat capacity ratio (ϒ) decreases consistently throughout concentrations and compositions. Solute-solvent dynamics intensify as solute concentrations rise. These interactions impact energy distribution in the solution, lowering specific heat at constant volume [33].

$$(r) = \{1 - \left(\frac{U}{U^{\infty}}\right)^2\} \quad (4)$$

The decline in relaxation strength (r) values with increasing weight fraction of l-isoleucine with salts is attributed to the formation of solute-solvent interaction, wherein solvent molecules surround the amino acid molecules, as depicted in Fig. 7. Equation 4 calculates the relaxation strength of L-isoleucine in aqueous solutions of $Mg(NO_3)_2$ and $MgSO_4$ across various temperatures. Shows the presence of solute-solvent interactions between the system's amino acid and electrolyte components. This research highlights enhanced interactions among amino acids, electrolytes, and water constituents, revealing strong interaction between these components [34].

4. Conclusion

This thermodynamic research yields insights into the likely intermolecular interactions inside a mixture. Common thermodynamic studies involve the determination of density and the velocity of sound. Stronger electrostatic contacts, like H-bonding, are suggested by positive acoustic impedance values. Conversely, higher values in salt solutions indicate the existence of more powerful interactions caused by the presence of charged surfaces on micelles in electrolyte solutions. The positive free-length results indicate that L-isoleucine can form structures in aqueous solutions containing $Mg(NO_3)_2$ and $MgSO_4$. Furthermore, the solute-solvent interactions between (L-isoleucine + $Mg(NO_3)_2$) exhibit greater interaction than those between (L-isoleucine + $MgSO_4$). This is because the former molecules possess a greater number of hydroxyl groups compared to the latter. The interaction order is verified by all of the parameters, which are listed as follows: be L-isoleucine + water + $Mg(NO_3)_2$ > L-isoleucine + water + $MgSO_4$ > L-isoleucine + water.

Table 1. Densities, velocity, and acoustic impedance values of L-isoleucine in $MgSO_4$ and $Mg(NO_3)_2$ at temperature, T= (288.15 and 298.15)K.

Conc. (M) mol/kg	U			ρ			Z		
	H_2O	$MgSO_4$	Mg $(NO_3)_2$	H_2O	$MgSO_4$	Mg $(NO_3)_2$	H_2O	$MgSO_4$	Mg $(NO_3)_2$
					288.15K				
0	1466.032	1466.03	1466.03	999.1	999.1	999.1	1464712	1464713	1464715
0.02	1470.632	1477.77	1486.85	1004.8	1005.65	1008.75	1477691	1484642	1499860
0.04	1473.174	1484.80	1488.83	1006.13	1009.98	1013.21	1482204	1499618	1508497
0.06	1477.265	1490.31	1492.88	1008.56	1011.62	1017.65	1489910	1507627	1519229
0.08	1481.794	1492.28	1494.79	1009.68	1013.48	1019.88	1496138	1512396	1524506
0.1	1485.474	1494.66	1497.84	1011.85	1014.06	1021.81	1503076	1515675	1530508
0.12	1487.177	1497.65	1499.78	1012.99	1016.71	1023.51	1506495	1522676	1535040

0.14	1488.933	1498.25	1500.83	1014.00	1019.09	1025.35	1509778	1526852	1538876
0.16	1491.665	1500.81	1502.78	1016.25	1022.64	1027.9	1515904	1534788	1544708
0.18	1493.143	1504.23	1507.00	1018.87	1024.8	1029.1	1521319	1541535	1550854
0.2	1495.206	1505.87	1509.51	1020.99	1026.45	1032.45	1526590	1545700	1558494
					298.15K				
0	1498.10	1498.10	1498.10	997.00	997.00	997.00	1493606	1493607	1493607
0.02	1501.42	1508.97	1510.06	998.18	999.56	1001.50	1498687	1508306	1512325
0.04	1503.01	1509.97	1513.04	999.15	1001.89	1004.56	1501732	1512824	1519939
0.06	1504.62	1511.52	1515.29	999.98	1005.56	1007.82	1504589	1519924	1527153
0.08	1507.25	1514.71	1517.70	1000.16	1008.87	1010.06	1507491	1528145	1532972
0.1	1510.48	1517.51	1520.16	1001.83	1010.12	1013.52	1513244	1532867	1540716
0.12	1512.08	1520.11	1523.97	1003.86	1013.43	1016.62	1517916	1540525	1549304
0.14	1516.60	1523.32	1526.05	1005.13	1015.45	1020.94	1524380	1546855	1558012
0.16	1517.14	1524.77	1528.51	1007.16	1018.09	1023.73	1528002	1552353	1564787
0.18	1518.23	1526.40	1530.86	1009.12	1020.98	1026.37	1532076	1558424	1571239
0.2	1520.22	1530.00	1533.85	1011.22	1023.54	1029.43	1537276	1566016	1579002

Table 2. specific heat (γ), relaxation strength (r), and Free length values (Lf) of L-isoleucine in $MgSO_4$ and Mg $(NO_3)_2$ at temperature, T= (288.15 and 298.15)K.

Conc. (M) mol/kg	γ			r			Lf *10^{-11}		
	H_2O	$MgSO_4$	Mg $(NO_3)_2$	H_2O	$MgSO_4$	Mg $(NO_3)_2$	H_2O	$MgSO_4$	Mg $(NO_3)_2$
					288.15K				
0	0.13802654	0.1380265	0.1380264	0.1604492	0.1604492	0.1604515	4.36	4.36	4.36
0.02	0.13776505	0.1377719	0.1375850	0.1551724	0.1469514	0.1364363	4.33	4.31	4.27
0.04	0.13770432	0.1375291	0.1373828	0.1522493	0.138816	0.1341348	4.32	4.28	4.26
0.06	0.13759364	0.1374547	0.1371827	0.1475344	0.1324125	0.1294176	4.30	4.26	4.24
0.08	0.13754274	0.1373706	0.1370826	0.1422989	0.1301173	0.1271886	4.29	4.25	4.23
0.1	0.13744435	0.1373444	0.1369963	0.1380339	0.1273404	0.1236231	4.27	4.24	4.22
0.12	0.13739277	0.1372250	0.1369204	0.1360564	0.1238455	0.1213515	4.26	4.23	4.21
0.14	0.13734714	0.1371180	0.1368384	0.1340150	0.1231433	0.1201208	4.26	4.22	4.20
0.16	0.13724570	0.1369592	0.1367252	0.1308337	0.1201442	0.1178329	4.25	4.21	4.19
0.18	0.13712796	0.1368629	0.1366720	0.1291104	0.1161297	0.1128714	4.24	4.19	4.18
0.2	0.13703298	0.1367895	0.1365240	0.1267027	0.1142013	0.1099138	4.23	4.19	4.16
					298.15K				
0	0.13604489	0.1360449	0.1360448	0.1233177	0.1233177	0.1233177	4.35	4.35	4.35
0.02	0.13599126	0.1359286	0.1358408	0.1194289	0.1105506	0.1092651	4.33	4.31	4.30
0.04	0.13594724	0.1358232	0.1357027	0.1175628	0.1093713	0.1057460	4.33	4.30	4.29
0.06	0.13590962	0.1356577	0.1355558	0.1156713	0.1075419	0.1030844	4.32	4.29	4.27
0.08	0.13590146	0.1355092	0.1354558	0.1125771	0.1037709	0.1002291	4.31	4.27	4.27
0.1	0.13582591	0.1354533	0.1353015	0.1087695	0.1004544	0.0973099	4.30	4.27	4.25
0.12	0.13573429	0.1353056	0.1351638	0.1068804	0.0973693	0.0927794	4.29	4.25	4.24
0.14	0.13567710	0.1352159	0.1349729	0.1015329	0.0935531	0.0903013	4.28	4.24	4.22
0.16	0.13558588	0.1350989	0.134850	0.1008930	0.0918267	0.0873660	4.27	4.23	4.21
0.18	0.13549804	0.1349713	0.1347343	0.0996006	0.0898840	0.084557	4.27	4.22	4.20
0.2	0.13540418	0.1348587	0.134600	0.0972387	0.0855859	0.080978	4.26	4.20	4.18

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