Ultrasonic Characterization on the Solutions of L-Histidine and Electrolyte Salts to Understand Their Interaction in View to Maintained Blood Pressure

Pooja Sonune, Urvashi Manik and Paritosh Mishra

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Pooja R. Sonune [a*], Urvashi P. Manik[b], and Paritosh L. Mishra[c]

[*a]Ph.D. Scholar, Department of Physics, Sardar Patel Mahavidyalaya, Chandrapur, Maharashtra, India
[b]Professor, Department of Physics, Sardar Patel Mahavidyalaya, Chandrapur, Maharashtra, India.
[c]Department of Physics, Sardar Patel Mahavidyalaya, Chandrapur, Maharashtra, India.

Abstract

The ability to forecast different types of intermolecular interaction and the degree of relationship between solute and solvent using thermo-acoustical and volumetric parameters is extremely advantageous. As human body contains lots of nutrients available in the form of amino acids as well as salts. And their interactions of them decide the capacity to absorb such nutrients. It is revealed that the amino acids (L-Histidine) are one of the necessary nutrients for maintaining blood pressure. Hence, the application of L-Histidine amino acid could be a remedy for maintaining the level of blood pressure. In this consideration, numerous thermos-acoustical and volumetric properties of the systems L-Histidine+H_2O and L-Histidine+H_2O+NaCl/$MgCl_2$ solutions at 283 & 293K temperature with different concentrations (0.02-0.2M) have been examined in this work. The result of the concentration-dependent variation of these volumetric and thermo-acoustical characteristics strongly indicates that there are molecular association exists in all systems. The amino acid: L-Histidine exhibit maximum molecular interaction at higher concentration in all three solvents, but the amino acid L-Histidine demonstrates maximal molecular interaction with $MgCl_2$ solvents and this can be suggested that the molecules of L-Histidine easily bind up with the molecules of magnesium as compared to water and sodium.

Keywords: Amino acid, density, electrolyte salts, thermo-acoustical properties, ultrasonic

1. Introduction

Ultrasonic analysis is currently one of the finest techniques to identify the specific molecular interactions (ion-ion, ion-solvent, and solvent-solvent) in liquid mixtures. The goal of thermo-acoustical and volumetric research is to evaluate structure and molecular interaction using data from compounds and their interaction with other solutes and solvents that have been collected and calculated [1-4]. Numerous researchers have used the ultrasonic method to assess the thermo-acoustical characteristics of amino acids [5-12].

The components of protein known as amino acids have both acidic and basic characteristics. Both amino and the carboxylic acid functional group can be found in amino-acid, which are organic molecules. α-amino acid, which makes up protein, is by far the most significant amino acid in nature, even though there are hundreds of them. The genetic coding contains only 22 essential and non-essential α-amino acids. Histidine is an essential amino acid that the body uses extensively, it lacks resulting in a drop in blood pressure levels. In this regard, we need to keep Histidine levels in the human body for a healthy body from the viewpoint to maintain the right blood pressure level. However, a biological study has shown that some electrolyte salt components, such as Na and Mg, are very effective in regulating blood pressure in the human body. Thus it can be inferred from this situation that the interaction between amino acid and specific salt combination is important to absorb this amino acid in the human body for fast remediation of the defect.

To overcome this difficulty, in this work an attempt has been carried out to provide a vision of the molecular interactions that occurred in the solutions and could help to pick out a suitable and specific salt for maintaining blood pressure at a proper level under ambient circumstances of temperature. Therefore, the present work is pointed to reconnoitrer the molecular interactions between L-Histidine, water, and salts using electrolytic (NaCl and $MgCl_2$) [13].

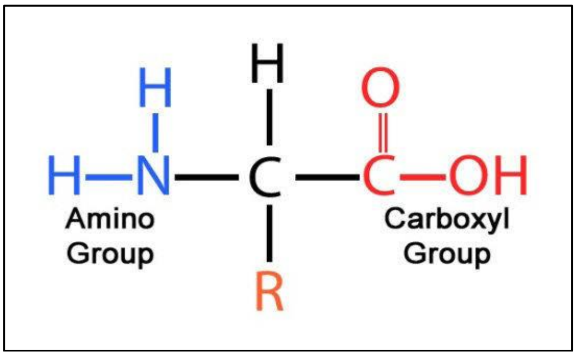

Fig. (a) Conventional formula of amino acid

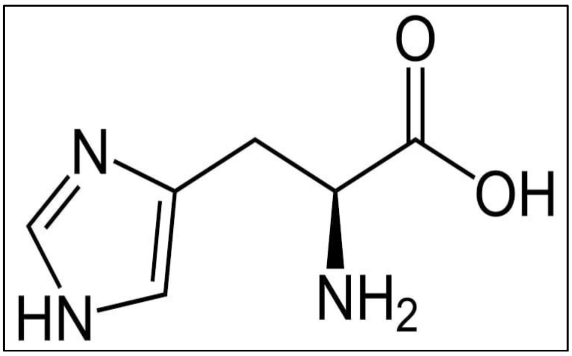

Fig.(b) Structural formula of amino acid: L-Histidine

2. Materials and Method

2.1Chemicals:

The chemicals listed below were obtained from Himedia Pvt. Ltd., Mumbai, and used in the present research without any further raffination. They are all AR-grade chemicals with a mass fraction purity >> 99.8%

- Essential amino acid (solute) – L-Histidine
  Molecular formula: $C_6H_9N_3O_2$, molecular weight: 155.16 g/mol & CAS no.: 71-00-1
- Universal solvent (solvent 1) – Water
  Molecular formula: H_2O & molecular weight: 18.01528 g/mol.
- Saline salt (solvent 2) – Sodium chloride
  Molecular formula: NaCl, molecular weight: 58.44 g/mol & CAS no.: 7647-15-5
- Ionic salt (solvent 3) – Magnesium chloride
  Molecular formula: $MgCl_2$, molecular weight: 203.30g/mol & CAS no.: 7791-18-6

2.2 Equipment and procedure:

2.2.1 Equipment

- Ultrasonic velocity digital interferometer
- Automatic thermostatic water bath
- Quartz crystal cell
- 10 ml specific gravity density bottle
- Electronic weighing balance machine

2.2.2 Procedure

Using an ultrasonic velocity interferometer in digital form, the ultrasonic velocity at a frequency of 2 MHz was measured with an overall precision of 0.0001m/s. The radio frequency oscillator is used to excite the ultrasonic wave in the quartz crystal. Using a very accurate digital electronic weighing scale with an accuracy of ±0.0001g and a 10 ml specific gravity density bottle with a precision of $\pm 2*10^{-2}$kg/m^{-3}, the density of the solution was precisely calculated. The temperature experimental solutions were kept constant by continuously running water through it with an automated thermostatic water bath with a temperature of accuracy around ±1K.

3. Defining relations

Utilizing density and ultrasonic velocity measurement, the following volumetric and thermo-acoustical parameters were calculated using the accepted formula from the literature.

- *Adiabatic compressibility (β):* Using the Newton-Laplace equation, it may be estimated from the sound speed and solution density data [14].
  $\beta = \frac{1}{\rho * U^2}$
- *Acoustic impedance (Z):* Equation presented by relating the specific acoustic impedance to density and velocity [15].
  $Z = \rho U$
- *Relative association (R_A):* Utilizing the relationship below which depends on ultrasonic velocity and density [16].
  $R_A = (\frac{\rho}{\rho_0})(\frac{U_0}{U})^{1/3}$

- *Relaxation strength (r):* Calculating Relaxation strength using the formula immediately relates it to adiabatic compressibility [17].

  $r = 1-(\frac{U}{U_\infty})^2$
- *Surface tension (σ):* The well-known Auerbach connection has been applied to estimate the surface tension of a combination using the Flory theory [18].

  $\sigma = (6.3*10^{-4})\ \rho U^{3/2}$
- *Specific heat ratio (γ):* The equation for the simplified link between isothermal compressibility and adiabatic compressibility is [16].

  $\gamma = \frac{17.1}{T^{\frac{4}{9}} * \rho^{1/3}}$

4. Result and discussion

The following table of data shows the experimentally determined value of density and ultrasonic velocity of distilled water at different temperatures, which provides a good accord after comparison with the observed and published/literature.

Temperature (T) K	**Obtained data**		**Literature data**	
	U. Velocity (U) m/s	Density (ρ) kg/m^3	U. Velocity (U) m/s	Density (ρ) kg/m^3
283	1447.427	999.70	1448.16[19]	999.891[19]
293	1481.496	998.200	1482.63[20]	998.202[20]

Table 1: Ultrasonic velocities and densities of freshly distilled water at 283 and 293K.

4.1 Ultrasonic velocity (U)

Having structural dependencies, ultrasonic velocity is a crucial physical metric. The ultrasonic velocity of the essential amino acid: L-Histidine, which has a range of concentration (0.02–0.2 mol/kg). In the current study 0.1M solutions of both electrolyte salt solvents, NaCl and $MgCl_2$were examined at various temperatures (i.e. 283 and 293K). Fig. 1 and also Table 2 list the observed data showing that ultrasonic velocity increases as temperature and concentration both rise. The system's concentration and temperature affect the ultrasonic velocity. With increasing ultrasonic velocity, the association of the medium's component particles is seen to grow, and this association is brought on by molecular contact. [21,22].

4.2 Density (ρ)

One significant Physicochemical characteristic that is temperature and pressure-dependent is density. In addition, the density of a metric of solute-solvent contact can be ascribed to the increase in density with concentration which suggests a rise in solute-solvent interaction, whereas a decline in density implies a fall in solute-solvent interaction. Volume shrinkage brought on by the presence of solute molecules is what causes the increase in density with concentration. The fact that the density value in the current study is growing to suggests that the solvent is becoming more structured as a result of the solute addition, according to one interpretation of the data shown in Fig. 2 [23].

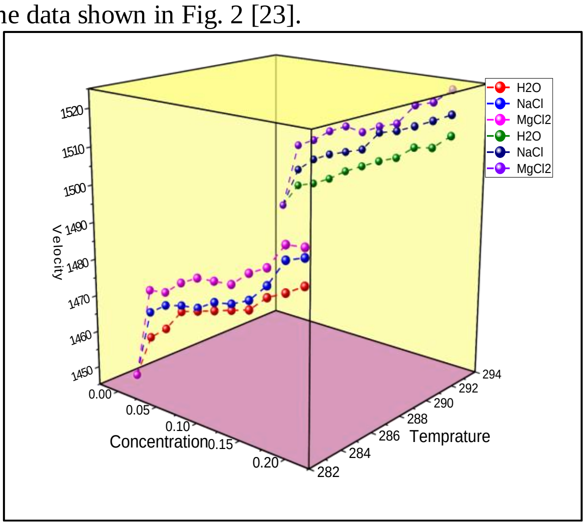

Figure 1 Concentration, Temperature-related changes in ultrasonic velocity

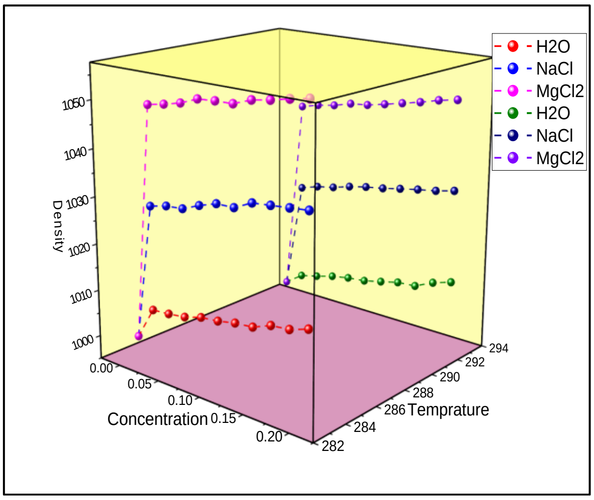

Figure. 2 Concentration, Temperature-related changes in density

4.3 Adiabatic compressibility (β)

As adiabatic compressibility increases with compressibility in the solution, the hydrogen bonds between the various components break down., explaining the physicochemical features of liquids. In this instance, it is discovered that the adiabatic compressibility of the solute can be represented as the degree of hydration compression that is possible around the solute molecule. The value of adiabatic compressibility, which can be shown in Fig. 3, is found to decrease with an increase in the molal concentration of the solute (amino acid), as well as the amount of aqueous NaCl and $MgCl_2$ (solvent). The weakening of the hydrogen bond in the solution may be the cause of the observed drop in adiabatic compressibility in the solvent [24].

4.4 Acoustic Impedance (Z)

In 0.1M of aqueous electrolyte salt solution of NaCl and $MgCl_2$, the value of acoustic impedance for amino acid: l-histidine of different weight fractions (0.02-0.2 mol/kg) was computed and tabulated in Table 3. Increased acoustic impedance values demonstrate that the distance between molecules in mixtures is decreasing, indicating that the solute-solvent interaction is effectively completed through hydrogen bonding. Therefore, an increase in the potential energy of the contact between the molecules is what is responsible for the observed rise in ultrasonic velocity and decrease in intermolecular free length. [25-27]

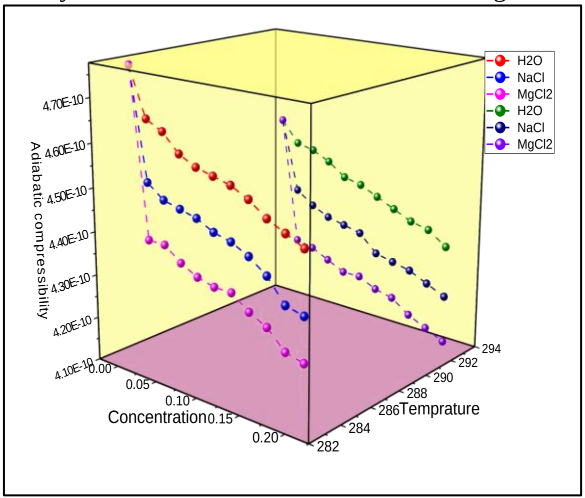

Figure 3 Concentration, Temperature-related changes in Adiabatic compressibility

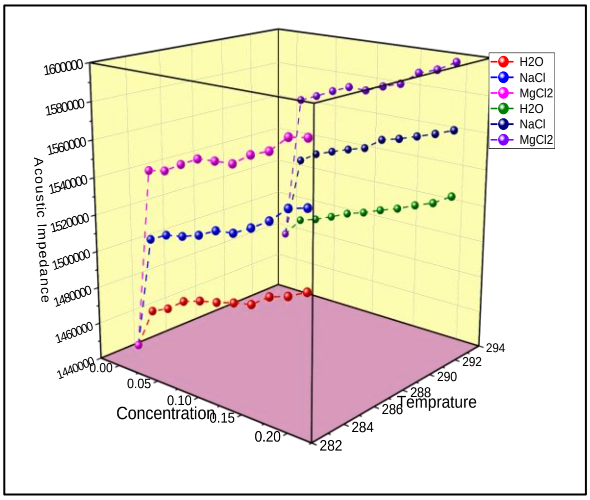

Figure 4 Concentration, Temperature-related changes in Acoustic Impedance

4.5 Relative association (R_A)

The attribute that helps us comprehend the interaction is the relative connection. Two key factors affect the relative association.

1. Dissolving the solute's associated solvent molecule as well as the solute itself.
2. The molecule of an amino acid is solvated.

As seen in Fig. 5, the correlation between R_A and concentration indicates that there is a close intermolecular association between the components of molecules as well as a higher influence of the second factor than the first [26-28]. As a result, the growing relative association of l-histidine in water and both electrolyte solutions are observed in the following order: (L-Histidine+$MgCl_2$) > (L-Histidine+NaCl) > (L-Histidine+H_2O)

4.6 Relaxation strength (r)

A direct relationship exists between relaxation strength and adiabatic compressibility. The factor $1-U/U_\infty$, where U is the ultrasonic speed and U_∞, is a constant with a value of 1600 m/s, determines the entire answer. Clarifying the molecular interactions that are present in the system is a crucial property. If the value of relaxation strength decreases with increasing concentration and temperature after adding a solute to solvent, this confirms solute-solvent interaction in the system, as depicted by Fig. 6. Which may imply a stronger connection between salts and amino acids [29,30].

4.7 Surface tension (σ)

Many biological and commercial processes depend on the surface tension of liquids and liquid mixtures. The surface tension of a solution increases as a solute is added; Figure 7 shows the increasing trends of surface tension. It is exposed that surface tension is typically higher due to hydrogen bonding and dipolar interactions [31].

4.8 Specific heat ratio (γ)

The specific heat of a liquid determines the amount of heat required for each degree of temperature rise. The specific heat ratio of several weight fractions (0.02-0.2M) of the amino acid (l-histidine) in water and also in 0.1M aqueous solutions of NaCl and $MgCl_2$ at various temperatures are listed in Table 4. It is clear from Fig. 8 that with the increasing concentration of solution; the heat capacity continuously declines to confirm the existence of intermolecular interaction [16].

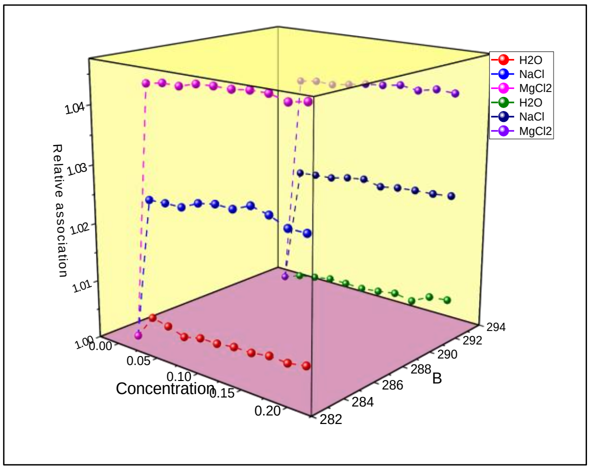

Figure 5 Concentration, Temperature-related changes in Relative association

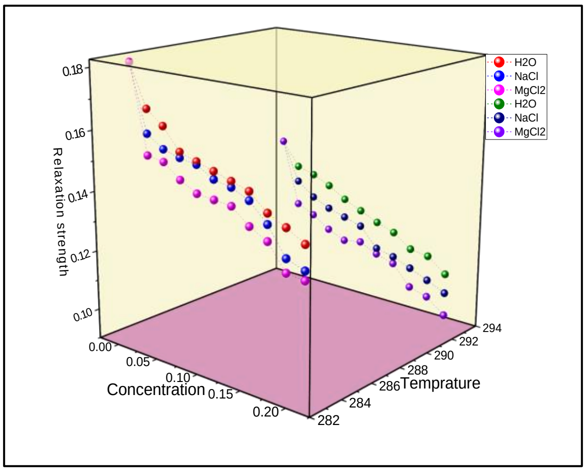

Figure 6 Concentration, Temperature-related changes in Relaxation strength

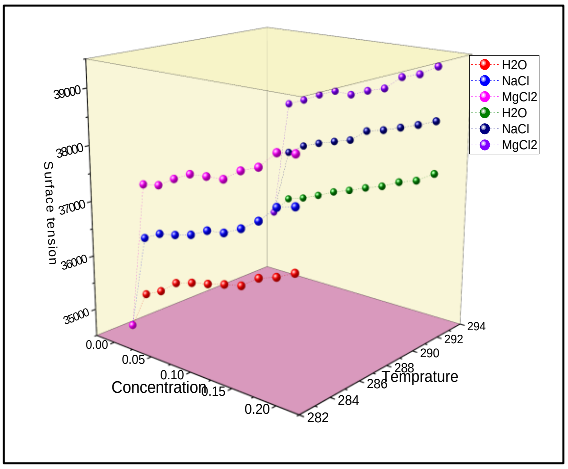

Figure 7 Concentration, Temperature-related changes in Surface tension

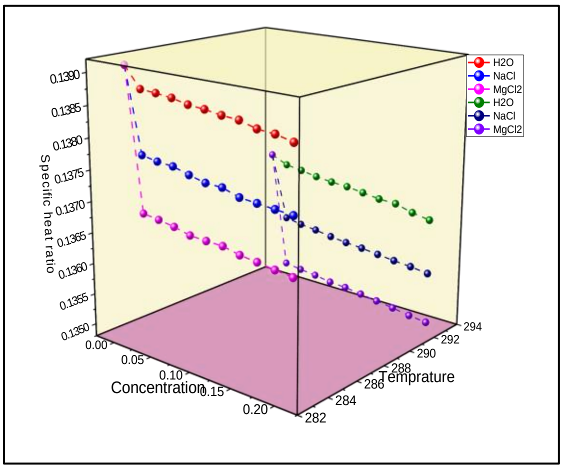

Figure 8 Concentration, Temperature-related changes in Specific heat ratio

5. Conclusion

By measuring the density and ultrasonic velocity of solutions of l-histidine in both electrolyte salt solutions and water, numerous volumetric and thermo-acoustical parameters were calculated. From the above results and observations, it is found that: the weight fraction, temperature, composition of the solute and solvent, and its position play significant roles in determining the interaction occurring in the liquid mixture. Additionally, it can be concluded from the various volumetric and thermo-acoustical properties that H-bonding is strong at higher concentrations. The order of interaction obtained for the L-Histidine amino acid in all of the three solvents (water, sodium chloride, and magnesium chloride) is as follows:

$$(C_6H_9N_3O_2+MgCl_2+H_2O) > (C_6H_9N_3O_2+NaCl+H_2O) > (C_6H_9N_3O_2+H_2O)$$

From the above order of interaction, it is explored that when the salts are added to the water the interaction between amino acid and solvent (NaCl, $MgCl_2$) increases due to the stronger hydrogen bonding. And from this, it is clear that the amino acid is interact much more with Mg^{++} as compared to Na^+ ions. Thus, the overall scenario led to the conclusion that, if we supply the L-Histidine with Mg^{++} content solvent then it rapidly interacts and quickly controls the blood pressure level than Na^+ content solvent.

Interest conflicts:

Concerning the current study project, the authors disclose no conflicts of interest.

Author Contribution:

PRS and UPM conceived the study, PRS, UPM, and PLM developed the theoretical and experimental model, and PRS perform the entire experimental work and analyzed the results. All authors wrote the manuscript. UPM and PLM reviewed the manuscript.

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Conc. (M) mol/kg	Ultrasonic Velocity(U) (m/sec)			Density(ρ) (kg/m³)		
	H_2O	NaCl	$MgCl_2$	H_2O	NaCl	$MgCl_2$
			283 K			
0.00	1447.427	1447.427	1447.427	0999.700	0999.700	0999.700
0.02	1459.633	1466.575	1472.658	1006.679	1028.847	1049.593
0.04	1463.483	1469.902	1473.435	1007.017	1029.787	1050.325
0.06	1469.619	1471.234	1477.326	1007.551	1030.135	1051.208
0.08	1471.174	1472.014	1479.942	1008.681	1031.704	1052.641
0.10	1472.729	1474.919	1480.452	1009.122	1032.974	1052.920
0.12	1474.288	1475.919	1480.952	1009.939	1033.109	1053.024
0.14	1475.811	1478.257	1485.120	1010.333	1034.936	1054.376
0.16	1480.337	1483.319	1487.789	1011.899	1035.377	1055.017
0.18	1482.850	1490.923	1494.720	1012.330	1035.817	1055.860
0.20	1485.860	1492.743	1495.270	1013.643	1036.261	1056.551
			293 K			
0.00	1481.496	1481.496	1481.496	0998.200	0998.200	0998.200
0.02	1488.577	1493.329	1500.606	1000.864	1022.204	1041.301
0.04	1490.158	1497.310	1503.014	1001.785	1023.348	1042.271
0.06	1492.536	1499.707	1506.428	1002.865	1024.031	1042.887
0.08	1495.716	1501.308	1508.658	1003.570	1025.080	1043.912
0.10	1498.108	1502.914	1507.849	1003.988	1025.847	1044.277
0.12	1500.507	1508.553	1510.277	1004.887	1026.405	1045.101
0.14	1502.363	1509.839	1511.890	1005.819	1027.170	1045.974
0.16	1506.131	1511.959	1517.712	1006.122	1027.867	1046.839
0.18	1506.938	1514.229	1519.237	1007.971	1028.459	1047.891
0.20	1510.980	1516.672	1523.339	1009.198	1029.325	1048.619

Table 2: The measured data of ultrasonic velocity and density of the system's L-Histidine + water and 0.1M concentration of the aqueous solution of NaCl/$MgCl_2$ at 283 & 293K temperatures.

Conc. (M) mol/kg	Adiabatic Compressibility (β) (m^2N^{-1})			Acoustic Impedance (Z) (kg-m^2s^{-1})			Relative Association (R_A) (----)		
	H_2O	NaCl	$MgCl_2$	H_2O	NaCl	$MgCl_2$	H_2O	NaCl	$MgCl_2$
				283K					
0.00	4.77E-10	4.77E-10	4.77E-10	1446993	1446993	1446993	1.00000	1.00000	1.00000
0.02	4.66E-10	4.52E-10	4.39E-10	1469381	1508882	1545692	1.00417	1.02466	1.04388
0.04	4.64E-10	4.49E-10	4.39E-10	1473752	1513686	1547585	1.00362	1.02482	1.04442
0.06	4.60E-10	4.48E-10	4.36E-10	1480717	1515570	1552977	1.00275	1.02486	1.04438
0.08	4.58E-10	4.47E-10	4.34E-10	1483945	1518682	1557848	1.00353	1.02623	1.04519
0.10	4.57E-10	4.45E-10	4.33E-10	1486163	1523554	1558798	1.00361	1.02682	1.04535
0.12	4.56E-10	4.44E-10	4.33E-10	1488941	1524785	1559478	1.00407	1.02673	1.04533
0.14	4.54E-10	4.42E-10	4.30E-10	1491060	1529902	1565875	1.00411	1.02800	1.04569
0.16	4.51E-10	4.39E-10	4.28E-10	1497951	1535795	1569642	1.00465	1.02727	1.04570
0.18	4.49E-10	4.34E-10	4.24E-10	1501133	1544323	1578215	1.00451	1.02595	1.04492
0.20	4.47E-10	4.33E-10	4.23E-10	1506132	1546871	1579830	1.00513	1.02597	1.04547
				293K					
0.00	4.56E-10	4.56E-10	4.56E-10	1478829	1478829	1478829	1.00000	1.00000	1.00000
0.02	4.51E-10	4.39E-10	4.26E-10	1489863	1526487	1562582	1.00108	1.02134	1.03873
0.04	4.50E-10	4.36E-10	4.25E-10	1492819	1532269	1566548	1.00164	1.02157	1.03914
0.06	4.48E-10	4.34E-10	4.23E-10	1496812	1535747	1571034	1.00219	1.02171	1.03897
0.08	4.45E-10	4.33E-10	4.21E-10	1501055	1538961	1574906	1.00218	1.02239	1.03948
0.10	4.44E-10	4.32E-10	4.21E-10	1504082	1541760	1574612	1.00207	1.02279	1.04003
0.12	4.42E-10	4.28E-10	4.19E-10	1507840	1548387	1578391	1.00243	1.02207	1.04029
0.14	4.40E-10	4.27E-10	4.18E-10	1511105	1550862	1581398	1.00295	1.02254	1.04079
0.16	4.38E-10	4.26E-10	4.15E-10	1515351	1554093	1588801	1.00241	1.02276	1.04032
0.18	4.37E-10	4.24E-10	4.13E-10	1518950	1557323	1591995	1.00407	1.02284	1.04101
0.20	4.34E-10	4.22E-10	4.11E-10	1524878	1561148	1597402	1.00440	1.02315	1.04080

Table 3: The computed data for Adiabatic compressibility, Acoustic Impedance, and Relative association of the system's L-Histidine + water and 0.1M concentration of the aqueous solution of NaCl/$MgCl_2$ at 283 & 293K temperatures.

Conc. (M) mol/kg	Relaxation Strength (r) (----)			Surface Tension (σ) (Nm^{-1})			Specific Heat Ratio (γ) $(K^{4/9})^{-1}(kg^{1/3}m^{-1})^{-1}$		
	H_2O	NaCl	$MgCl_2$	H_2O	NaCl	$MgCl_2$	H_2O	NaCl	$MgCl_2$
				283K					
0.00	0.181623	0.181623	0.181623	34682.09	34682.09	34682.09	0.139109	0.139109	0.139109
0.02	0.167762	0.159827	0.152843	35366.89	36403.90	37369.26	0.138787	0.137783	0.136869
0.04	0.163366	0.156011	0.151949	35518.83	36561.21	37424.90	0.138772	0.137741	0.136838
0.06	0.156336	0.154481	0.147464	35761.43	36623.29	37604.83	0.138747	0.137726	0.136799
0.08	0.154550	0.153584	0.144442	35858.36	36708.22	37756.18	0.138695	0.137656	0.136737
0.10	0.152761	0.150240	0.143852	35930.92	36862.29	37785.71	0.138675	0.137599	0.136725
0.12	0.150967	0.149087	0.143274	36017.14	36904.58	37808.57	0.138638	0.137594	0.136721
0.14	0.149212	0.146389	0.138445	36087.02	37057.75	38017.06	0.138620	0.137512	0.136662
0.16	0.143985	0.140533	0.135345	36309.36	37264.13	38142.73	0.138548	0.137493	0.136634
0.18	0.141077	0.131699	0.127270	36417.36	37566.98	38440.28	0.138529	0.137473	0.136598
0.20	0.137586	0.129577	0.126628	36575.69	37651.91	38486.69	0.138469	0.137454	0.136568
				293K					
0.00	0.142644	0.142644	0.142644	35859.88	35859.88	35859.88	0.137048	0.137048	0.137048
0.02	0.134429	0.128894	0.120383	36213.67	37163.06	38134.38	0.136926	0.135966	0.135130
0.04	0.132590	0.124243	0.117558	36304.77	37353.52	38261.83	0.136884	0.135916	0.135088
0.06	0.129819	0.121437	0.113545	36430.93	37468.25	38414.96	0.136835	0.135885	0.135061
0.08	0.126107	0.119560	0.110918	36573.11	37566.70	38538.13	0.136803	0.135839	0.135017
0.10	0.123310	0.117676	0.111872	36676.15	37655.16	38520.60	0.136784	0.135805	0.135002
0.12	0.120500	0.111042	0.109009	36797.20	37887.88	38644.13	0.136743	0.135781	0.134966
0.14	0.118322	0.109526	0.107105	36899.69	37964.61	38738.42	0.136701	0.135747	0.134928
0.16	0.113894	0.107023	0.100215	37049.75	38070.41	38994.61	0.136687	0.135716	0.134891
0.18	0.112944	0.104340	0.098406	37147.67	38178.15	39092.64	0.136603	0.135690	0.134846
0.20	0.108179	0.101448	0.093531	37342.64	38302.79	39278.33	0.136548	0.135652	0.134815

Table 4: The computed data for Relaxation strength, Surface tension, and Specific heat ratio of the system's L-Histidine + water and 0.1M concentration of the aqueous solution of NaCl / $MgCl_2$ at 283 & 293K temperatures.