



A VOLUMETRIC AND ACOUSTICAL STUDIES ON INTERMOLECULAR INTERACTION BETWEEN ISOLEUCINE AND AQUEOUS SACCHARIDES SOLUTION

Neha S. Pathan¹, Urvashi P. Manik², Paritosh L. Mishra³

¹Department of Physics, Sardar Patel Mahavidyalaya, Chandpur, Maharashtra, India

²Sardar Patel Mahavidyalaya, Chandrapur, Maharashtra, India

³Department of Physics, Professor, Sardar Patel Mahavidyalaya, Chandpur, Maharashtra

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ABSTRACT:

Different non-covalent interactions can be investigated using measurements of physical properties. Accurate volumetric and acoustical data are necessary for improved comprehension. The nature of interactions between amino acids and saccharides regulates the functionalization process. Because of this, we present data on the densities and ultrasonic speed of l-isoleucine in a solution of glucose and fructose in water obtained over the range of (283.15 and 288.15) K at atmospheric pressure. The experimental results have also been used to derive volumetric and acoustic parameters, such as isothermal compressibility (KT), specific heat (σ), nonlinear parameters, relaxation strengths (r), acoustic impedance (Z), and relative association (RA) have been evaluated using the information on ultrasonic speed. Positive values for the acoustic impedance and negative values for the isothermal compressibility point to a strong intermolecular electrostatic interaction between the isoleucine ions and water molecules. The presence of saccharide molecules in the micellar form in isoleucine often increases the degree of intermolecular interaction among the solution's constituents. Additionally, it was shown that amino acids can form structures in both water and an aqueous saccharide solution by positive values for the expansibility factor.

Keywords :- Isoleucine; Glucose; Fructose; volumetric and acoustical parameters.

INTRODUCTION :

Amino acids, which are the basic building blocks of proteins, are necessary for the functional and structural stability of every biological process. Amazingly, amino acids also function as neurotransmitters in addition to being structural, hormonal, and enzyme-active substances. There are extraordinarily intricate molecules called proteins in [1] all living things. Proteins are essential biomolecules for human survival. Proteins function as Signaling molecules that link the activity of various cells, tissues, and organs. They take part in transcription, DNA replication, catalysis, digestion, and many other biological processes. [2] The interactions of these complex biomolecules with the environment affect their capacity to corroborate. These interactions indeed exist between the protein molecules and

the solvent's ions. Isoleucine is an essential branch-chain amino acid [3] for both people and other animals. Proteins function as a transmission element that enhances the integration of biological activity among various cells, tissues, and organs. They also play a part in digestion, DNA replication, catalysis, and transcription. How successfully these complex biomolecules can reinforce one another depends on how they interact with their surroundings. Branched-chain amino acids, including isoleucine, which seem to be essential for both human beings and other animals, interact with the ions in the solvents and the cellular proteins. [5] [6] The volumetric and acoustic characteristics of the interaction of amino acids and saccharides in an aqueous medium can be used to learn more about how solutes and solvents interact. Hydrogen bonding,

electrostatic contact, and electrostatic contacts in solution are only a handful of the interactions that support protein confirmation. Several thermos-acoustic characteristics will be used to investigate the intermolecular interactions of a specific amino acid in aqueous and other saccharide solutions. The intermolecular interactions of particular isoleucine in water and glucose and fructose solutions will be researched using various thermos-acoustic parameters.[7-8] The influence of the solvent medium on this biomolecule interaction has also been studied. [9]

In the current study, the densities and speed of sound of iso-leucine in an aqueous solution of saccharides were investigated at different temperatures and concentrations. The volume of isoleucine transferred from water to glucose and fructose was calculated using measured data for acoustical and volumetric parameters such as isothermal compressibility (KT), specific heat (σ), nonlinear parameters, relaxation strengths (r), acoustic impedance (Z), and relative association (RA). These factors have been used to investigate solute-solute and solute-solvent associations in solutions, in addition to the possibility of the constituents forming and breaking structures in viable solutions. [10] This research aims to fill gaps in our understanding of the interactions of active pharmaceutical aqueous solutions as well as amino acids in aqueous media.

EXPERIMENTAL DETAILS :

Materials.

The mass fraction purification of the respective AR grade compounds, 99.7%, was obtained and immediately put to use. Chemical sample requirements

The mole fraction of isoleucine differed between (0.02-0.2) mol·kg⁻¹ and 0.1 mol·kg⁻¹ to create an investigational liquid (mixture) with different compositions. To reduce the risk of errors, all glassware had been carefully left to dry before

use and cleaned with acetone and newly double-distilled water.

METHOD :

In the proposed work, we want to assess the ultrasonic velocity at different solutions using an electronic ultrasonic interferometer going to operate at 2MHz and 0.0001 m·s⁻¹ frequencies, in addition to a pulse-echo overlap process with temperature and concentration functions.

The density of the double-distilled water as well as the experimental liquid was calculated using a 10 mL specific gravity bottle with a 2*10⁻² Kg·m⁻³ and very precise and accurate digital weighing balance with a frequency of 0.0001 g. The temperature of an experimental solution was kept constant using an electrically controlled fully automated thermostatic water bath with an accuracy of ±1 K.

THEORY :

The complete list of volumetric and acoustic parameters was determined by calculating from measured data of speed of sound (U) and density (ρ) using standard formulae derived from the literature.

Equation (I) simplifies the calculation of an Acoustic impedance by incorporating values for such medium's density (ρ) and sound speed (U). [9]

- (Z): $U\rho$ (I)
- Relative Association (RA) is derived using the formulae

$$(RA) : \frac{\rho}{\rho_0} \left(\frac{U_0}{U} \right)^2 \dots\dots (II)$$

Where (U) has a specific value (1600) m/s [11] and (U) is the solvent or solution's ultrasonic sound velocity.

- The specific Heat Ratio is calculated as
- $$(\gamma) : \frac{17.1}{T^{0.9} \times \rho^3} \dots\dots (III)$$

- Surface tension can be calculated using the relation

$$(\sigma) : \{(6.3 \times 10^{-4}) \rho U^2\} \dots (IV)$$

- The term isothermal compressibility [12] is derived from the equation

$$(k_{T1}) : \frac{1.33 \times 10^{-8}}{(6.4 \times 10^{-4} U^2 p)^{3/2}} \dots (V)$$

In theory, the intermolecular potential energy determines the sound speed and its variation in liquids. as demonstrated by Hartmann-Balizar [12]. The sentence of Hartmann- Balizar and P. L. Mishra is as follows. [13]

- $(B/A)_1 : \left\{ 2 + \left[\frac{0.98 \times 10^4}{U} \right] \right\} \dots (VI)$
- Relaxation Strength (r)[14] seems to have been calculated using the formula.

$$(r) : 1 - \left(\frac{U}{U_\infty} \right)^2 \dots (VII)$$

RESULT AND DISCUSSION:

At 283.15K and 288.15K temperatures, the density (ρ) and sound velocity (U) of isoleucine probably depend on its weight fraction ranges (0.02-0.2mol-kg⁻¹) in water and are within 0.1mol-kg⁻¹ aqueous solution containing glucose and fructose.

[Table 2] shows the density (ρ) and sound speed (U) of isoleucine at different molar concentrations (0.02 to 0.2) mol-kg⁻¹ in water, glucose, and fructose solutions. Examining the density (ρ), as well as velocity (U) data, velocity data indicates that these values rise as the isoleucine concentration in the solution rises. [15] The increase in density and ultrasonic sound velocity is caused by strong molecular interactions due to an increase in cohesive force. Because of these coordinating factors. Isoleucine molecules form a more compact structure than water when combined with glucose and fructose. [16] The results indicate that as the concentration of isoleucine in a solution increases, so does the density. The presence of an isoleucine-containing solute may also have increased density, improving the structure of water, glucose, and fructose. While density decreases as temperature rises, revealing that such kinetic energy of the molecule increases, this Density increase may be due to the incorporation of the isoleucine-containing

solute. As a result, there is less interaction between both the molecules of a solute and the molecules of a solvent. [17]

The acoustic impedance is focused on the system's molecular packing and the numerous molecular interactions (Z). The (Z) values of isoleucine in water, and saccharides solution are shown in [Table 2]. Increases with changes in temperature and concentration. The increase in acoustical impedance with concentration confirms the increased interaction due to the formation of H-bonds in the solvent. As the temperature increases, the value increases, indicating that the system has a greater tendency to form structures. [18]

The acoustic impedance (Z) explained the molecular packing of such a system in terms of the various types of molecular interactions that have been present. [Table 2] shows the isoleucine (Z) values in water, as well as saccharide solutions. Increases as both concentration and temperature rise. The fact that the acoustic impedance increases with concentration indicate that there is more interaction in the solution due to the formation of H-bonds. The value increases as the temperature rises, confirming that as the temperature rises, the system becomes more structured. [19] This also implies that the molecules of the components in the mixture could very well interact in a specific way. Furthermore, these same Values for Isoleucine in Glucose are higher compared to those for Isoleucine in Fructose, which can be explained by the greater positive intermolecular interaction observed in the case of Isoleucine in Glucose. [9] RA is an important characteristic that can be used to learn more about molecular interactions. The solubility of the solute molecule as well as the dispersion of associated solvent molecules associated solvent molecules of the solute's interaction with it are two governing factors. [20]

When the concentrations of isoleucine in water, glucose, and fructose rise, so does (RA) increase as well [Table 3]. The increase in RA value with solute concentration is caused by the solvation of the solute molecule. The solvent molecules compact closer together when the solute dissolves in the solvent and the solvent travels near the electrostatic field within the vital solvation shell. This type of medium compression generated either by the electric field of the solutes is referred to as electrostriction. [21] The specific heat ratio and relaxation strength decrease as the weight fraction of isoleucine increases. [21] This is due to the solvent molecule forming a complex, indicating isoleucine interaction in the system [Tables 3 and 4]. This demonstrates that isoleucine, water, glucose, and fructose have a stronger relationship. [22] The measured values are listed in the Supplementary material [Table 3]. The surface tension of isoleucine was measured at atmospheric pressure and temperatures ranging from (283.15 to 288.15 K). [13] The surface tensions of isoleucine decrease as the hydrogen bond network is disturbed by increasing temperature. Furthermore, isoleucine in fructose has much less surface tension than isoleucine in fructose due to the length of the branch chain in the alkyl group. [Table 3] illustrates the increasing surface tension with concentration, which is due to hydrogen bonding with dipolar interaction. [23]

The nonlinearity of the fluid state equation is measured using nonlinearity parameters, which already have much more applications in acoustics and medicine. [Table 4] shows the non-linear parameters B/A derived from the (Paritosh Mishra and Ballou) relations. It should be noted that the nonlinearity parameter values for isoleucine in the Hartmann and Ballou instance are a significant benefit. This means that a molecule's spacing is reduced because its clustering is greater. [24] Isothermal

compressibility refers to the amount of pressure fluid can withstand without increasing its temperature. [Table 4] displays KT trends for total isothermal compressibility. The KT values of the amino acid system are decreasing. This demonstrates a stronger molecular association. The KT values of (isoleucine + fructose) are higher than those of (isoleucine + glucose), indicating a stronger molecular association compared to either of the other two solutions. In a neutral solution, it exists in dipolar form, which has more interactions with nearby water molecules. The compressibility of the solution decreases further as the water's electrostrictive compression around all over the molecules increases. [26]

CONCLUSION :

The current study's findings suggest that interactions between amino acids in water and saccharide solutions decrease in the following order: isoleucine in Glucose > isoleucine in Fructose > isoleucine in Water.

The association between both the trend in acoustical parameters as well as concentration indicates the presence of significant interactions between solutes, and the magnitude and direction of excess parameters indicate the possibility of electrostatic interactions between solute molecules. Surface tension values increase for each component of a solution. This indicates that the solution contains a high concentration of H-bonds and dipole-dipole interactions.

Finding

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Conflict of Interest

The authors (N.S.Pathan, U.P.Manik, and P.L.Mishra) assert that there are no conflicts of interest (COI) in the current research work.

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Table-1

Chemicals Mol. Wt	CAS number	source	mass fraction purity
Iso-leucine 131.17 g-mol ⁻¹	73-32-5	HI Media chem. Pvt. Ltd India	≥0.99
Glucose 180.16 g-mol ⁻¹	50-99-7	HI Media chem. Pvt. Ltd India	≥0.99
Fructose 180.16 g-mol ⁻¹	57-48-7	HI Media chem. Pvt. Ltd India	≥0.99

Table [2] lists the values for velocity, density, and acoustic impedance for Isoleucine + water + 0.1 mol kg⁻¹ aq saccharides solutions (glucose/ fructose) at 283.15, and 288.15K, respectively.

Conc. (M) mol/kg	Velocity (U) m/s			Density(ρ) (Kg/m ⁻³)			Acoustic impedance (Z) (kgm ² s ⁻¹)	
	H ₂ O	Fructose	Glucose	H ₂ O	Fructose	Glucose	H ₂ O	Fructose
	283K							
0	1447.427	1447.427	1447.427	999.703	999.703	999.70	1446999	1446997
0.02	1453.160	1468.637	1469.529	1021.1041	1025.123	1031.24	1489667	1505533
0.04	1454.428	1471.412	1472.730	1025.427	1026.125	1033.56	1492429	1509852
0.06	1458.851	1473.861	1479.130	1028.790	1029.456	1038.929	1501822.92	1517275.05
0.08	1463.461	1477.012	1482.008	1031.9956	1032.125	1041.256	1510474.68	1524461.01
0.1	1465.00	1481.832	1483.131	1034.5543	1034.458	1044.452	1515480.97	1532892.97
0.12	1467.321	1483.281	1485.903	1036.3591	1037.874	1046.178	1522894.32	1539458.78
0.14	1469.645	1485.618	1487.466	1039.0818	1042.894	1049.127	1532683.95	1549342.1
0.16	1472.057	1487.236	1492.194	1042.2254	1045.253	1051.75	1538672	1554537.89
0.18	1474.741	1491.602	1497.287	1044.6610	1047.216	1056.725	1544372.37	1562029.48
0.2	1477.483	1493.245	1499.326	1048.3428	1052.21	1061.487	1554622.39	1571207.32
	288.15K							
0	1466.032	1466.032	1466.032	999.103	999.103	999.103	1464716.969	1464716.969
0.02	1470.632	1483.803	1489.803	1019.596	1022.024	1023.487	1499450.505	1516482.277
0.04	1473.174	1484.586	1490.884	1022.572	1025.584	1025.879	1506426.484	1522567.648
0.06	1477.265	1488.517	1491.636	1027.618	1028.254	1029.458	1518064.105	1530573.559
0.08	1481.794	1490.094	1493.478	1032.622	1035.897	1037.897	1530133.084	1543583.904
0.1	1485.474	1493.245	1498.023	1035.092	1039.154	1040.457	1537602.254	1551711.515
0.12	1487.177	1496.431	1500.616	1038.485	1042.458	1044.254	1544411.007	1559966.467
0.14	1488.933	1498.023	1502.014	1040.367	1046.561	1048.169	1549036.758	1567772.449
0.16	1491.665	1500.825	1506.256	1041.484	1047.154	1049.547	1553545.231	1571594.902
0.18	1493.143	1502.181	1507.498	1043.425	1049.475	1052.147	1557982.735	1576501.405
0.2	1495.206	1503.423	1509.639	1046.171	1050.124	1054.128	1564241.156	1578780.574

Table.[3]: Table 3 gives the values for Relative Association, Specific Heat, and Surface Tension at 283.15, and 288.15K for isoleucine + water + 0.1 mol kg⁻¹ aq saccharides solutions (glucose/fructose), respectively.

Conc (mol·kg ⁻¹)	Relative Association (R _A)			Specific heat (γ)			Surface tension(σ)		
	----			[K ^{4/9}] ⁻¹ (kg ^{1/3} m ⁻¹) ⁻¹			Nm ⁻¹		
	H ₂ O	Fructose	Glucose	H ₂ O	Fructose	Glucose	H ₂ O	Fructose	Glucose
283.15K									
0.00	1	1	1	0.139076	0.139076	0.13907	34682.19	34682.19	34682.089
0.02	1.02275	1.020	1.018	0.138098	0.137917	0.13764	35635.32	36348.64	36598.859
0.04	1.026998	1.0208	1.0210	0.13790374	0.137872467	0.137540	35833.04	36487.34	36801.12
0.06	1.031796	1.0235	1.0244	0.137753315	0.137723602	0.13730373	36114.67	36697.22	37233.678
0.08	1.0361	1.0254	1.032426	0.137610537	0.137604785	0.13720138	36399.06	36910.41	37426.041
0.10	1.039033	1.0266	1.033925	0.137496995	0.137501261	0.13706129	36546.88	37175.08	37583.594
0.12	1.041395	1.0297	1.0371	0.137417132	0.137350241	0.13698587	36697.67	37352.56	37751.292
0.14	1.044682	1.0341	1.040665	0.137297003	0.137129507	0.1368574	36881.53	37621.96	37917.455
0.16	1.048415	1.0361	1.041054	0.137158824	0.137026268	0.13674353	37084.22	37768.68	38193.636
0.18	1.051504	1.0370	1.043346	0.137052147	0.136940596	0.1365286	37272.59	38006.36	38570.93
0.20	1.055863	1.0416	1.044816	0.136891515	0.136723603	0.13632413	37508.32	38250.72	38823.916
288.15K									
0.00	1	1	1	0.13802641	0.13802641	0.13802641	35331.818	35331.818	35331.818
0.02	1.019446	1.018841	1.018928	0.13709541	0.13698676	0.13692145	36226.359	36801.542	37077.987
0.04	1.021833	1.02221	1.021063	0.13696228	0.13682807	0.13681495	36426.338	36958.967	37205.099
0.06	1.025927	1.023969	1.024453	0.13673773	0.13670954	0.13665622	36758.676	37202.46	37363.149
0.08	1.029871	1.031216	1.032426	0.1365165	0.13637248	0.13628483	37107.669	37538.561	37739.231
0.10	1.031482	1.03373	1.033925	0.13640783	0.13622986	0.13617297	37335.08	37776.095	38005.146
0.12	1.034468	1.03628	1.0371	0.13625911	0.13608578	0.13600772	37521.895	38017.553	38242.921
0.14	1.035935	1.03999	1.040665	0.13617689	0.13590771	0.13583818	37656.491	38228.109	38439.952
0.16	1.036413	1.039932	1.041054	0.13612819	0.13588205	0.1357787	37800.723	38357.137	38653.66
0.18	1.038002	1.041923	1.043346	0.13604373	0.13578181	0.13566677	37927.472	38494.266	38797.352
0.20	1.040255	1.04228	1.044816	0.1359246	0.13575383	0.13558173	38106.124	38565.851	38953.238

Table. [4]: Table 4 lists the results for the non-linear parameter, isothermal compressibility relaxation strength, for isoleucine + water + 0.1 mol kg⁻¹ aq saccharides solutions (glucose/fructose), at 283.15 and 288.15K, respectively.

Con c. (M) mol /kg	Non-linearity Parameter (B/A)			Isothermal compressibility Δβ*10 ⁻¹¹ (m ² N ⁻¹)			Relaxation Strength		
	H ₂ O	Fructose	Glucose	H ₂ O	Fructose	Glucose	H ₂ O	Fructose	Glucose
283K									
0	8.770635	8.770635065	8.7706351	6.35776	6.38523	6.35967	0.18162307	0.18162	0.181623078
0.02	8.743923	8.672853809	8.6688034	6.10621	5.92734	5.86666	0.17512734	0.15746	0.156439265
0.04	8.738044	8.660269184	8.6543087	6.05574	5.89358	5.81837	0.17368718	0.15428	0.152760292
0.06	8.717615	8.649202333	8.6255164	5.98504	5.84309	5.71727	0.16865381	0.15146	0.145380642
0.08	8.696454	8.635017183	8.6126499	5.91503	5.79254	5.67325	0.16339136	0.14783	0.142051675
0.1	8.689419	8.613435261	8.6076429	5.87918	5.73079	5.63761	0.16163085	0.14226	0.140750952
0.12	8.678838	8.606974673	8.5953161	5.84298	5.69	5.60009	0.15897229	0.14058	0.137536045
0.14	8.668277	8.596581355	8.5883859	5.79935	5.69938	5.56332	0.15630608	0.13787	0.135720664
0.16	8.657350	8.589404775	8.5675107	5.75187	5.68349	5.50308	0.15353444	0.13599	0.130217604
0.18	8.645234	8.57011723	8.5451714	5.70832	5.54381	5.42253	0.15044491	0.13091	0.124270172
0.2	8.632902	8.562888207	8.5362703	5.65459	5.49068	5.36962	0.14728280	0.12899	0.121883416
288.15K									
0	8.684710	8.684710839	8.6847108	6.18505	6.18505	6.18505	0.16045	0.16045	0.16045
0.02	8.663801	8.604650348	8.5780509	5.95738	5.81826	5.75332	0.15517	0.13997	0.133
0.04	8.652303	8.601166925	8.5732814	5.90839	5.78113	5.72386	0.15225	0.13906	0.13174
0.06	8.633880	8.583734012	8.5699675	5.82845	5.72447	5.68758	0.14753	0.1345	0.13087
0.08	8.613604	8.576766298	8.5618643	5.74642	5.64776	5.60277	0.1423	0.13266	0.12872
0.1	8.597220	8.562888207	8.5419556	5.69399	5.59457	5.54407	0.13803	0.12899	0.12341
0.12	8.589666	8.548915386	8.5306514	5.65152	5.54136	5.49245	0.13606	0.12527	0.12037
0.14	8.581894	8.541955631	8.524573	5.62125	5.49564	5.45027	0.13402	0.12341	0.11873
0.16	8.569839	8.529741975	8.5061981	5.58911	5.46793	5.40514	0.13083	0.12013	0.11375
0.18	8.563336	8.523847659	8.5008378	5.56111	5.43874	5.37513	0.12911	0.11854	0.11229
0.2	8.554280	8.518458212	8.4916182	5.522	5.42361	5.3429	0.1267	0.11708	0.10976

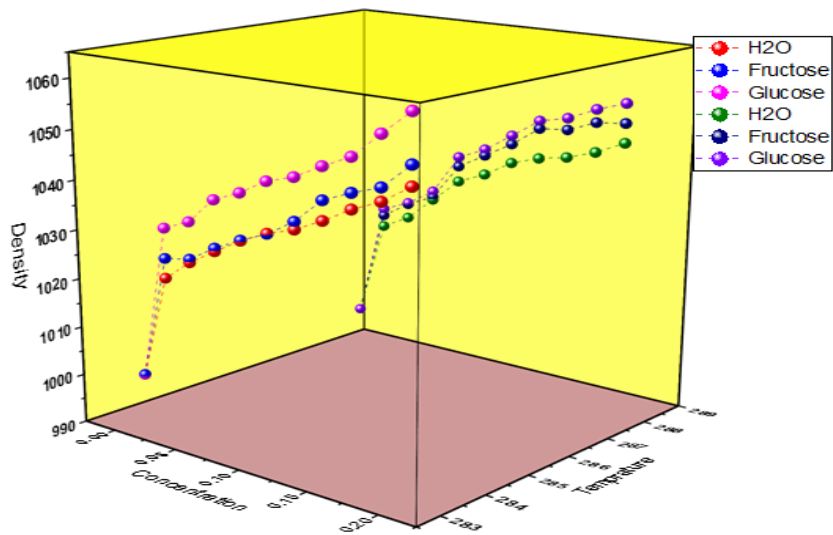


Fig.1. shows a plot of the Density(ρ) [17]of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

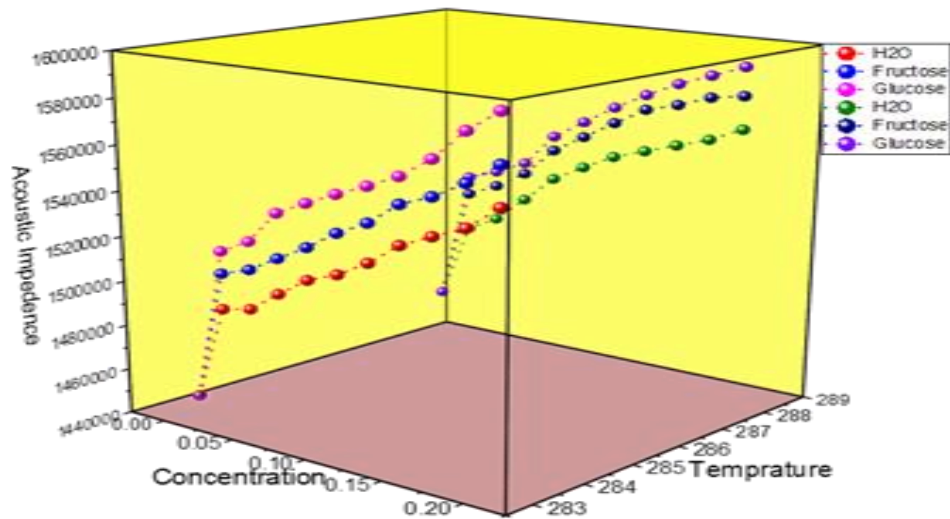


Fig.2. shows a plot of the acoustic impedance (Z) [15] of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

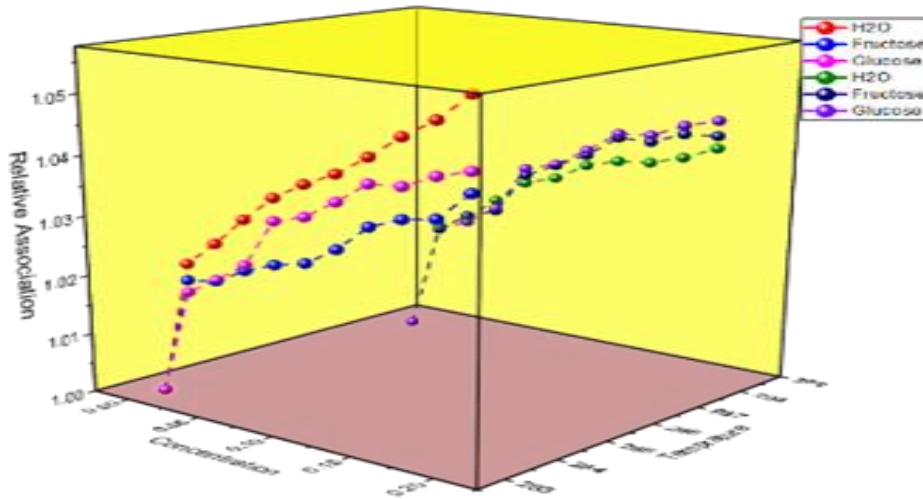


Fig.3. shows a plot of the Relative Association [17] of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

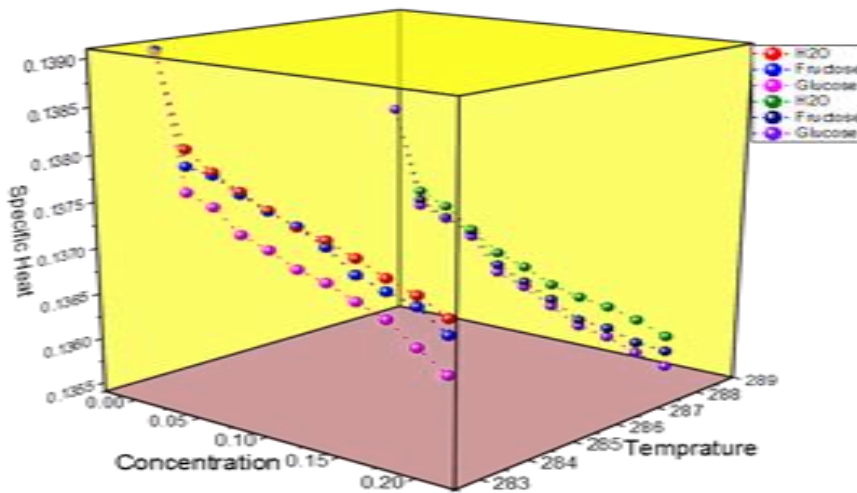


Fig.4. shows a plot of the Specific Heat [18-19] of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

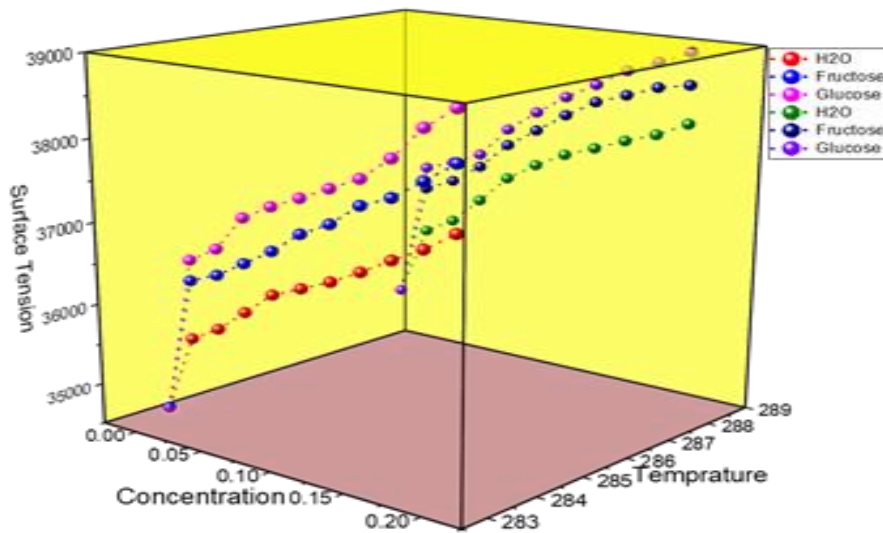


Fig.5. shows a plot of the surface tension of isoleucine in water, fructose, and glucose at various temperatures and concentration.

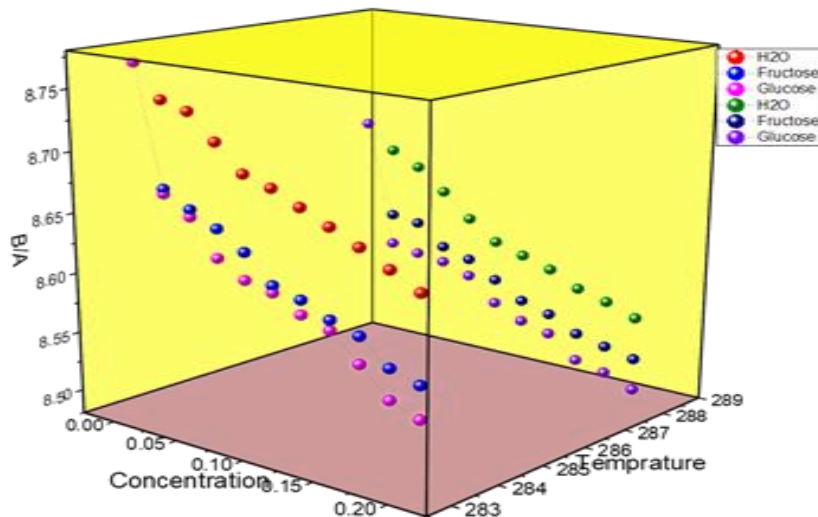


Fig.6. shows a plot of the Non-Linearity parameters of isoleucine in water, fructose, and glucose at various temperatures and concentrations.[21]

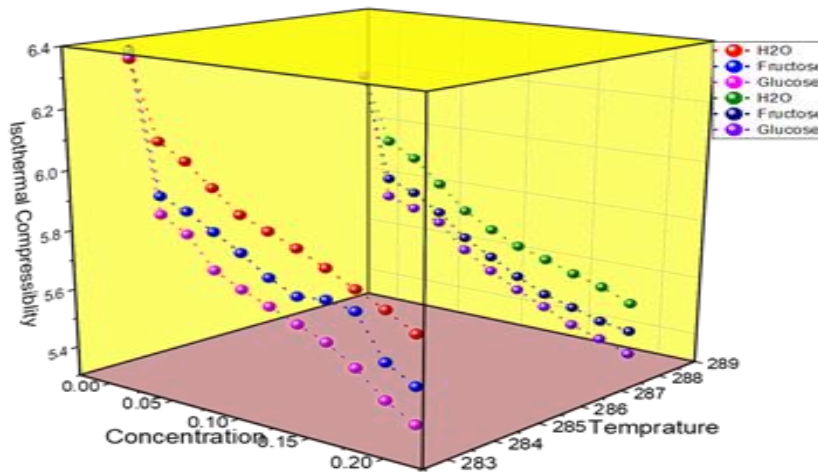


Fig.7. shows a plot of the [22] Isothermal Compressibility of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

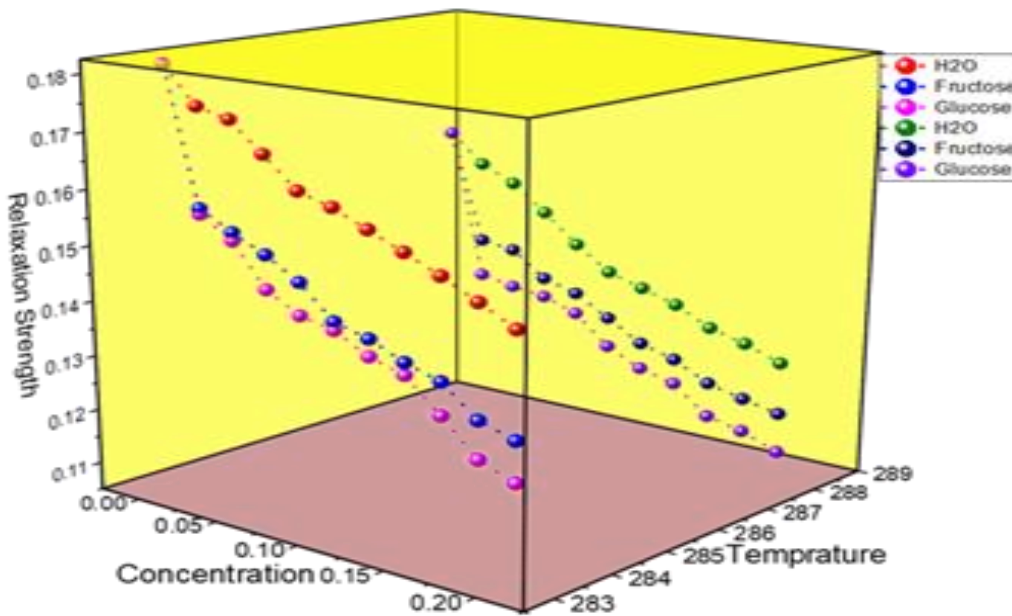


Fig.8. shows a plot of the Relaxation Strength of isoleucine in water, fructose, and glucose at various temperatures and concentrations.