An Acoustical Study in View to Determine Intermolecular Interaction Between Isoleucine and Saccharides Solution

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November 29, 2022

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Abstract

In the current work, amino acids have been considered and physical characteristics like sound velocities and densities have been obtained to better understand intermolecular interactions. We evaluated the density and speed of sound of isoleucine at various concentrations [0.02-0.20 mol Kg-1] in saccharide solutions (fructose and glucose) at different temperatures. Additionally, volumetric and acoustic parameters including acoustic impedance (Z), isothermal compressibility (KT), relative association (RA), specific heat (ϒ), nonlinear parameters, and relaxation strengths have been derived from the experimental data (r). The outcome of the various acoustical and volumetric parameters revealed by the calculation of the type and vitality of the intermolecular interactions that are found within the system under these conditions, as well as the correlation between the concentration trend, and the acoustical parameters, illustrate the significance of the interactions between the solvent and the solutes.

Key-words- isoleucine, glucose, fructose; volumetric and acoustical Parameters

1 Introduction

The structural and functional integrity of all biological processes depends on amino acids, which are the fundamental components of proteins. Aside from amino acids that can act as enzymes, hormones, and structural elements, they amazingly also act as neurotransmitters.[1]all living things have incredibly complex molecules called proteins. The biomolecules required for human life are proteins. Proteins participate in transcription, DNA replication, catalysis, and digestion, and operate as signaling molecules that link the activity of numerous cells, tissues, and organs.[2]

These intricate biomolecules' interactions with the surrounding environment have an impact on their ability to corroborate. These interactions between the ions of the solvent and the molecules of proteins exist. Isoleucine is a branch-chain amino acid[3] that is crucial for humans and other animals. Proteins play a role in digestion, DNA replication, catalysis, and transcription, and operate as a signaling component that enables the integration of biological activity among distinct cells, tissues, and organs.[4]these intricate biomolecules' interactions with the surrounding environment determine how well they can corroborate one another. The ions in the solvent and the protein molecules interact with one Branch chain amino acids, such as isoleucine, which are vital for both humans and other animals.[5] [6]

Information about the interactions between solutes and solvents can be obtained from the volumetric and acoustic properties of the mixture of amino acids, and saccharides in an aqueous solution. Only a few of the interactions that contribute to protein confirmation include hydrogen bonds, electrostatic contact, and hydrophobic interactions in solution. The intermolecular interaction of a particular amino acid in water and other saccharide solutions will be studied using various thermos-acoustic parameters.[2]With the help of different thermos-acoustic parameters, the intermolecular interaction of specific amino acids in water and other saccharide solutions will be investigated.[7][8] It has also been investigated how the solvent medium affects this biomolecule interaction.[9]

The densities and sound velocity of iso-leucine in a liquid solution of glucose and fructose have been studied in the current work at various temperatures and concentrations. Using measured data for acoustical and volumetric parameters including acoustic impedance, isothermal compressibility, specific heat, nonlinear parameters, relative association, relaxation strengths, and nonlinear parameters, the volume of isoleucine that is transferred from water to glucose and fructose was calculated. Solute-solute as well as solute-solvent interactions in solutions, as well as the tendency of the components to form and break structures in working solutions, have all been explored with these factors.[10] This study aims to fill in the gaps in our knowledge of the interactions between pharmaceutically active ionic liquids and amino acids in an aqueous media.

2.Experimental details

2.1 Materials.

The mass fraction purity of the following mentioned AR grade compounds, which is 99.7%, was acquired and put to use right away. Chemical sample specifications

Table.. 1

Chemicals	CAS number	source	mass fraction purity	Purification	Mol. Wt
Iso-leucine	73-32-5	HI Media chem. Pvt. Ltd India	≥0.99	Used as such	131.17 $g\text{-}mol^{-1}$
Glucose	50-99-7	HI Media chem. Pvt. Ltd India	≥0.99	Used as such	180.16 $g\text{-}mol^{-1}$
Fructose	57-48-7	HI Media chem. Pvt. Ltd India	≥0.99	Used as such	180.16 $g\text{-}mol^{-1}$

The mole fraction of amino acids were altered over the ranges (0.02-0.2) $mol\text{-}kg^{-1}$ in 0.1 $mol\text{-}kg^{-1}$ to produce an experimental liquid (mixture) with various compositions. All glassware was carefully dried before use and rinsed with acetone and freshly double-distilled water to eliminate the possibility of errors.

2.2 Method

With the help of a digital ultrasonic interferometer operating at a 2MHz frequency and 0.0001 $m\text{-}s^{-1}$ frequency, as well as a pulse-echo overlap method with functions for temperature and concentration, we want to estimate the ultrasonic velocity at various solutions in the proposed work.

Using a 10 ml specific gravity bottle with a± $2*10^{-2}$ $Kg\text{-}m^{-3}$ Correctness and very accurate and precise digital electronic weighing balance with a frequency of± 0.0001 g, the densities of the double-distilled water and the experimental liquid were calculated. The temperature of the experimental solution was maintained at a constant value using an electrically controlled automatic thermostatic water bath with a precision of± 1 K.

2.3 Theory

Using the conventional formulae derived from the literature, the following list of acoustic and volumetric parameters was calculated from observed data of ultrasonic sound velocity (U) and density (ρ):

- Equation (1) makes it easier to calculate the Acoustic impedance by utilizing the values for the medium's density (ρ) and sound speed (U).[9] $(Z) = U\rho$ …………………………..1

- Relative Association can be calculated from the relation $(R_A) = \frac{\rho}{\rho_o}\left(\frac{U_0}{U}\right)^2$ ….2
- Where (U) has a fixed value and U is the ultrasonic sound velocity of the solvent or solution $(1600)\frac{m}{s}$ [11]
- The value of (ϒ) derived from the relation [11]Specific Heat Ratio $(\Upsilon)\ \frac{17.1}{T^{\frac{4}{9}}\times\rho^{\frac{1}{3}}}$ … … … … … … … … … . .3
- The Surface tension is given by the relation $(\sigma) = \{(6.3^{*}\times10^{-4})\ \rho\ U^{\frac{3}{2}}\}$ …………4

- Isothermal compressibility[12] derived from the relationship **(**k_{T1}):
- $(k_{T1}) = \frac{1.33\times10^{-8}}{\left(6.4\times10^{-4}\ U^{\frac{3}{2}}\ p\right)^{3/2}}$ ….5
- Theoretically, the sound speed and its variation in liquids are mostly determined by the intermolecular potential energy. [10], as shown by Hartmann-Balizar [12]. Hartmann- Balizar and P. L. Mishra's sentence is as follows [13],

- $(B/A)_1 = \left\{2+\left[\frac{0.98\times10^4}{U}\right]\right\}$………6
- Using the formula, [14] Relaxation Strength was determined. (r)= $1-\left(\frac{U}{U_\infty}\right)^2$ 7

3… Result and discussion:

The results for isoleucine's density (ρ) and sound velocity (U), which vary depending on its weight fraction (0.02-0.2mol-kg-1), in water as well as within 0.1mol-kg-1 solutions containing glucose and fructose at 283.15K and 288.15K temperatures**.**

[Table 2] lists the values for isoleucine's density (ρ) and sound speed (U) at various molar concentrations (0.02 to 0.2) mol-kg^{-1} in water, fructose, and glucose aqueous solution. Reviewing the density and sound speed data reveals that these numbers increase when the solution's isoleucine concentration increases.[15][4]

Strong molecular interactions attributed to the improvement in cohesive force are what cause the rise in density and ultrasonic sound velocity. Owing to these coordinating factors. When associated with glucose and fructose, isoleucine molecules form a structure that is more compact than water.[16] The findings suggest that density rises with increasing isoleucine concentration in a solution. The addition of an isoleucine-containing solute may have increased density, which may have improved the structure of water, glucose, and fructose. While density [17] drops with rising temperature, indicating that the kinetic energy of the molecule rises with rising temperature, this increase in density may be due to the addition of the isoleucine-containing solute. Consequently, a lesser contact between the molecules of the solute and solvent is seen.[9]

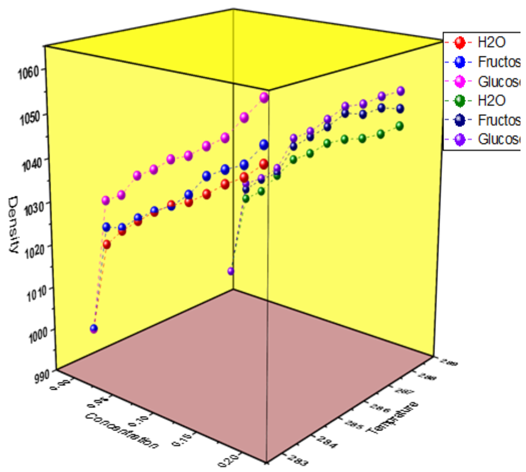

Fig.1. shows a plot of the Density(ρ) [17]of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

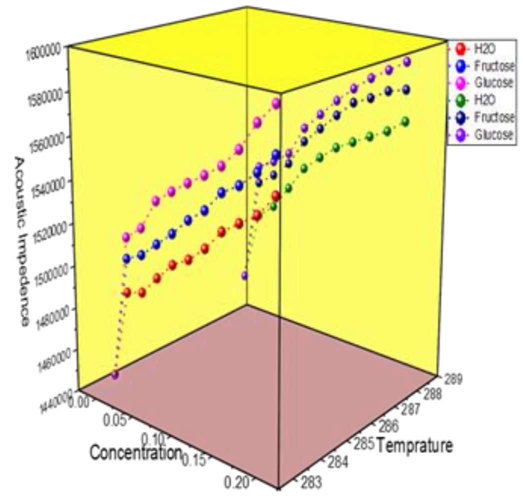

Fig.2. shows a plot of the acoustic impedance (Z) [15] of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

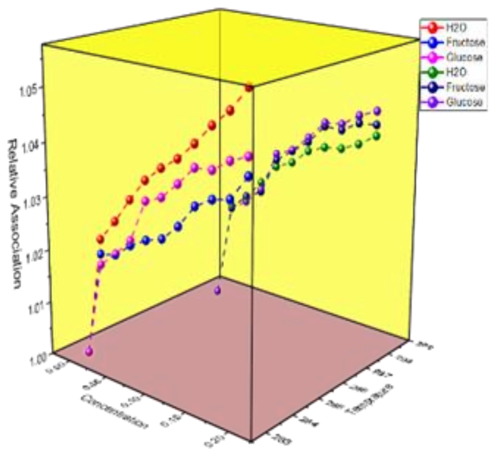

Fig.3. shows a plot of the Relative Association [17] of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

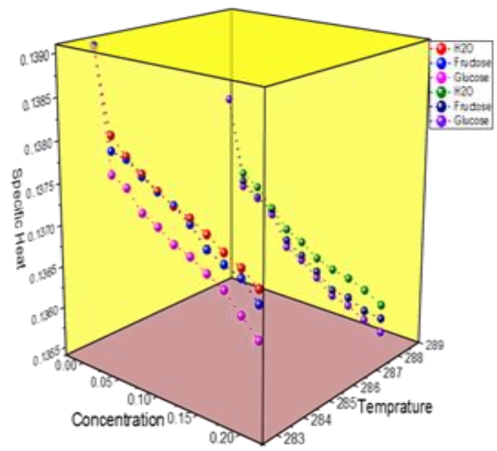

Fig.4. shows a plot of the Specific Heat [18-19] of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

The molecular packing of the system and the many molecular interactions that are present are the focus of the acoustic impedance (Z). Table 2 contains the (Z) values of isoleucine in water, fructose, and glucose solutions. Increases along with temperature and concentration changes. The greater interaction caused by the formation of H-bonds in the solvent is confirmed by the rise in acoustical impedance with concentration. The value grows as the temperature rises, confirming that the system has an increased propensity to form structures as the temperature rises.[18]

In terms of the many types of molecular interactions that were present, the acoustic impedance (Z) addressed the molecular packing of such a system.[9]**[Table 2]** lists the (Z) values of isoleucine in water, fructose, and glucose solutions. Increases along with both a rise in concentration and temperature. The fact that the acoustical impedance increases with concentration indicate a greater interaction caused by the formation of H-bonds in the solution. The value grows as the temperature rises, confirming that the system tends to become more structured as the temperature rises.[19] This also suggests that the elements in the mixture may interact with one another's molecules in a specific way. Additionally, the Z values for Isoleucine in Glucose are greater than those for Isoleucine in Fructose, which may be interpreted by the stronger intermolecular interaction seen in the case of Isoleucine in Glucose.[9] R_A is a crucial attribute that can be considered to gather more knowledge about molecular interaction. Particularly, two governing factors are the solvation of the solute molecule and the dispersion of associated solvent molecules of the solute's interaction with it.[20]

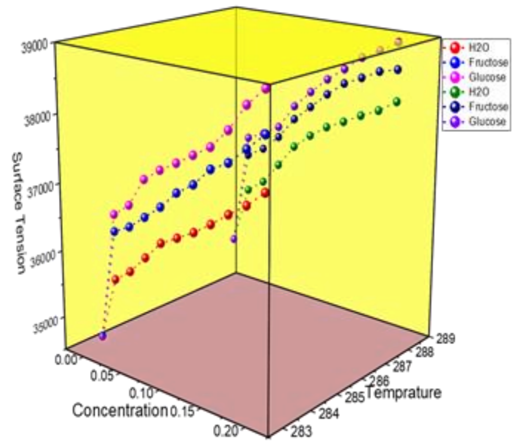

Fig.5. shows a plot of the surface tension of isoleucine in water, fructose, and glucose at various temperatures and

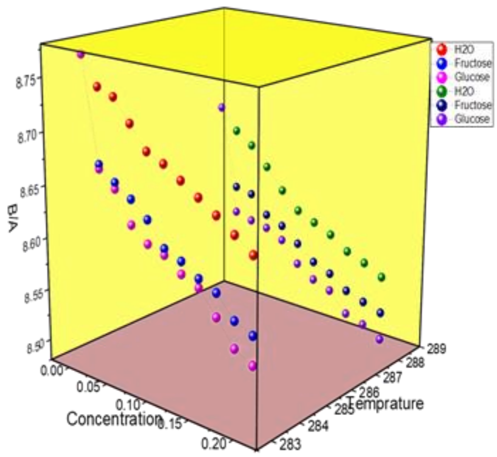

Fig.6. shows a plot of the Non-Linearity parameters of isoleucine in water, fructose, and glucose at various temperatures and concentrations.[21]

When isoleucine in water and isoleucine in glucose and fructose concentrations are elevated, (R_A) [Table 3] increases as well. The solvation of the solute molecule is responsible for the rise in R_A value with solute concentration. As the solute is dissolved in the solvent and the solvent travels near its electrostatic field in the fundamental solvation shell, the solvent molecules compact closer together than they otherwise would have. Electrostriction is the word used to describe this type of medium compression caused by the electric field of the solutes.[21]

When the weight fraction of isoleucine increases, the values of relaxation strength[11] and specific heat ratio drop. This is because the solvent molecule forms a complex, indicating the interaction of isoleucine in the system **[Tables 3 and 4]** This demonstrates that isoleucine, water, as well as glucose, and fructose have a stronger association.[22]

In the Supplementary material [Table 3], the measured values are listed. At atmospheric pressure and temperatures between (283.15 and 288.15 K),[13] the surface tension of the isoleucine was measured. As the hydrogen bond network is disrupted with increasing temperature, the surface tensions of isoleucine also drop. Additionally, because of the length of the branch chain in the alkyl group, isoleucine in fructose has less surface tension than isoleucine in fructose. **[Table 3]**shows the increasing surface tension trend with concentration, which is attributed to hydrogen bolding with dipolar interaction.[23]

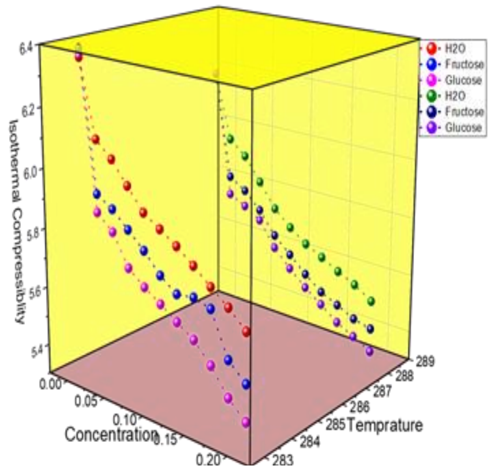

Fig.7. shows a plot of the [22] Isothermal Compressibility of isoleucine in water, fructose, and glucose at various temperatures and concentrations.

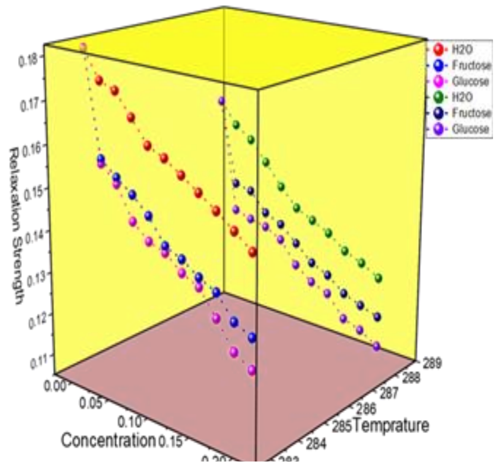

Fig.8. shows a plot of the Relaxation Strength of isoleucine in water, fructose, and glucose at various temperatures and concentrations

The fluid state equation's nonlinearity is measured by the nonlinearity parameters, which have applications in acoustics, and medicine[18]. The (Paritosh Mishra and Ballou) [11] relations were used to derive the non-linear parameters B/A, which are shown in [Table 4]. It should be emphasized that the Hartmann and Ballou[13] instance's nonlinearity parameter values for isoleucine constitute a significant benefit. This implies that a molecule's spacing is less since its clustering is stronger.[24]

Isothermal compressibility is a concept used to define how much pressure a fluid can withstand without raising its temperature. **[Table 4]** shows K_T trends for total isothermal compressibility are shown. The amino acid system's K_T values exhibit a trend toward decline. The greater molecular association is demonstrated by this. (Isoleucine + fructose) has higher K_T values than (isoleucine + glucose), revealing a stronger molecular association than either of the other two solutions. [25]existing in the dipolar form in the neutral solution, which thus has greater interactions with the nearby water molecules. The compressibility of the solution decreases more as a result of the water's rising electrostrictive compression around the molecules.[26]

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 (kgm^{2}s^{-1})**	
	H2O	**Fructose**	**Glucose**	**H_2O**	**Fructose**	**Glucose**	**H_2O**	**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_2O	**Fructose**	**Glucose**	**H_2O**	**Fructose**	**Glucose**	**H_2O**	**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.

Conc. (M) mol/kg	(B/A) Non-linearity Parameter			Isothermal compressibility $\Delta\beta*10^{-11}$ (m^2N^{-1})			Relaxation Strength		
	H2O	Fructose	Glucose	H_2O	Fructose	Glucose	H_2O	Fructose	Glucose
					283K				
0	8.770635	8.770635065	8.7706351	6.35776	6.38523	6.35967	0.18162307	0.18162	0.18162307
0.02	8.743923	8.672853809	8.6688034	6.10621	5.92734	5.86666	0.17512734	0.15746	0.15643926
0.04	8.738044	8.660269184	8.6543087	6.05574	5.89358	5.81837	0.17368718	0.15428	0.15276029
0.06	8.717615	8.649202333	8.6255164	5.98504	5.84309	5.71727	0.16865381	0.15146	0.14538064
0.08	8.696454	8.635017183	8.6126499	5.91503	5.79254	5.67325	0.16339136	0.14783	0.14205167
0.1	8.689419	8.613435261	8.6076429	5.87918	5.73079	5.63761	0.16163085	0.14226	0.14075095
0.12	8.678838	8.606974673	8.5953161	5.84298	5.69	5.60009	0.15897229	0.14058	0.13753604
0.14	8.668277	8.596581355	8.5883859	5.79935	5.69938	5.56332	0.15630608	0.13787	0.13572066
0.16	8.657350	8.589404775	8.5675107	5.75187	5.68349	5.50308	0.15353444	0.13599	0.13021760
0.18	8.645234	8.57011723	8.5451714	5.70832	5.54381	5.42253	0.15044491	0.13091	0.12427017
0.2	8.632902	8.562888207	8.5362703	5.65459	5.49068	5.36962	0.14728280	0.12899	0.12188341
					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

4. Conclusion

The results of the current study lead to the conclusion that interactions between the amino acids in water and saccharide solutions decrease in the order of isoleucine in Glucose > isoleucine in Fructose > isoleucine in Water.

The relationship between the trend in acoustical parameters and concentration shows the presence of prominent interactions between the solutes, and the direction and magnitude of excess parameters show the potential for electrostatic interactions between the solute molecules. Surface tension values turn positive for every component of the solution. This shows that the system has a lot of hydrogen bonds and dipole-dipole interactions happening in the solution.

Finding

No specific grant for this research was provided by funding organizations in the public, private, or nonprofit sectors.

Conflict of Interest:

The authors (NSP, UPM, PLM) Assert no conflict of interest (COI) in the existing research work

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