



## Molecular Interactions Study in between Amino Acids (Glycine) and Vitamins using Ultrasonic Technique

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### ARTICLE INFO

Published Online:  
19 April 2023

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### ABSTRACT

Sound (ultrasonic) velocity and density have been determined at 2 MHz frequency for the Thermo-Acoustical Investigation of the system (binary mixture) Amino acid (Glycine) vitamins at 283.15-298.15K temp the various thermoacoustical characteristics, such as adiabatic Compressibility, relaxation Strength, surface tension and relative Association have been calculated using the obtained ultrasonic velocity and density. This study aims to characterise the kind and strength of molecular interactions in a binary mixture of aqueous vitamin C solution (0.2) and amino acid solution (0.02 - 0.2 mol/kg). The obtained result supports the occurrence of moderate potential of intermolecular interaction follows by association in the adopted liquid mixture.

**KEYWORDS:** Amino acid, Vitamin C, Ultrasonic Velocity, Density, Acoustical Parameter, Thermodynamical Parameter.

### INTRODUCTION

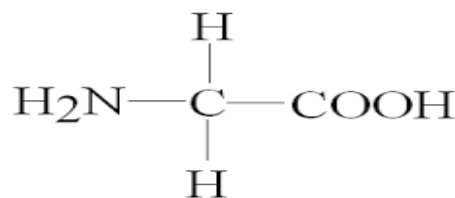
Ultrasonic is the science of acoustic and the technology of sound in the frequency range of the ultrasonic wave is higher than 20 KHz. Which beyond the audible limit, ultrasonic method has become a power full tool to providing the information about the physicochemical properties of liquid system.[1] The ultrasonic velocity gives information about structure and strength of molecular interactions in solution.[2] and the value of ultrasonic velocity, density and adiabatic compressibility which help to providing the wealth information about the interaction between the dipoles, hydrogen bonding etc. The 20% of the living organisms is made by the protein, which are play an important functions in all the biological processes and the glycine is the building blocks of this.[3]

Amino acid is the fundamental units of protein peptides and certain types of Harmons and antibiotics. Protein cannot be existed without any combination of the amino acid. most of the studies on amino acid and biomolecules have been carried out in pure and mix aqueous solution.[4] mixing of the various vitamins and water the different behavior of the two mixtures is shown. when the binary solution is equal to its components counterpart is arises from the nature of vitamin and glycine interaction.[5] the interaction of amino acid with the vitamins the result evaluation of the hydrogen is form. in the present paper we have determined or calculate different thermo-acoustic parameter depends on ultrasonic velocity and density which are acoustic impedance, specific

heat ratio, relative association, surface tension, adiabatic compressibility and molal volumes etc. [6]

### MATERIAL AND METHOD

➤ Currently at Work, Amino acid (Glycine) is used as analytical reagent {[ CAS No - 56 -40.- 6, EC No. - 200 - 272 - 2]} [ Molecular Weight 75.07 g/mol] distilled water is utilised as a solute and has a purity grade of 99% [ Molecular Weight 18.01528 g/mol] and aqueous solution vitamins [ Molecular Weight 122.13 g/mol] with density 1000 kg/m<sup>3</sup> and 2170 kg/m<sup>3</sup> is used as a solvent.



glycine

- This method has taken place at various temperatures (283.15 - 298.15K) is maintained constant by electronic thermostat.
- The Wight of substance has measured by utilising a precise digital weighing scale 0.1 Mg.
- Analog the ultrasonic velocity is Measured using an ultrasonic interferometer with 2 MHz frequency and 0.1% accuracy.

## “Molecular Interactions Study in between Amino Acids (Glycine) and Vitamins using Ultrasonic Technique”

- The density of solution has perfectly determined or calculate by using 10 ml gravity density bottle.
- By using these two parameters, we can determine or calculate different thermal acoustic parameter at different temperatures and concentration.

### DEFINING RELATIONS

The following defining relations from the literature are utilised to calculate the various Acoustical and Thermodynamical parameters

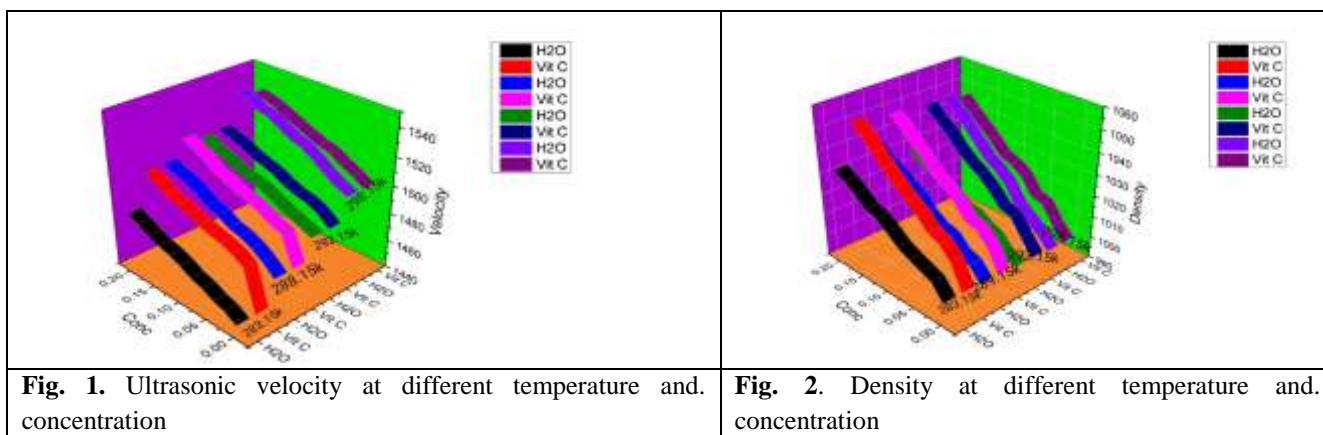
- ❖ Adiabatic Compressibility ( $\beta$ ) =  $1 / (U^2\rho)$
- ❖ Acoustic Impedance ( $Z$ ) =  $U \rho$
- ❖ Relative Association ( $R_A$ ) =  $(\rho/\rho_0) (U_0/U)^{1/3}$
- ❖ Isothermal Compressibility ( $K_T$ ) =  $17.1 \cdot 10^{-4} / (T^{4/9} U^2 \rho^{1/3})$
- ❖ Specific Heat Ratio ( $\gamma$ ) =  $\{17.1 / (T^{4/9} \rho^{1/3})\}$
- ❖ Relaxation Strength ( $r$ ) =  $1 - (U/U_\infty)^2$
- ❖ Molal Volume ( $V_m$ ) =  $M_{eff}/\rho$
- ❖ Surface Tension ( $\sigma$ ) =  $\{(6.3 \cdot 10^{-4}) \rho U\}$
- ❖ Nonlinear parameter ( $B/A$ ) =  $\{2 + [0.98 \cdot 10^4 / U]\}$
- ❖ Lenard Jones Potential =  $\{6(V_m/V_a) - 13\}$

### RESULT AND DISCUSSION

In present work, the obtained various in ultrasonic velocity and density at different temp. 283.15-298.15k and mole fraction for aqueous system of ( Glycine, vitamin) is showing in fig 1.2.

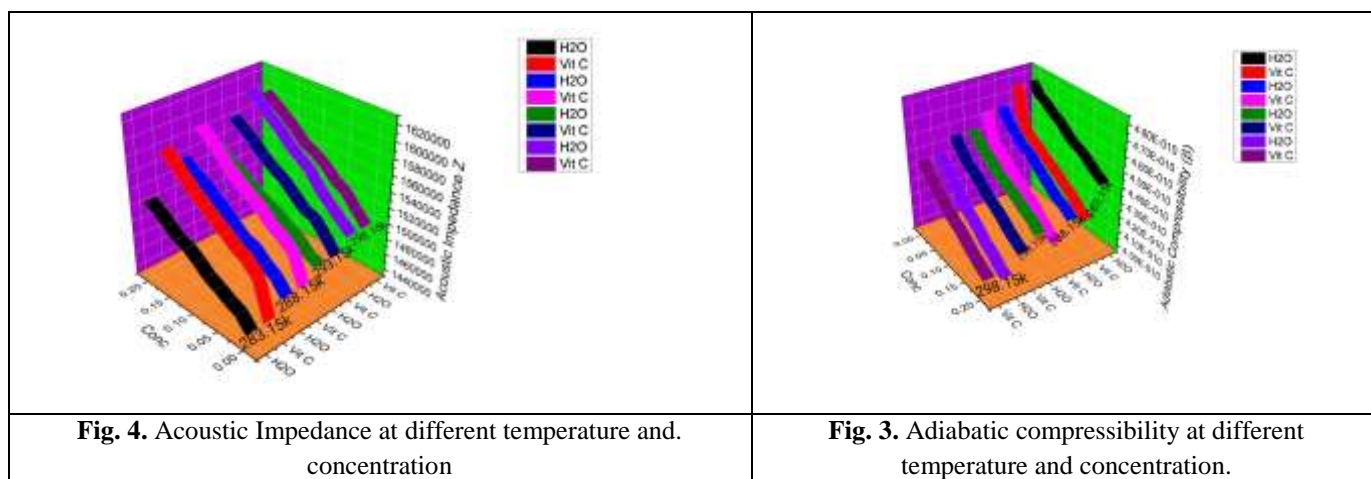
The plot between ultrasonic velocity and concentration at different temperatures is shown that the ultrasonic velocity increase with an rise in conc. of Amino acid (Glycine) in a water -based mixture of vitamins, result indicates association in the molecules of the component. The molecule - level interaction in the constituent , may involve due to dipole interaction and due to the hydrogen bonding between the constituent molecules the peak at molar concentration because of containing the strong hydrogen bond.[7]

It is observed that the density of mixture of Aqueous Solution of vitamin and Amino acid (glycine) is increase with concentration and decrease with rise of the temperature.[8]



The adiabatic compressibility was a reverse trend of ultrasonic velocity, thus in the given binary mixture association take place. An ionic interaction among the molecules and the development and breaking in the hydrogen bonds that solution.[9]

From given table, it is observed that for a given concentration, with increases concentration; the values of acoustic impedance ( $z$ ) increases. of solution due to the interaction between solute and solvent molecules.[10]

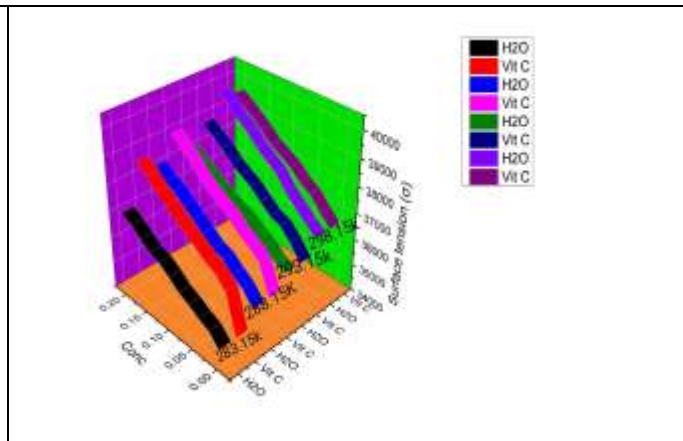
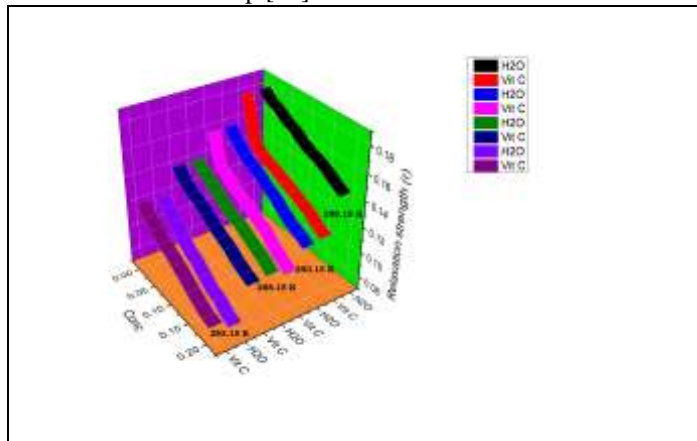


“Molecular Interactions Study in between Amino Acids (Glycine) and Vitamins using Ultrasonic Technique”

It is observed that, the drop in values of relaxation Strength along with rise in conc. shows that the interaction between solute and solvent in the system, which indicate the greater association between vitamin and Amino acid (Glycine) [11]

The surface tension for both the system (glycine + vita C + water and glycine + water) increases as concentration of tension should also drop.[12]

Amino acid (glycine) increases, this behavior forms the strong film due to the increase in molecular association. As temperature increases, this attractiveness must be drop and therefore surface



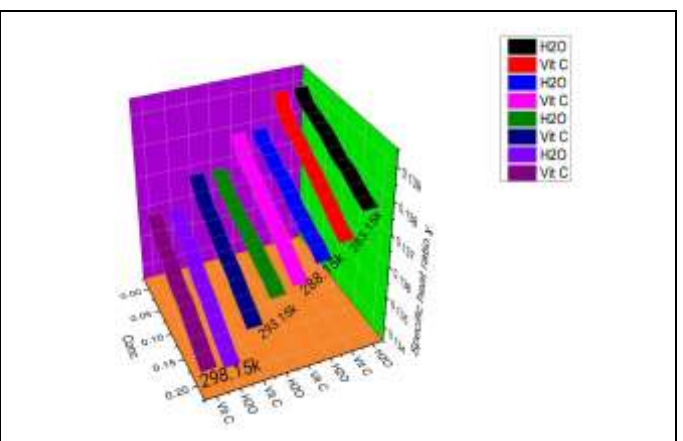
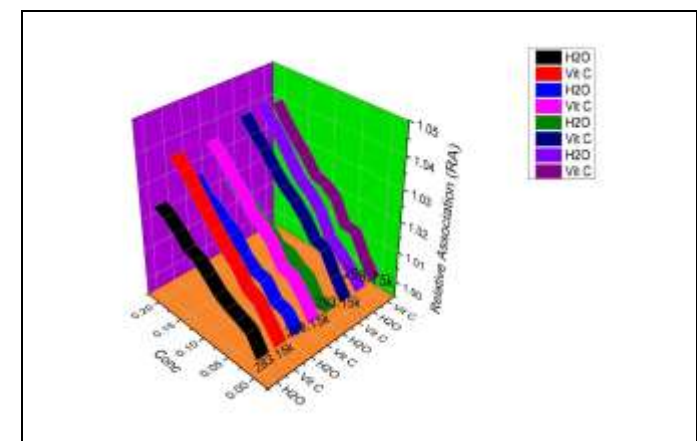
**Fig. 5.** Relaxation strength at different temperature and concentration.

**Fig. 6.** Surface Tension at different temperature and concentration.

It is observed that , The value of Relative association rises with conc. indicating that there is intermolecular interaction and that the components of the molecule are closely related , it shows th the close association of components of molecule and there exists intermolecular interaction it also indicate that

when the temp. rises the data of Relative Association increases which shows that , the molecular interactions of the system increases.[13]

A steady decrease in the specific heat ratio of a solution of vit. and the (283.15-298.15k) indicates that the specific heat at constant Valume is dropping as conc. increases.[14]



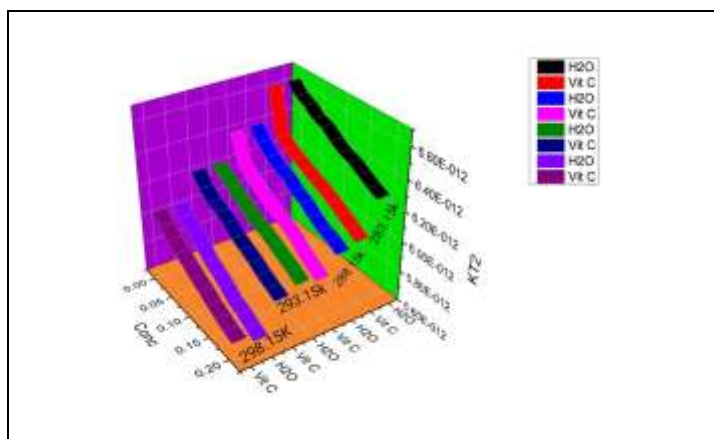
**Fig. 7.** Relative association at different temperature and concentration

**Fig. 8.** Specific heat ratio relation at different temperature and concentration

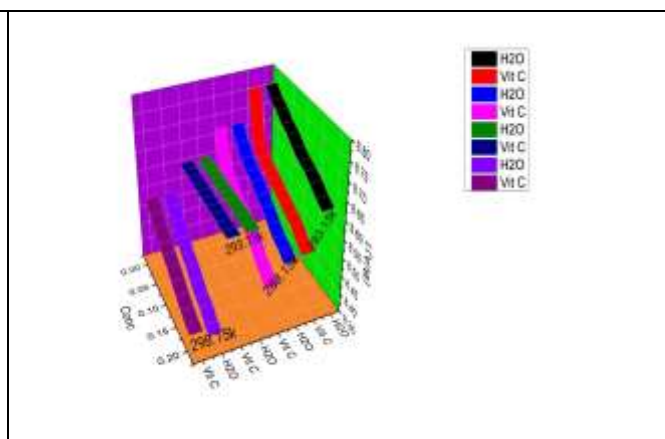
At all temp. It has been found that the isothermal compressibility decreases as the solute's conc. rises This demonstrates how the electrostatic field of the particle has an impact on how a protein of the surrounding dissolvable atoms

is securely attached to the particles when a solute breaks down vit. (dissolvable).[15]

The non-linear parameters' declining trends demonstrate that the interaction between the solvent and solute components during mixing is stronger at higher conc.[16]



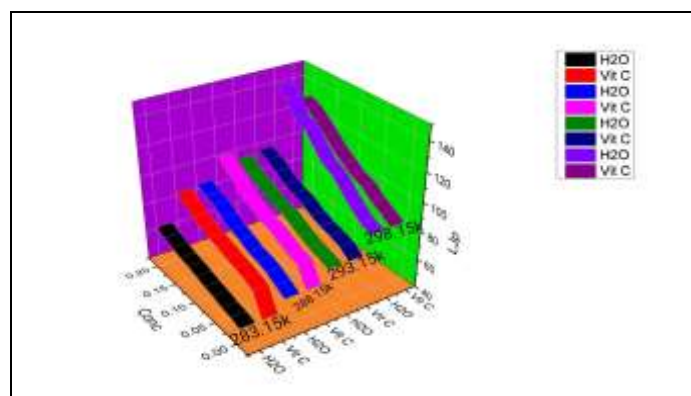
**Fig. 9.** Isothermal Compressibility at different temperature and concentration.



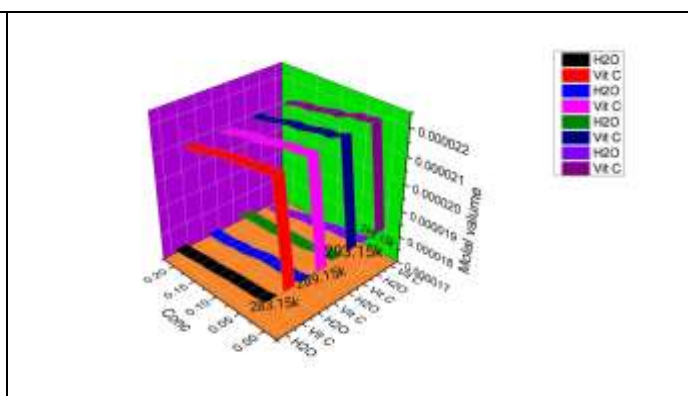
**Fig. 10.** Non linearity parameter at different temperature and concentration

From the given table, it is observed that for a given concentration the values of Lenard Jones Potential increases with increases in concentration. It is observed that the molal

volume decrease with increases in solute concentration with slight deviation. confirms that the highest value of free volume indicates the weak solute solvents interaction.[17]



**Fig. 11.** LJP at different temperature and concentration.



**Fig. 12.** Molal Volume at different temperature and concentration.

## CONCLUSION

All parameters are non - linearly varied with rise in molar concentration of Glycine along vitamins solution. So that association, and molecular interactions takes place in the solution perhaps due to the formation of hydrogen bond also ionic interaction among solute and solvent molecules. These interaction shows the result in the attractive force which pramote the structure forming tendency.

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**Table 1:** The value of ultrasonic velocity, density and molal volume at different temperatures and concentration.

Conc.	Velocity		Density		Molal Volume	
	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C
<b>283.15 K</b>						
0	1447.427	1447.427	999.7	999.7	1.80E-05	1.80E-05
0.02	1452.689	1476.516	1006.627	1011.2673	1.79E-05	2.18E-05
0.04	1455.25	1481.616	1008.801	1016.801	1.79E-05	2.17E-05
0.06	1459.531	1484.537	1011.1	1019.011	1.79E-05	2.17E-05
0.08	1462.015	1486.586	1013.64	1024.4693	1.79E-05	2.16E-05
0.1	1466.482	1489.345	1017.91	1028.1923	1.78E-05	2.16E-05
0.12	1469.739	1492.103	1021.78	1032.7013	1.78E-05	2.15E-05
0.14	1471.812	1494.892	1023.24	1037.4239	1.78E-05	2.14E-05
0.16	1474.963	1497.62	1027.56	1042.631	1.77E-05	2.13E-05
0.18	1479.304	1502.379	1031.28	1047.892	1.77E-05	2.12E-05
0.2	1482.512	1505.578	1033.68	1051.8826	1.76E-05	2.12E-05
<b>288.15 K</b>						
0	1466.032	1466.032	999.103	999.103	1.80E-05	1.80E-05
0.02	1473.379	1486.517	1005.29	1009.3145	1.79E-05	2.19E-05
0.04	1478.928	1489.275	1007.32	1014.836	1.79E-05	2.18E-05
0.06	1482.667	1493.904	1012.91	1016.192	1.79E-05	2.18E-05
0.08	1484.783	1497.155	1014.08	1022.8	1.79E-05	2.17E-05
0.1	1489.392	1499.31	1017.88	1026.823	1.78E-05	2.16E-05

“Molecular Interactions Study in between Amino Acids (Glycine) and Vitamins using Ultrasonic Technique”

<b>0.12</b>	1492.2	1503.068	1023.7	1030.079	1.77E-05	2.15E-05
<b>0.14</b>	1497.307	1505.443	1026.39	1035.061	1.77E-05	2.15E-05
<b>0.16</b>	1501.447	1511.827	1030.43	1040.114	1.76E-05	2.14E-05
<b>0.18</b>	1503.612	1515.428	1032.38	1045.235	1.76E-05	2.13E-05
<b>0.2</b>	1507.23	1519.421	1037.68	1049.077	1.76E-05	2.12E-05
<b>293.15 K</b>						
<b>0</b>	1481.496	1481.496	998.2	998.2	1.81E-05	1.81E-05
<b>0.02</b>	1484.992	1488.556	999.31	1005.289	1.81E-05	2.20E-05
<b>0.04</b>	1488.361	1492.301	1005.83	1012.8309	1.80E-05	2.18E-05
<b>0.06</b>	1492.132	1494.217	1008.35	1014.5306	1.79E-05	2.18E-05
<b>0.08</b>	1496.296	1497.421	1011.94	1020.4992	1.79E-05	2.17E-05
<b>0.1</b>	1499.883	1501.869	1013.1	1025.1002	1.79E-05	2.16E-05
<b>0.12</b>	1500.999	1504.484	1016.58	1028.3018	1.78E-05	2.16E-05
<b>0.14</b>	1504.3	1507.205	1019.36	1032.6309	1.78E-05	2.15E-05
<b>0.16</b>	1507.612	1511.314	1022.82	1038.2836	1.78E-05	2.14E-05
<b>0.18</b>	1510.589	1514.172	1025.09	1042.2103	1.78E-05	2.13E-05
<b>0.2</b>	1515.122	1516.39	1029.52	1047.0999	1.77E-05	2.13E-05
<b>298.15 K</b>						
<b>0</b>	1498.101	1498.101	997	997	1.81E-05	1.81E-05
<b>0.02</b>	1501.639	1503.273	1002.38	1002.9306	1.80E-05	2.20E-05
<b>0.04</b>	1506.83	1507.371	1007.02	1010.893	1.79E-05	2.19E-05
<b>0.06</b>	1512.92	1512.515	1011.23	1012.3208	1.79E-05	2.19E-05
<b>0.08</b>	1518.21	1514.62	1019.439	1019.8906	1.78E-05	2.17E-05
<b>0.1</b>	1520.63	1517.826	1023.98	1023.3689	1.77E-05	2.17E-05
<b>0.12</b>	1525.27	1521.39	1027.45	1025.1178	1.77E-05	2.16E-05
<b>0.14</b>	1529.89	1525.369	1033.11	1030.8321	1.76E-05	2.15E-05
<b>0.16</b>	1531.401	1528.97	1038.85	1035.3601	1.75E-05	2.15E-05
<b>0.18</b>	1536.321	1531.832	1043.87	1040.1543	1.74E-05	2.14E-05
<b>0.2</b>	1538.361	1533.08	1047.92	1045.2309	1.74E-05	2.13E-05

**Table 2:** The value of Acoustic Impedance, specific Heat Ratio and isothermal Compressibility at different temperatures and concentration.

Conc.	Acoustic Impedance		Specific Heat ratio		KT2	
	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C
<b>283.15 K</b>						
<b>0</b>	1446992.772	1446992.77	0.13907670	0.13907670	6.64E-12	6.64E-12
<b>0.02</b>	1462315.97	1493151.90	0.13875696	0.13854441	6.58E-12	6.35E-12
<b>0.04</b>	1468057.655	1506508.63	0.13865721	0.13829261	6.55E-12	6.30E-12
<b>0.06</b>	1475731.794	1512759.53	0.13855204	0.13819256	6.50E-12	6.27E-12
<b>0.08</b>	1481956.885	1522961.71	0.13843621	0.13794670	6.48E-12	6.24E-12
<b>0.1</b>	1492746.693	1531333.06	0.13824237	0.13778000	6.43E-12	6.21E-12
<b>0.12</b>	1501749.915	1540896.70	0.13806762	0.13757918	6.39E-12	6.18E-12
<b>0.14</b>	1506016.911	1550836.68	0.13800192	0.13737010	6.37E-12	6.15E-12
<b>0.16</b>	1515612.98	1561465.03	0.13780825	0.13714103	6.33E-12	6.11E-12
<b>0.18</b>	1525576.629	1574330.93	0.13764235	0.13691114	6.29E-12	6.07E-12
<b>0.2</b>	1532443.004	1583691.30	0.13753575	0.13673778	6.26E-12	6.03E-12
<b>288.15 K</b>						
<b>0</b>	1464716.969	1464716.96	0.13802640	0.13802640	6.42E-12	6.42E-12
<b>0.02</b>	1481173.175	1500363.16	0.13774266	0.13755934	6.35E-12	6.23E-12
<b>0.04</b>	1489753.753	1510631.20	0.13765007	0.13733179	6.29E-12	6.19E-12
<b>0.06</b>	1501808.231	1518093.29	0.13739639	0.13724831	6.25E-12	6.15E-12
<b>0.08</b>	1505688.745	1531290.14	0.13734353	0.13695213	6.23E-12	6.11E-12
<b>0.1</b>	1516022.329	1539525.99	0.13717240	0.13677301	6.18E-12	6.08E-12

“Molecular Interactions Study in between Amino Acids (Glycine) and Vitamins using Ultrasonic Technique”

<b>0.12</b>	1527565.14	1548278.78	0.13691195	0.13662875	6.15E-12	6.05E-12
<b>0.14</b>	1536820.932	1558225.33	0.13679224	0.13640919	6.10E-12	6.02E-12
<b>0.16</b>	1547136.03	1572472.42	0.13661323	0.13618793	6.06E-12	5.96E-12
<b>0.18</b>	1552298.957	1583978.38	0.13652716	0.13596515	6.04E-12	5.92E-12
<b>0.2</b>	1564022.426	1593989.62	0.13629433	0.13579897	6.00E-12	5.88E-12
<b>293.15 K</b>						
<b>0</b>	1478829.30	1478829.30	0.13701639	0.13701639	6.24E-12	6.24E-12
<b>0.02</b>	1483967.356	1496428.97	0.13696564	0.13669356	6.21E-12	6.17E-12
<b>0.04</b>	1497038.145	1511448.56	0.13666905	0.13635342	6.17E-12	6.12E-12
<b>0.06</b>	1504591.302	1515928.87	0.13655510	0.13627723	6.13E-12	6.10E-12
<b>0.08</b>	1514161.774	1528116.93	0.13639343	0.13601103	6.09E-12	6.07E-12
<b>0.1</b>	1519531.467	1539566.21	0.13634135	0.13580724	6.06E-12	6.02E-12
<b>0.12</b>	1525885.563	1547063.60	0.13618560	0.13566615	6.04E-12	5.99E-12
<b>0.14</b>	1533423.248	1556386.45	0.13606168	0.13547630	6.01E-12	5.96E-12
<b>0.16</b>	1542015.706	1569172.54	0.13590808	0.13522999	5.98E-12	5.92E-12
<b>0.18</b>	1548489.678	1578085.65	0.13580769	0.13505995	5.95E-12	5.89E-12
<b>0.2</b>	1559848.401	1587810.45	0.13561262	0.13484943	5.91E-12	5.86E-12
<b>298.15 K</b>						
<b>0</b>	1493606.697	1493606.69	0.13604489	0.13604489	6.06E-12	6.06E-12
<b>0.02</b>	1505212.901	1507678.49	0.13580106	0.13577620	6.02E-12	6.01E-12
<b>0.04</b>	1517407.947	1523790.79	0.13559216	0.13541878	5.97E-12	5.96E-12
<b>0.06</b>	1529910.092	1531150.39	0.13540373	0.13535508	5.92E-12	5.92E-12
<b>0.08</b>	1547722.484	1544746.70	0.13503931	0.13501938	5.86E-12	5.89E-12
<b>0.1</b>	1557094.707	1553295.92	0.1348394	0.13486623	5.83E-12	5.85E-12
<b>0.12</b>	1567138.662	1559603.97	0.13468743	0.13478949	5.79E-12	5.82E-12
<b>0.14</b>	1580544.658	1572399.33	0.13444101	0.13453997	5.74E-12	5.78E-12
<b>0.16</b>	1590895.929	1583034.53	0.13419294	0.13434355	5.72E-12	5.75E-12
<b>0.18</b>	1603719.402	1593341.64	0.13397748	0.13413683	5.68E-12	5.72E-12
<b>0.2</b>	1612079.259	1602422.58	0.13380466	0.13391931	5.65E-12	5.70E-12

**Table 3:** Lenard Jones Potential, Relative Association and Relaxation Strength at different temperatures and concentration.

Conc.	LJP		Relative Association		Relaxation Strength	
	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C
<b>283.15 K</b>						
<b>0</b>	49.79069767	49.7906976	1	1	0.18162307	0.181623078
<b>0.02</b>	52.09090909	64.8571428	1.00571182	1.00488334	0.17566198	0.148398633
<b>0.04</b>	53.2962963	67.8695652	1.00729226	1.00922176	0.17275290	0.14250548
<b>0.06</b>	55.40764331	69.9299363	1.00859977	1.0107515	0.16787861	0.139121053
<b>0.08</b>	56.74025974	71.7058823	1.01056052	1.01569847	0.16504380	0.136742994
<b>0.1</b>	58.67785235	73.9798657	1.01378610	1.01875974	0.15993380	0.133535731
<b>0.12</b>	60.65517241	75.9655172	1.01688815	1.02259654	0.15619815	0.130323686
<b>0.14</b>	61.68531469	78.0638297	1.01786284	1.02663367	0.15381618	0.127069495
<b>0.16</b>	63.95652174	80.9705882	1.02143173	1.03115975	0.15018912	0.1238806
<b>0.18</b>	66.25373134	85.6046511	1.02412582	1.03526743	0.14517956	0.118303649
<b>0.2</b>	68.86046512	88.76	1.02576821	1.03847341	0.14146803	0.114544877
<b>288.15 K</b>						
<b>0</b>	58.52317881	58.5231788	1	1	0.16044928	0.160449287
<b>0.02</b>	62.63380282	71.7741935	1.00451730	1.00555872	0.15201340	0.136823128
<b>0.04</b>	66.55555556	73.6225165	1.00528530	1.00994131	0.14561405	0.133617177
<b>0.06</b>	68.98473282	77.2068965	1.01001356	1.01073916	0.14128850	0.128222984
<b>0.08</b>	70.25581395	80.6690647	1.01069963	1.01657482	0.13883572	0.124424573
<b>0.1</b>	73.82926829	82.2941176	1.01343942	1.02008414	0.13348104	0.121902158
<b>0.12</b>	76.24369748	86.2307692	1.01859430	1.02246522	0.13021060	0.117494761

“Molecular Interactions Study in between Amino Acids (Glycine) and Vitamins using Ultrasonic Technique”

<b>0.14</b>	80.15789474	88.5748031	1.02010845	1.02686982	0.12424677	0.114703662
<b>0.16</b>	84.77777778	95.8135593	1.02318157	1.03042834	0.11939722	0.107179345
<b>0.18</b>	86.62264151	100.097345	1.02462561	1.03468081	0.11685584	0.102921085
<b>0.2</b>	90.52941176	105.878504	1.02906108	1.03757351	0.11260067	0.098187432
<b>293.15 K</b>						
<b>0</b>	68.04477612	68.0447761	1	1	0.14264437	0.142644376
<b>0.02</b>	70.53846154	73.2745098	1.00032577	1.00550708	0.13859326	0.134453529
<b>0.04</b>	72.71428571	75.9795918	1.00609213	1.01220247	0.13468028	0.130092861
<b>0.06</b>	75.76033058	77.8333333	1.00776239	1.01346756	0.13028988	0.127857639
<b>0.08</b>	79.5862069	80.6690647	1.01041128	1.01870231	0.12542901	0.124113417
<b>0.1</b>	82.89285714	85.1818181	1.01076249	1.02228399	0.12123085	0.118902151
<b>0.12</b>	84.09090909	87.4651162	1.01398303	1.02488231	0.11992265	0.115831208
<b>0.14</b>	87.75471698	90.2	1.01601167	1.02857730	0.11604746	0.112630112
<b>0.16</b>	90.68932039	94.8991596	1.01871322	1.03326968	0.11215080	0.107785154
<b>0.18</b>	94.33668342	99.1052631	1.02030297	1.03652445	0.10864096	0.104407482
<b>0.2</b>	100.0990415	102.135135	1.023689343	1.04087849	0.10328333	0.101781784
<b>298.15 K</b>						
<b>0</b>	81.43478261	81.4347826	1	1	0.12331773	0.123317732
<b>0.02</b>	84.2972973	86.2481203	1.00460596	1.00479346	0.11917199	0.117254019
<b>0.04</b>	90.26923077	90.4645669	1.00809598	1.01185203	0.11307162	0.112434636
<b>0.06</b>	97.26694045	96.5	1.01095035	1.01213117	0.10588791	0.106366553
<b>0.08</b>	104.3626374	99.2413793	1.01797200	1.01922695	0.09962437	0.103877444
<b>0.1</b>	107.9567198	104.297297	1.02196376	1.02198242	0.09675172	0.100079779
<b>0.12</b>	115.4159613	109.264150	1.02438606	1.02292893	0.09123102	0.09584862
<b>0.14</b>	123.9649805	116	1.0289913	1.02773583	0.08571741	0.091113052
<b>0.16</b>	127	122.220125	1.03436799	1.03143922	0.08391053	0.086816695
<b>0.18</b>	137.6493506	127.789473	1.03825564	1.03556952	0.07801476	0.083394814
<b>0.2</b>	142.8208955	130.434343	1.04182293	1.04034130	0.07556462	0.081900669

**Table 4:** The value of surface tension, adiabatic compressibility and Non linearity parameter at different temperatures and concentration.

Conc.	Surface Tension		Adiabatic Compressibility		(B/A)1	
	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C	H <sub>2</sub> O	Vitamin C
<b>283.15 K</b>						
<b>0</b>	34682.08881	34682.0888	4.77E-10	4.77E-10	8.77063506	8.770635065
<b>0.02</b>	35113.01293	36146.2810	4.71E-10	4.54E-10	8.74611014	8.637246058
<b>0.04</b>	35281.94068	36532.5513	4.68E-10	4.48E-10	8.73423810	8.614399413
<b>0.06</b>	35518.50236	36720.2780	4.64E-10	4.45E-10	8.71448568	8.601384809
<b>0.08</b>	35698.66968	36993.4261	4.62E-10	4.42E-10	8.70307760	8.592285949
<b>0.1</b>	36013.47552	37231.2711	4.57E-10	4.38E-10	8.68265958	8.580073791
<b>0.12</b>	36270.89523	37498.4639	4.53E-10	4.35E-10	8.66785055	8.567911196
<b>0.14</b>	36399.59636	37775.6133	4.51E-10	4.31E-10	8.65845909	8.555657532
<b>0.16</b>	36670.71928	38069.1894	4.47E-10	4.28E-10	8.64423446	8.543716029
<b>0.18</b>	36966.07091	38443.8019	4.43E-10	4.23E-10	8.62473703	8.522987875
<b>0.2</b>	37172.68992	38713.5244	4.40E-10	4.19E-10	8.61040180	8.509128056
<b>288.15 K</b>						
<b>0</b>	35331.81823	35331.8182	4.66E-10	4.66E-10	8.68471083	8.684710839
<b>0.02</b>	35818.18913	36443.6512	4.58E-10	4.48E-10	8.65137754	8.592591945
<b>0.04</b>	36093.46306	36727.0841	4.54E-10	4.44E-10	8.6264213	8.580383072
<b>0.06</b>	36431.48218	36965.821	4.49E-10	4.41E-10	8.60971074	8.559993145
<b>0.08</b>	36551.6719	37327.7159	4.47E-10	4.36E-10	8.60029108	8.545748436
<b>0.1</b>	36859.60321	37555.4779	4.43E-10	4.33E-10	8.57986614	8.53634005
<b>0.12</b>	37175.24216	37816.2992	4.39E-10	4.30E-10	8.56748425	8.519997765



“Molecular Interactions Study in between Amino Acids (Glycine) and Vitamins using Ultrasonic Technique”

<b>0.14</b>	37464.43988	38089.2980	4.35E-10	4.26E-10	8.54508394	8.509711759
<b>0.16</b>	37768.00575	38518.9675	4.30E-10	4.21E-10	8.52703691	8.482223164
<b>0.18</b>	37921.35146	38846.9971	4.28E-10	4.17E-10	8.51763885	8.466819935
<b>0.2</b>	38253.68615	39143.9909	4.24E-10	4.13E-10	8.50199372	8.449825295
<b>293.15 K</b>						
<b>0</b>	35859.88065	35859.8806	4.56E-10	4.56E-10	8.614935174	8.614935174
<b>0.02</b>	36026.90496	36373.0103	4.54E-10	4.49E-10	8.599362151	8.583561519
<b>0.04</b>	36385.43375	36784.2696	4.49E-10	4.43E-10	8.584424075	8.567039759
<b>0.06</b>	36615.31026	36916.9837	4.45E-10	4.41E-10	8.567783547	8.558618996
<b>0.08</b>	36899.59376	37253.6729	4.41E-10	4.37E-10	8.54950624	8.544585658
<b>0.1</b>	37074.81042	37588.4958	4.39E-10	4.32E-10	8.53384297	8.52520293
<b>0.12</b>	37243.69102	37804.4135	4.37E-10	4.30E-10	8.52898502	8.513861231
<b>0.14</b>	37468.80312	38066.6058	4.34E-10	4.26E-10	8.51465798	8.502101572
<b>0.16</b>	37720.21325	38431.6120	4.30E-10	4.22E-10	8.50034624	8.484423488
<b>0.18</b>	37915.95709	38686.4364	4.28E-10	4.18E-10	8.48753565	8.472184138
<b>0.2</b>	38251.34793	38953.3364	4.23E-10	4.15E-10	8.46812599	8.462717375
<b>298.15 K</b>						
<b>0</b>	36420.62117	36420.6211	4.47E-10	4.47E-10	8.54161501	8.541615018
<b>0.02</b>	36746.94598	36827.1590	4.42E-10	4.41E-10	8.52620237	8.519108638
<b>0.04</b>	37108.63953	37271.4228	4.37E-10	4.35E-10	8.50371972	8.501385525
<b>0.06</b>	37489.91371	37515.2845	4.32E-10	4.32E-10	8.47754012	8.479274586
<b>0.08</b>	37992.6481	37874.7408	4.26E-10	4.27E-10	8.45496999	8.470269771
<b>0.1</b>	38253.16336	38124.6395	4.22E-10	4.24E-10	8.44469726	8.456603063
<b>0.12</b>	38558.60723	38324.3819	4.18E-10	4.21E-10	8.42509195	8.441477859
<b>0.14</b>	38947.30608	38689.2986	4.14E-10	4.17E-10	8.40568929	8.424674948
<b>0.16</b>	39221.73338	38996.9301	4.10E-10	4.13E-10	8.39936894	8.40954368
<b>0.18</b>	39601.34318	39287.5570	4.06E-10	4.10E-10	8.37887524	8.397568402
<b>0.2</b>	39834.19734	39527.5609	4.03E-10	4.07E-10	8.37041630	8.392360477