# Studies of Thermo-Chemical Interactions of Aqueous L-Proline with 2-Ethoxyethanol System at 308.15K and at Various Concentrations

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**Abstract:** The thermo-chemical parameters viz. density  $(\varrho)$ , viscosity  $(\eta)$ , and ultrasonic velocity (u) have been measured for aqueous *l*-proline with 2-ethoxyethanol system at 0.1 to 1 mole fractions and at 308.15K. The concentration increases of 2-ethoxyethanol the density, viscosity and ultrasonic velocity decreases; due to weak solute-solvent interactions. It results structure-breaking of the solvent. Thus it is confirmed from the above parameters that; there is a weak association between present systems showing hydrophobic nature.

Keywords: Acoustical impedance, adiabatic compressibility, relaxation time, Rao's constant, Wada's constant.

#### 1. Introduction

The correlation of physical parameters in aqueous amino acid and glycol ether system at various concentrations and at given temperature gives information about intermolecular interactions. The thermo physical parameters are very easy tool for understanding and correlation of result. These results predict direct correlation of physical parameters of liquid system. The study of ultrasonic velocity is found to be useful in measuring number of physicochemical parameters [1-4]. From a long time researcher interested in studies of solubility and stability of complex molecules like proteins but because of complex nature of molecules, low molecular weight compounds are preferred [5]; hence the physical properties of amino acids in aqueous solution have been studied to understand solute-solvent interaction and their role in the stability of proteins [6]. The random coil, unfolded, forms of denatured proteins these studies in the form of thermodynamic stability of protein [7-8]. To study volumetric and compressibility parameter of amino acids in aqueous salt system shows molecular interactions [9-22]. The amino acid like 1-proline shows solute solvent interactions [23]. The data of density of glycine, 1-alanine and 1-serine in aqueous glucose solutions discussed by Li, et al [24]. The data of the ultrasonic velocity of glycine, dl-alanine, diglycine and triglycine in aqueous solution of glucose discussed by Banipal et al [25]. To study the molecular interactions of ions and proteins are useful in the separation and purification processes and to understand the physiological systems [26-30]. In proteins the amino acids are building blocks compounds. Their studies provide important information about nature of larger biomolecules. The proteins as amino acids play an important role in metabolism and neurochemical mechanisms such as pain transmission, reflex action, hormones mechanism [31-32]. They have many applications in pharmaceutical industries and also used as food additives. To study the effect of temperature and concentration of salt on the thermodynamic properties of amino acids have been proved by researcher to useful in elucidating the various interactions [33-41]. The thermo physical parameter shows the molecular interactions of aqueous glycine. This data useful to understand the nature of biological molecules[42]. The electrolyte in aqueous solution has been studied under thermo dynamical property [43-44].

#### 2. Experimental

#### a) Source and purity of sample

All the chemicals are analytical reagent (AR) and spectroscopic reagent (SR) grades from Sigma-Aldrich, Merck, AVARA, Sd Fine and Alfa-Aesar. The purities of the above chemicals were checked by density determination.

#### b) Experimental Method

The liquid mixtures of different known compositions were prepared in stopper volumetric flasks. The density, viscosity and ultrasonic velocity values were measured as a function of composition of the liquid mixture of aqueous amino acid with glycol ether at various temperatures and concentrations. The density was determined using a bi-capillary pycnometer. The weight of the sample measured using electronic digital balance with an accuracy of ±0.1 mg (Model: Shimadzu AX-200). An Ubbelohde viscometer (20ml) was used for the viscosity measurement and efflux time determined with digital clock ±0.01s. An ultrasonic interferometer having the frequency of 3 MHz (Mittal Enterprises, New Delhi, Model: F-05) with an overall accuracy of  $\pm 0.1\%$  was used for velocity measurement. An electronically digital operating constant temperature water bath (RAAGA Industries) was used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desired temperature with an accuracy of  $\pm 0.1$  °C [45].

#### 3. Theory and Calculation

The present measured values of density ( $\rho$ ), ultrasonic velocity (u) and viscosity ( $\eta$ ). We were calculated the physical parameters viz. acoustical impedance (z), adiabatic compressibility ( $\beta$ ), relaxation time ( $\tau$ ), Rao's constant (R),Wada's constant (W), free volume (V<sub>f</sub>), molar volume(V<sub>m</sub>), intermolecular free length (L<sub>f</sub>), relaxation strength(r) by using following standard relation [42,45-49].

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1) z = \rho u
2) \beta = 1/u_2 \rho
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3) $\tau = 4/3 \eta \beta$ 

#### $(4)R = u_{1/3}v$

- 5) W =  $\beta_{1/7}$ v
- 6)  $V_f = M_{eff} u/K\eta (K=4.28 \times 10^9)$  is a temperature independent constant)(M<sub>eff</sub> –effective molecular wt. of soln. M<sub>eff</sub> = x1M1+x2M2+x3M3; where, x1, x2, x3, M1, M2, M3) are mole fractions and molar masses of the pure components 1, 2 & 3)

$$7) V_m = M_{eff} / \rho$$

8)  $L_f = K_j \beta_{1/2} (K_j = 6.0816 \times 104)$  (K<sub>j</sub> is Jacobson's constant which is temperature dependent constant but independent of the nature of the liquid.)

9)r =  $1 - (U/U_{\infty})^2$  where,  $U_{\infty} = 1.6 \text{ x} 10^5$ 

#### 4. Results and Discussion

The present research work is a system of aqueous 1-proline with 2-ethoxyethanol.The present systems correlated by physical parameters viz. density, viscosity and ultrasonic velocity. It is proved by experimental data. These physical properties correlated with various concentrations 0.1 to 1.0 and at 308.15 K. The present experimental data clearly reveals that as concentration increases of 2-ethoxyethanol; in which particle-particle frictional resistance leads intermolecular interaction. It shows increasing and decreasing trend of the measured parameters. Density is a parameter giving information about solute-solute, solutesolvent and solvent-solvent interactions [50]. The higher compressibility values (present work) predict that the medium is loosely packed where as the lower compressibility is an indication of maximum interaction. The intermolecular free length (Lf) is again a predominant factor in determining the existing interactions in liquid system. Analyzing the table (L<sub>f</sub>) reflects a similar trend as that of  $(\beta)$ . The aqueous amino acid in system there is hydrogen bonding between H-atom of water with O-atom of C=O group of amino acid, H-atom of water molecule and N-atom of -NH<sub>2</sub> group of amino acid, H-atom of -OH group of amino acid with O-atom of water molecule this condition only when aqueous amino acid in the system but when start addition of 2-ethoxyethanol in the system then concentration of aqueous amino acid decreases and concentration of 2-ethoxyethanol increases thus Hbonding interactions decreases it results interactions becomes weak. The temperature increases it results decrease interactions within the system; due to increase in thermal energy of the system which causes a volume expansion and density, viscosity and ultrasonic velocity decreases; hence an increase in intermolecular free length and compressibility. The regular increase in intermolecular free length is due to the loose packing of the molecules inside the shield; it may be brought by weakening of molecular interaction.

The molar sound velocity (R) indicates the cube root of sound velocity through one molar volume of solutions called as Rao's constant. The 'R' measure of interaction existing in the solution. Further the trend of molar adiabatic compressibility (W) called as Wada's constant which depends on the adiabatic compressibility of one molar volume solutions may be taken as a confirmation for existing interactions. The observed values of molar sound velocity and molar compressibility in the present system show trends

which indicating that the trends of interactions. The molar compressibility or molar sound velocity with increasing glycol ether indicates the loose packing of the medium and thereby decrease the interactions. The acoustic impedance that the specific interactions are of solute-solute and solutesolvent type. The decrease in acoustic velocity in the aqueous solution of amino acid may be attributed to the weak cohesion brought by the ionic hydration. The trends of density with molar concentration suggest a solute-solvent interaction exist between water and amino acid [42]. In other words the density may be interpreted to the structure breaking of the solvent due to H-bonding [51-52]. The decrease in density indicates the decrease in solute-solvent and solvent-solvent interactions which results structurebreaking of the solvent. It shows that; solvent-solvent interactions bring about a bonding, probably H-bonding between them. Thus, size of the resultant molecule increases and there will be decrease in density[53]. The viscosity is a physical property in understanding the structure as well as molecular interaction occurring in the aqueous system. The trends of physical parameter related to aqueous system attributed to structural changes [52]. The values of adiabatic compressibility  $(\beta)$  show trend with concentration which suggest the making and breaking of H-bonding[42]. The intermolecular free length depends upon the intermolecular attractive and repulsive forces. The values of density and viscosity of any system vary with increase or decrease in concentration of solutions[53]. Eyring and Kincaid[54] have proposed that (Lf) is a predominating factor in determining the variation of ultrasonic velocity in aqueous system. The values of intermolecular free length listed in the tables show increasing trend with concentration. The increase in intermolecular free length and decrease in acoustic value shows solute-solvent interaction. The trends in relaxation strength suggest that presence of solute-solute interactions. Thus H-bond forming or dissociating properties can be correlated with change in density and viscosity [53]. Hence it can be concluded that there is significant interaction of solute-solute or solute-solvent or solvent-solvent type due to which the structural arrangement is also affected. Thus it is clear from the above parameters that there is a weak association between present systems showing hydrophobic nature.

## Applications

To study of the molecular interactions of ions and proteins are useful in the separation and purification processes and to understand the physiological systems[26-30]. The proteins as amino acids play an important role in metabolism and neurochemical mechanisms such as pain transmission, reflex action, hormones mechanism[31-32]. The various solution properties in recent studies consisting of polar as well as non polar components find applications in industrial and technology processes[42]. They have many applications in pharmaceutical industries and also used as food additives. The variations of physical parameter related to aqueous system attributed to structural changes[55]. This research work proved that some of the novel molecules can stabilize the biochemical part of living beings[56-59].The measured and calculated thermodynamic parameters are useful to know the interactions like solute-solute or solute-solvent or solvent-solvent type.

### 5. Conclusion

The parameters are correlated with aqueous 1-proline and 2ethoxyethanol. The system containing aqueous amino acid and glycol ether has weak intermolecular H-bonding. The decrease in density, viscosity and ultrasonic velocity indicates the decrease in solute-solvent and solvent-solvent interactions; it results structure-breaking of the solvent. The acoustical parameters proved that H-bonding interactions are weak at higher concentration. The increase in adiabatic compressibility with present work suggests that; the medium become more and least compressible. The  $L_f$  is again a predominant factor in determining the existing interactions among the components of the mixture.

<b>x</b> <sub>1</sub>	x <sub>2</sub>	<b>X</b> <sub>3</sub>	X	ρ	η (×10 <sup>-3</sup> )	u	z (×10 <sup>6</sup> )	β (×10 <sup>-10</sup> )
				kgm <sup>-3</sup>	Nsm <sup>-2</sup>	ms <sup>-1</sup>	kgm <sup>-2</sup> s <sup>-1</sup>	$N^{-1} m^2$
0.9884	0.0116		0.0000	1024.2	0.8928	1564.3	1.6022	3.9900
0.9665	0.0113	0.0222	0.1056	1020.5	0.8116	1520.0	1.5512	4.2413
0.9412	0.0110	0.0478	0.2113	1007.1	0.7491	1491.5	1.5021	4.4636
0.9115	0.0107	0.0778	0.3068	996.0	0.6277	1457.1	1.4513	4.7289
0.8735	0.0103	0.1163	0.4110	982.3	0.5119	1431.1	1.4058	4.9707
0.8287	0.0097	0.1616	0.5168	971.1	0.4544	1385.0	1.3450	5.3683
0.7672	0.0900	0.2238	0.6115	955.4	0.3731	1365.7	1.3048	5.6118
0.6841	0.0080	0.3079	0.7130	938.1	0.2905	1343.4	1.2602	5.9066
0.5715	0.0067	0.4218	0.8044	929.0	0.2553	1326.2	1.2320	6.1202
0.3628	0.0043	0.6330	0.9057	925.6	0.2089	1305.0	1.2079	6.3439
		1.0000	1.0033	912.1	0.1827	1280.1	1.1676	6.6907

 Table 1: (Aqueous L-Proline and 2-Ethoxyethanol system at 308.15 K)

Where, mole fraction of water  $(x_1)$ , mole fraction of 1-proline  $(x_2)$ , mole fraction of 2-ethoxyethanol  $(x_3)$ , mole fraction of aqueous 1-proline and 2-ethoxyethanol system (x), density

( $\rho$ ), viscosity ( $\eta$ ), ultrasonic velocity (u), acoustical impedance (z), adiabatic compressibility ( $\beta$ ).

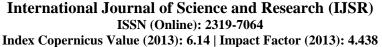
Table 1: (continued) ...

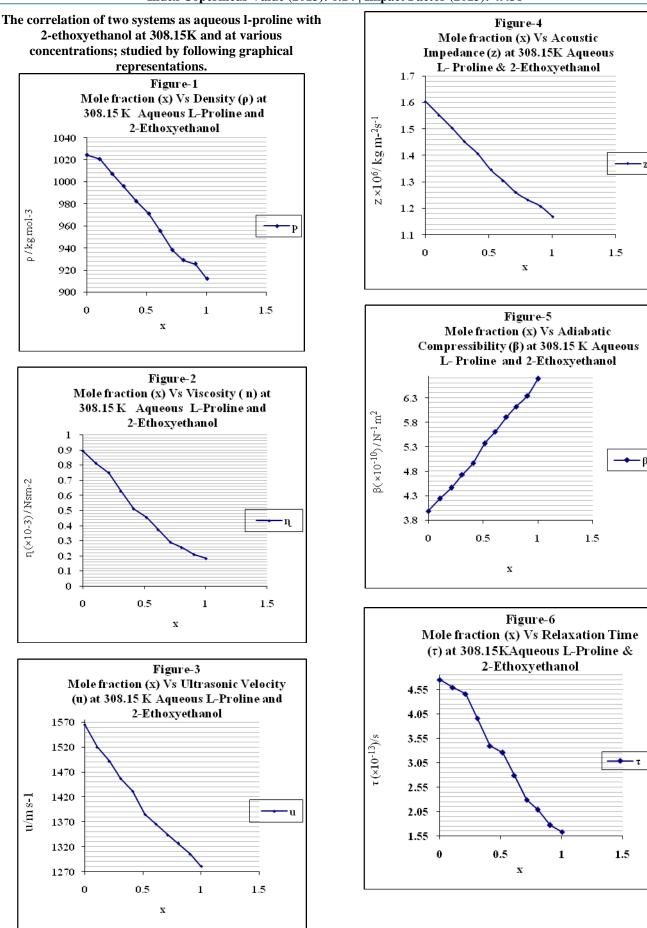
$\tau$ (×10 <sup>-13</sup> )	<b>R</b> (×10 <sup>3</sup> )	W	V <sub>f</sub>	Vm	L <sub>f</sub>	r	σ (x10 <sup>4</sup> )
s	ms <sup>-1</sup> mol <sup>-1</sup>	$m^3$	$m^3$	cm <sup>3</sup>	A		Nm <sup>-1</sup>
		mol <sup>-1</sup>	mol <sup>-1</sup>	mol <sup>-1</sup>			
4.7497	1.5454	6.0473	0.01272	0.1300	1.2148	0.999904413	3.9921
4.5897	2.5669	10.2297	0.03053	0.2188	1.2525	0.999909750	3.8099
4.4582	2.5507	10.3046	0.03347	0.2217	1.2849	0.999913103	3.6547
3.9578	2.5310	10.3900	0.04213	0.2241	1.3225	0.999917065	3.4901
3.3927	2.5158	10.4642	0.05569	0.2273	1.3559	0.999919998	3.3503
3.2525	2.4885	10.5799	0.06339	0.2299	1.4091	0.999925069	3.1534
2.7917	2.4769	10.6472	0.08343	0.2337	1.4407	0.999927143	3.0378
2.2878	2.4634	10.7254	0.11847	0.2380	1.4780	0.999929503	2.9100
2.0833	2.4528	10.7799	0.14105	0.2403	1.5045	0.999931297	2.8266
1.7670	2.4397	10.8353	0.18601	0.2412	1.5318	0.999933476	2.7490
1.6299	2.4240	10.9180	0.22094	0.2448	1.5731	0.999935990	2.6318

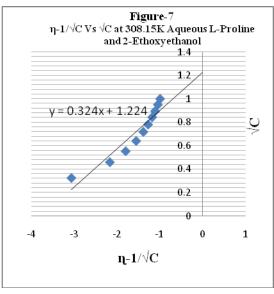
Relaxation time ( $\tau$ ), Rao's constant (R), Wada's constant (W), free volume (V<sub>f</sub>), molar volume (V<sub>m</sub>), intermolecular free length (L<sub>f</sub>), relaxation strength (r), surface tension ( $\sigma$ ).

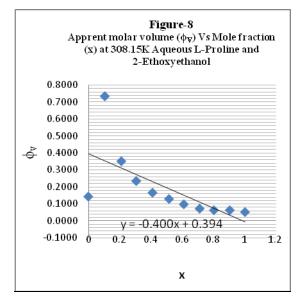
Table 1 (continued)								
φ <sub>v</sub>	$(\alpha/f_2)Cl$ (x10 <sup>-12</sup> )	$\pi_{\rm i}$ (x10 <sup>4</sup> )	ղ -1/√C	√C	VE			
		Nm <sup>-2</sup>						
0.1421	9.3661	8.5548	000000000	000000000	-19.10796551			
0.7341	9.0504	4.5160	-3.074789748	0.324961536	-20.97384507			
0.3505	8.7912	4.3415	-2.173826104	0.459673797	-23.07032655			
0.2342	7.8045	3.9912	-1.804262115	0.553895297	-25.56344889			
0.1650	6.6901	3.6035	-1.559038057 0.641092817		-28.72312469			
0.1283	6.4136	3.4248	-1.390405123	0.71888803	-32.60788962			
0.0967	5.5050	3.0914	-1.278320353	0.781984655	-37.45666435			
0.0710	4.5114	2.7171	-1.183938257	0.844393273	-43.99148348			
0.0618	4.1081	2.5470	-1.114687368	0.896883493	-53.59152629			
0.0617	3.4844	2.3169	-1.05055086	0.95168272	-66.8644694			
0.0507	3.2139	2.1664	-0.998171673	1.001648641				

Apparent molar volume ( $\phi_v$ ), classical absorption coefficient ( $\alpha/f2$ )Cl, internal pressure ( $\pi_i$ ), excess molar volume(V<sup>E</sup>).









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