



**INTERMOLECULAR INTERACTION STUDIES IN AQUEOUS AMINO ACID AND
GLYCOL ETHER SYSTEM AT 308.15K AND AT VARIOUS CONCENTRATIONS**

A. V. Kachare* and D. D. Patil

A.S.C.College, Chopda, Dist- Jalgaon (M.S.) India.

Corresponding Author: Prof. A. V. Kachare

A.S.C.College, Chopda, Dist- Jalgaon (M.S.) India.

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ABSTRACT

The physicochemical parameters as density, viscosity and ultrasonic velocity have been measured for aqueous amino acid and glycol ether at 0.1 to 1 mole fractions. The concentration increases of glycol ether the density, viscosity and ultrasonic velocity decreases as interactions becomes weak, it indicate decrease in solute-solvent and solvent- solvent interactions which results structure-breaking of the solvent. Thus it is clear 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 l-proline shows solute-solvent interactions^[23]. The data of density of glycine, l-alanine and l-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 ± 0.01 s. 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 $\pm 0.1^\circ\text{C}$ ^[45].

3. THEORY AND CALCULATION

The present measured values of density (ρ), ultrasonic velocity (u) and viscosity (η). We were calculated the physical parameters viz. acoustical impedance (z), adiabatic compressibility (β), relaxation time (τ), Rao's constant (R), Wada's constant (W), free volume (V_f), molar volume(V_m), intermolecular free length (L_f), relaxation strength(r) by using following standard relation^[42,45-49]. 1) $z = \rho u^2$ 2) $\beta = 1/u^2\rho$ 3) $\tau = 4/3 \eta \beta$ 4) $R = u^2/3V$ 5) $W = \beta V/7V$ 6) $V_f = M_{\text{eff}} u/K\eta$ ($K=4.28 \times 10^9$ is a temperature independent constant) (M_{eff} –effective molecular wt. of solution. $M_{\text{eff}} = x_1M_1+x_2M_2+x_3M_3$. Where x_1 , x_2 , x_3 , M_1 , M_2 , M_3) are mole fractions and molar masses of the pure components 1, 2 and 3.) 7) $V_m = M_{\text{eff}} / \rho$ 8) $L_f = K_j \beta^{1/2}$ ($K_j = 6.0816 \times 10^4$) (K_j 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, $U_\infty = 1.6 \times 10^5$

4. RESULTS AND DISCUSSION

The present research work is a system of aqueous glycine with 2-methoxyethanol. 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-methoxyethanol; 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, solute-solvent and solvent-solvent interactions^[50]. The higher compressibility values predict that the medium is loosely packed where as the lower compressibility is an indication of maximum interaction. The intermolecular free length (L_f) is again a predominant factor in determining the existing interactions among the components of the mixture. Analyzing the table (L_f) reflects a similar trend as that of (β). 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 -NH₂ 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-methoxyethanol in the system then concentration of aqueous amino acid

decreases and concentration of 2-methoxyethanol increases thus hydrogen bonding 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, which 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. It is also a 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 (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 solute-solvent type. The decrease in ultrasonic 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 structure-breaking of the solvent. It reveals 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 variations of physical parameter related to aqueous system attributed to structural changes^[52]. The values of adiabatic compressibility (β) 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 (L_f) 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. The system changes as a result of hydrogen bond formation or dissociation or hydrophobic (structure-breaking) or hydrophilic (structure-forming) nature of solute. Hence hydrogen 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.

Table 1
(Aqueous glycine and 2-methoxyethanol system at 308.15 K)

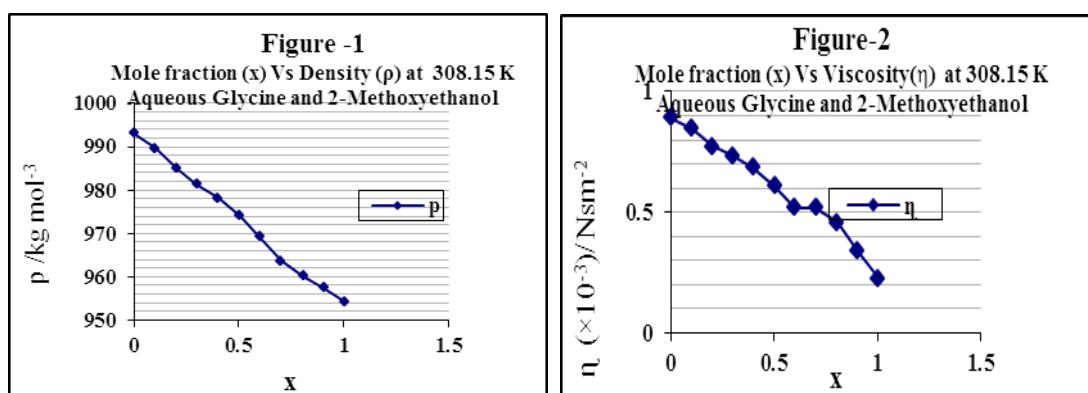
x_1	x_2	x_3	x	ρ	$\eta \times 10^{-3}$	u	$z \times 10^6$	$\beta \times 10^{-10}$
.....	kg m^{-3}	Nsm^{-2}	ms^{-1}	$\text{kg m}^{-2}\text{s}^{-1}$	N^{-1}m^2
0.9823	0.0177	0.0000	993.1	0.8905	1469.6	1.4595	4.6624
0.9571	0.0172	0.0257	0.1005	989.6	0.8479	1463.1	1.4479	4.7206
0.9276	0.0167	0.0557	0.2102	985.0	0.7731	1438.3	1.4167	4.9076
0.8935	0.0161	0.0904	0.3065	981.4	0.7355	1425.0	1.3985	5.0179
0.8505	0.0153	0.1341	0.4020	978.1	0.6848	1408.5	1.3777	5.1535
0.7963	0.0143	0.1894	0.5023	974.1	0.6084	1383.1	1.3473	5.3665
0.7291	0.0131	0.2578	0.6004	969.3	0.5182	1371.8	1.3297	5.4823
0.6379	0.0115	0.3507	0.7044	963.7	0.5760	1359.3	1.3100	5.6160
0.5173	0.0093	0.4734	0.8060	960.2	0.3377	1337.5	1.2843	5.8217
0.3225	0.0058	0.6717	0.9072	957.5	0.2245	1332.2	1.2756	5.8847
.....	1.0000	1.0008	954.3	0.1518	1315.4	1.2553	6.0562

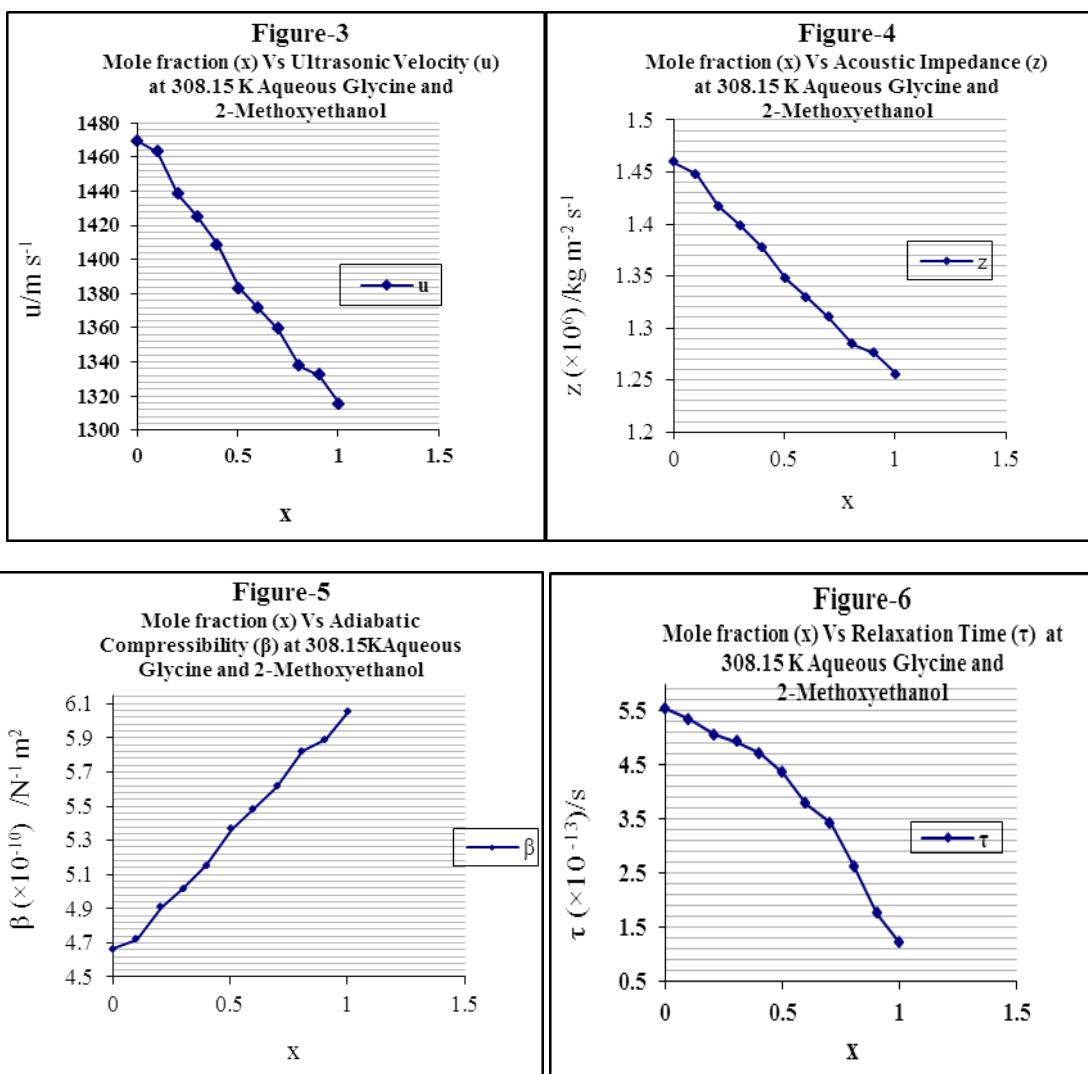
Where, mole fraction of water (x_1), mole fraction of glycine (x_2), mole fraction of 2-methoxyethanol (x_3), mole fraction of aqueous glycine and 2-methoxyethanol system (x), density (ρ), viscosity (η), ultrasonic velocity (u), acoustical impedance (z), adiabatic compressibility (β).

Table 1 (continued)...

$\tau \times 10^{-13}$	$R \times 10^3$	W	V_f	V_m	L_f	r
s	$\text{ms}^{-1}\text{mol}^{-1}$	$\text{m}^3\text{mol}^{-1}$	$\text{m}^3\text{mol}^{-1}$	$\text{cm}^3\text{mol}^{-1}$	A°	
5.5358	1.0581	4.3227	0.0067	0.0937	1.3132	0.999915636
5.3367	1.9204	7.8707	0.0178	0.1709	1.3213	0.999916380
5.0587	1.9095	7.9145	0.0199	0.1717	1.3473	0.999919191
4.9209	1.9036	7.9396	0.0211	0.1724	1.3623	0.999920679
4.7055	1.8962	7.9699	0.0231	0.1729	1.3806	0.999922505
4.3533	1.8847	8.0162	0.0269	0.1737	1.4088	0.999925275
3.7879	1.8796	8.0407	0.0338	0.1745	1.4240	0.999926491
3.4265	1.8739	8.0684	0.0402	0.1755	1.4412	0.999927824
2.6213	1.8638	8.1100	0.0619	0.1762	1.4674	0.999930121
1.7615	1.8613	8.1224	0.1135	0.1767	1.4753	0.999930674
1.2258	1.8535	8.1558	0.2004	0.1773	1.4966	0.999932411

Relaxation time (τ), Rao's constant (R), Wada's constant (W), free volume (V_f), molar volume (V_m), intermolecular free length (L_f), relaxation strength (r).





5. 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.

6. CONCLUSION

The parameters are correlated with aqueous amino acid and glycol ether. 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 which 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.

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