

Studies of Interactions of Aqueous Amino Acid and Glycol Ether System at 318.15 K and at Various Concentrations.

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ABSTRACT

The thermo physical parameters viz. density (ρ), viscosity (η), and ultrasonic velocity (u) have been measured for aqueous amino acid and glycol ether system at 0.1 to 1 mole fractions and at 318.15 K. Physical parameters viz. acoustical impedance (z), adiabatic compressibility (β), relaxation time (τ), intermolecular free length (L_f) have been obtained from experimental data which show intermolecular interaction. The measured and calculated thermodynamic parameters have been discussed in terms of solute-solute or solute-solvent or solvent-solvent interactions.

Keywords: - Acoustical impedance, Adiabatic compressibility, Relaxation time, Intermolecular free length.

INTRODUCTION

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 no. 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 of 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 bio-molecules. 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].

EXPERIMENTAL

2.1 Source and Purity of Sample:-

All the chemicals are analytical reagent (AR) and spectroscopic reagent (SR) grades from E-Merck, Germany, AVRA chemicals India. The purities of the above chemicals were checked by density determination at 318.15 K

2.2 Method:-

The liquid mixtures of different known compositions were prepared in stoppard volumetric flasks. The density, viscosity and ultrasonic velocity values were measured as a function of composition of the liquid mixture of amino acid with glycol ether at 318.15 K. The density was determined using a Bi-capillary pyknometer. 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 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 ± 0.01 K [45].

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), Intermolecular free length (L_f) by using following standard relation [42,45-49].

$$1) z = \rho u$$

$$2) \beta = 1/u^2 \rho$$

$$3) \tau = 4/3 \eta \beta$$

$$4) L_f = K_j \beta^{1/2} \quad (K_j = 6.0816 \times 10^4)$$

(K_j is Jacobson's constant which is temperature dependent constant but independent of the nature of the liquid.)

RESULTS AND DISCUSSION

The present work is a system of aqueous glycine with diethylene glycol and aqueous l-proline with diethylene glycol. To investigate the physical parameters viz. density (ρ), ultrasonic velocity (u) and viscosity (η), acoustical impedance (z), adiabatic compressibility (β), relaxation time (τ), intermolecular free length (L_f) gives information about interaction. It is proved by experimental data. These physical properties correlated with various concentrations 0.1 to 1.0 and at 318.15 K.

The present experimental data clearly reveals that as concentration increases the parameters viz. density, viscosity, ultrasonic velocity, acoustical impedance increases while adiabatic compressibility, relaxation time, intermolecular free length decreases. As concentration increases the no. of molecules in the medium increases making the medium to be denser which leads to increase of density, viscosity, ultrasonic velocity, acoustical impedance, Rao's constant, free volume increases and hence lesser intermolecular free length, adiabatic compressibility, relaxation time, Wada's constant. As the increase in the number of particles that increases the fractional resistance between the layers of medium and that leads to increase the coefficient of viscosity. The present system 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 solvent – solvent and ion - 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 gradual decrease in adiabatic compressibility in present work suggests that the medium become more and more less compressible. The intermolecular free length (L_f) is again a predominant factor in determining the existing interactions among the components of the mixture. Analyzing the respective table, (L_f) reflects a similar trend as that of (β).

The increasing trends in these parameters suggest the strengthening of interactions among the components. The interaction may be solute-solute or solute-solvent or solvent-solvent type. 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 amino acid are of increasing trend with glycol ether indicating that the magnitude of interactions are enhanced. The increasing trend of molar compressibility or molar sound velocity with increasing glycol ether indicates the availability of more number of components in a given region thus leads to a tight packing of the medium and thereby increase the interactions. The acoustic impedance that the specific interactions are of solute-solute and solute-solvent type. The increase in ultrasonic velocity in the aqueous solution of amino acid may be attributed to the cohesion brought by the ionic hydration. The increase in density with molar concentration suggests a solute-solvent interaction exist between water and amino acid [42]. In other words the increase in density may be interpreted to the structure making of the solvent due to H-bonding [51-52]. As concentration increases density increases due to the shrinkage in the volume. It results in increase in density is interpreted to the structure - maker of the solvent.

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 hydrogen 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 decreasing 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 decreasing trend with concentration. 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 strong association between present systems showing hydrophilic nature.

Table-1 (Aqueous Glycine and Diethylene glycol system at 318.15 K)

X_1	X_2	X_3	X	ρ	η ($\times 10^{-3}$)	u	z ($\times 10^6$)	β ($\times 10^{-10}$)	τ ($\times 10^{-13}$)	L_f
.....	kgm^{-3}	Nsm^{-2}	ms^{-1}	$\text{kg m}^{-2}\text{s}^{-1}$	$\text{N}^{-1} \text{m}^2$	s	A°
0.9809	0.01908	0.0000	987.0	0.8908	1511.1	1.4914	4.4371	5.2701	1.2810
0.9611	0.01870	0.02012	0.1327	991.2	0.8911	1515.0	1.5017	4.3956	5.2226	1.2750
0.9377	0.01824	0.04404	0.2241	996.0	0.8915	1518.0	1.5119	4.3571	5.1791	1.2695
0.9099	0.01770	0.07234	0.3100	999.1	0.8918	1522.0	1.5206	4.3208	5.1377	1.2642
0.8753	0.01702	0.1076	0.4013	1003.2	0.8921	1525.0	1.5299	4.2862	5.0983	1.2591
0.8303	0.01615	0.1535	0.5253	1006.0	0.8925	1528.1	1.5373	4.2569	5.0657	1.2548
0.7752	0.01484	0.2099	0.6102	1008.1	0.8929	1532.0	1.5444	4.2265	5.0318	1.2503
0.6915	0.01331	0.2950	0.7310	1011.1	0.8933	1534.2	1.5512	4.2019	5.0047	1.2466
0.5707	0.01105	0.4182	0.8221	1014.0	0.8936	1537.0	1.5585	4.1746	4.9739	1.2426
0.3792	0.00717	0.6136	0.9152	1017.0	0.8938	1540.1	1.5663	4.1455	4.9403	1.2382
.....	1.0000	1.0124	1019.0	0.8941	1544.0	1.5733	4.1165	4.9074	1.2339
...										

(Where, mole fraction of water (x_1), mole fraction of glycine (x_2), mole fraction of diethylene glycol (x_3), mole fraction of aqueous glycine and diethylene glycol system (x), density (ρ), viscosity (η), ultrasonic velocity (u), acoustical impedance (z), adiabatic compressibility (β), relaxation time (τ), intermolecular free length (L_f).

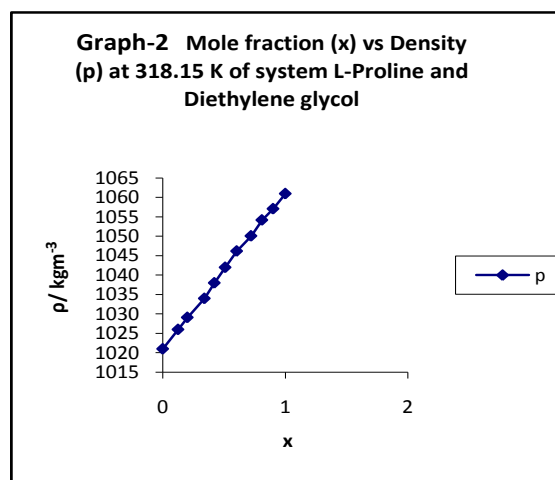
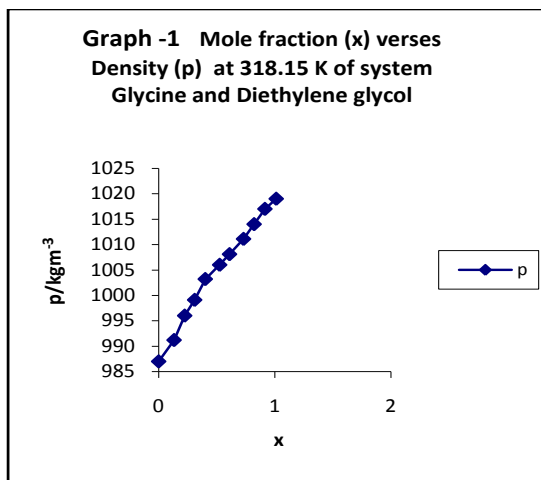
The table-1 data shows relative correlation as concentration increases. The parameter like density, viscosity, ultrasonic velocity, acoustical impedance increases while adiabatic compressibility, relaxation time, intermolecular free length decreases.

Table-2 (Aqueous L-Proline and Diethylene glycol system at 318 .15 K)

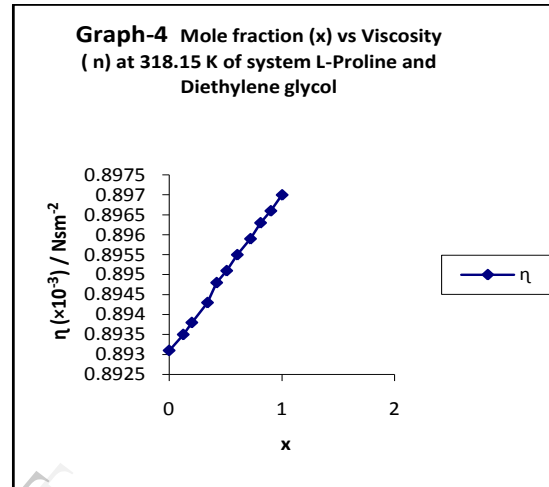
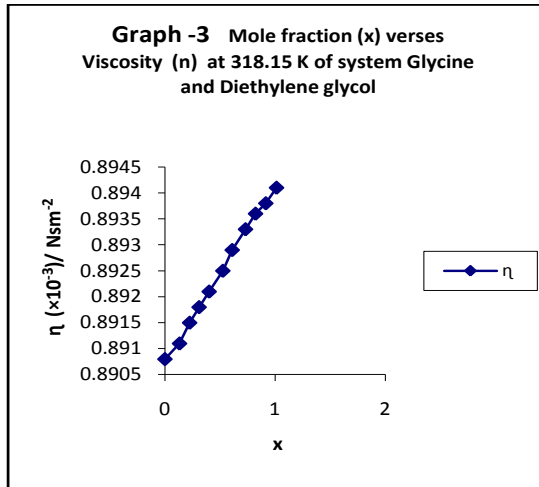
X_1	X_2	X_3	X	ρ	η ($\times 10^{-3}$)	u	z ($\times 10^6$)	β ($\times 10^{-10}$)	τ ($\times 10^{-13}$)	L_f
.....	kgm^{-3}	Nsm^{-2}	ms^{-1}	$\text{kg m}^{-2}\text{s}^{-1}$	$\text{N}^{-1} \text{m}^2$	s	A°
0.9800	0.01993	0.0000	1021.0	0.8931	1602.0	1.6356	3.8164	4.5446	1.1881
0.9602	0.01937	0.01970	0.1251	1026.0	0.8935	1605.0	1.6467	3.7836	4.5075	1.1830
0.9356	0.01903	0.04528	0.2010	1029.1	0.8938	1608.1	1.6549	3.7576	4.4781	1.1789
0.9073	0.01836	0.07435	0.3401	1034.0	0.8943	1611.0	1.6658	3.7264	4.4434	1.1740
0.8710	0.01771	0.1112	0.4214	1038.0	0.8948	1614.1	1.6754	3.6978	4.4117	1.1695
0.8243	0.01669	0.1590	0.5100	1042.0	0.8951	1618.0	1.6860	3.6659	4.3751	1.1644
0.7632	0.01552	0.2212	0.6041	1046.2	0.8955	1622.1	1.6970	3.6327	4.3374	1.1591
0.6829	0.01378	0.3032	0.7210	1050.1	0.8959	1626.0	1.7075	3.6019	4.3025	1.1542
0.5603	0.01133	0.4283	0.8102	1054.2	0.8963	1628.1	1.7163	3.5786	4.2767	1.1505
0.3749	0.007137	0.6179	0.9013	1057.1	0.8966	1633.0	1.7262	3.5474	4.2408	1.1454
.....	1.0000	1.0014	1061.0	0.8970	1635.0	1.7347	3.5257	4.2167	1.1419

(Where, mole fraction of water (x_1), mole fraction of l-proline (x_2), mole fraction of diethylene glycol (x_3), mole fraction of aqueous l-proline and diethylene glycol system (X), density (ρ), viscosity (η), and ultrasonic velocity (u), acoustical impedance (z), adiabatic compressibility (β), relaxation time (τ), intermolecular free length (L_f).

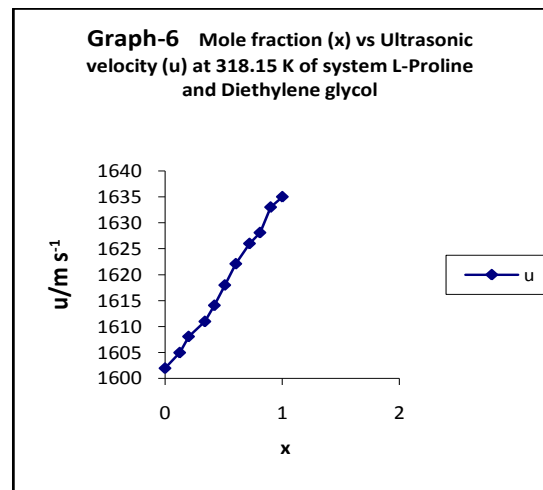
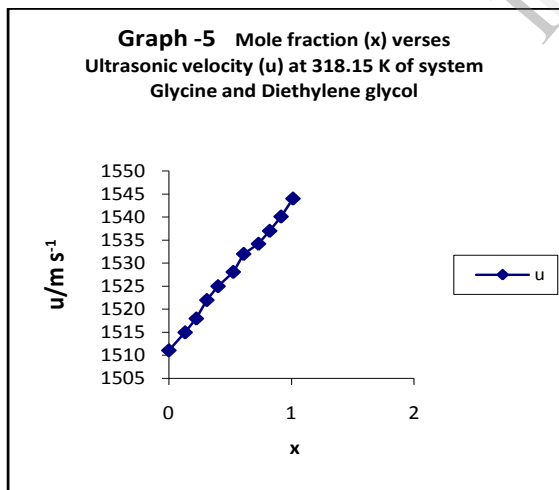
The table-2 data shows relative correlation as concentration increases. The parameter like density, viscosity, ultrasonic velocity, acoustical impedance increases while adiabatic compressibility, relaxation time, intermolecular free length decreases.



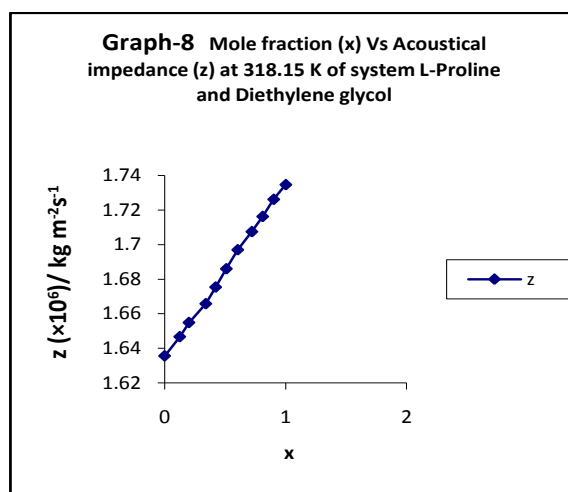
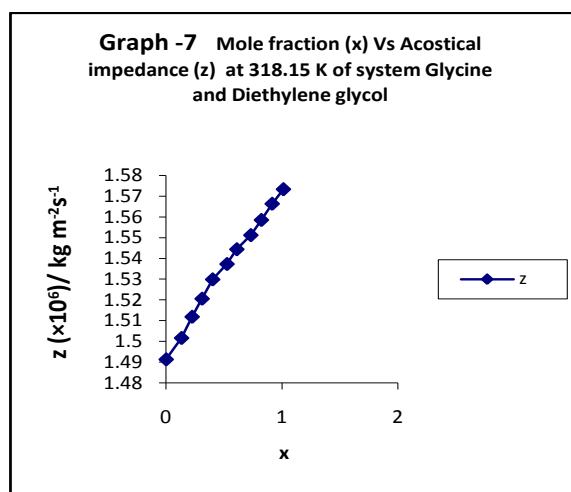
Density is a parameter giving information about solvent – solvent and ion - solvent interactions [50]. As concentration increases density increases due to the shrinkage in the volume. It results in increase in density is interpreted to the structure - maker of the solvent. The decrease in density indicates 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 hydrogen bonding between them. Thus, size of the resultant molecule increases and there will be decrease in density [53].



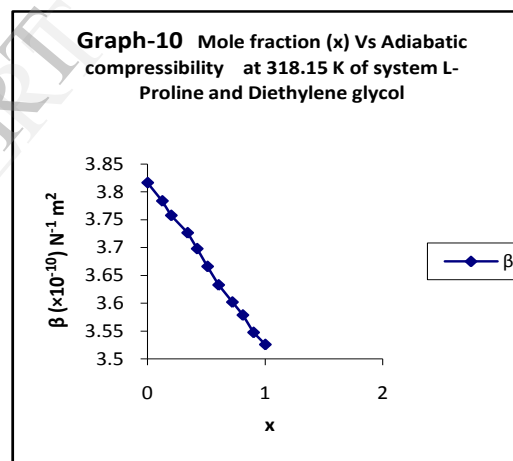
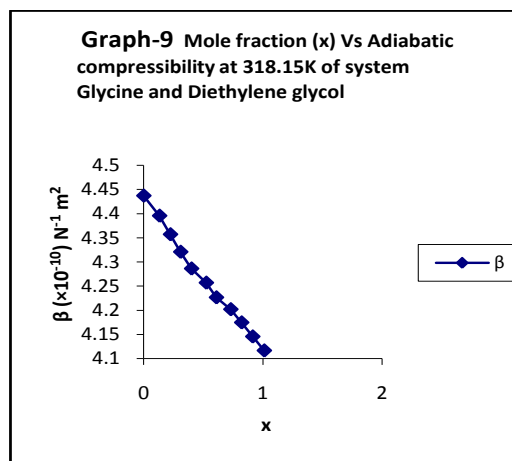
The viscosity is a physical property in understanding the structure as well as molecular interaction occurring in the aqueous system. The variations of physical parameter related to aqueous system attributed to structural changes [31]. The values of density and viscosity of any system vary with increase or decrease in concentration of solutions [53].



The nature of variation of ultrasonic velocity with mole fraction (x) at 318.15 K is evident from tables and figures 5,6 show the variation which indicates increasing trends in both the systems attributed to the cohesion brought by the ionic hydration it predict the interaction between aqueous glycine with diethylene glycol and aqueous l-proline with diethylene glycol.



The correlation of acoustic impedance (z) with mole fraction (x) at 318.15 K is evident from tables and figures 7, 8 show the variation which indicates increasing trends in both the systems. Hence it can be concluded that there is significant interaction between solute and solvent molecules due to which the structural arrangement is also affected. Thus it is clear from the above parameters that there is a strong association between water and amino acid molecules showing hydrophilic nature. The acoustic impedance that the specific interactions are of solute-solute and solute-solvent type.



The variation of adiabatic compressibility (β) with mole fraction (x) at 318.15 K is evident from data show the variation which indicating decreasing trends in both the systems. It suggests that making and breaking of H-bonding. The higher compressibility values predict that the medium is loosely packed whereas the lower compressibility is an indication of maximum interaction. The gradual decrease in adiabatic compressibility in present work suggests that the medium become more and more less compressible. The intermolecular free length (L_f) is again a predominant factor in determining the existing interactions among the components of the mixture. Analyzing the respective table, (L_f) reflects a similar trend as that of (β). Increasing trend in these parameters suggest the strengthening of interaction among the components. The interaction may be solute-solute or solute-solvent or solvent-solvent type. 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.

As concentration increases the number of molecules in the medium increases making the medium to be denser. It leads to increase of density, viscosity, ultrasonic velocity, acoustical impedance, Rao's constant, free volume and hence lesser intermolecular free length, adiabatic

compressibility, relaxation time, Wada's constant. The present system in which particle-particle frictional resistance leads to intermolecular interaction shows increasing and decreasing trend of the measured parameters. The interaction may be solute-solute or solute-solvent or solvent-solvent type. Variations of physical parameter related to aqueous system attributed to structural changes [55].

APPLICATION

The various solution properties in recent studies consisting of polar as well as non polar components find applications in industrial and technology processes [42]. 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.

CONCLUSION

The experimental data clearly reveals that the conclusion of system-1 aqueous glycine and diethylene glycol and system-2 aqueous l-proline and diethylene glycol in which as concentration increases the parameter like density, viscosity, ultrasonic velocity, acoustical impedance, Rao's constant, free volume, increases while adiabatic compressibility, relaxation time, Wada's constant, intermolecular free length decreases. These parameters are related with intermolecular correlation of aqueous amino acid and glycol ether. The system containing aqueous amino acid and glycol ether has strong intermolecular H-bonding. The acoustical parameters proved that H-bonding interaction is very strong at higher concentration. The gradual decreases in adiabatic compressibility with present work suggest that the medium become more and less compressible. The intermolecular free length (L_f) is again a predominant factor in determining the existing interactions among the components of the mixture. Analyzing the respective table, (L_f) reflects a similar trend as that of (β). Increasing trend in these parameters suggest the strengthening of interactions among the components. Thus molecular interactions are confirmed. The interactions may be solute-solute or solute-solvent or solvent-solvent type. As the increase in the number of particles that increases the fractional resistance between the layers of medium leads to increase the coefficient of viscosity. The present system in which particle-particle frictional resistance leads to intermolecular interaction.

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