

Investigation of physical parameters for aqueous amino acid and glycol ether system at 303.15 K and at various concentration

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Abstract

Density (ρ), viscosity (η), and ultrasonic velocity (u) have been measured for aqueous glycine and glycol ether at 0.1 to 1 concentrations and at 303.15 K temperatures. Physical parameters as 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) have been obtained from experimental data it shows intermolecular interaction of the present system. The measured and calculated thermodynamic parameters have been discussed in terms of interaction may be solute-solute or solute-solvent or solvent-solvent type.

Key words: acoustical impedance, adiabatic compressibility, relaxation time, Rao's constant, Wada's constant.

Introduction

The recent data about viscosity, density, ultrasonic velocity and other physical parameter to study interaction within the system, acoustic parameter and transport properties of aqueous amino acids electrolytes¹ are very helpful to obtain data about various types of interactions in solutions. In recent studies of solution properties of liquid system consisting of polar as well as non polar components find

applications in industrial and technology processes.² The investigation of physical parameters in aqueous amino acid and glycol ethers system to studies these parameter in correlation with various concentration and temperature. It shows information about intermolecular interaction. In amino acid water-protein system interaction give easy guide line about their correlation³. The physical parameter to study aqueous amino acid and organic solvent system it gives essential data about protein

unfolding⁴⁻⁶ and the hydrophobic interactions of non-polar side chains⁷. The aqueous amino acid behave as zwitterions⁸⁻¹² thus due to physiological conditions, the two functional groups of amino acid having both positive charge (amino group NH_3^+) and negative charge (Carboxyl group, COO^-)¹³. The intermolecular interaction with proteins have resemblances with those of electrolytes¹⁴. The interactions occurring between aqueous amino acid and other components are shown by their thermodynamic parameters^{2,15,16-18}. The aqueous amino acid system in which solute-solvent interactions verify by related thermo physical properties and that interaction decide the fate of that system, such interaction are responsible for physiological processes in a living cell¹⁹. Volumetric properties²⁰ and thermodynamic properties²¹ such as acoustical impedance, adiabatic compressibility, relaxation time, Rao's constant, Wada's constant, free volume, molar volume, intermolecular free length, apparent molar volume, molar hydration no., apparent molar compressibility, free energy, entropy and enthalpy of aqueous amino acid are plays important role to investigate the interaction between aqueous amino acid and related aqueous systems. Such research proved that some of the novel molecules can stabilize the biochemical part of living beings. The results of such molecules with their structure and functions of proteins in terms of structure making or breaking characteristics have been observed by various researchers^{13, 22-24}.

Experimental

All the chemicals required in the present research work are analytical reagent

(AR) and spectroscopic reagent (SR) grades of minimum assay of 99% to be obtained from E-Merck, Germany and Sd Fine, AVRA chemicals India. The liquid mixtures of different known compositions are to be prepared in stopper measuring flasks. The density, viscosity and ultrasonic velocity will be measured as a function of composition of the liquid mixture of amino acid with glycol ether at 303.15 K. The density will be determined using a Bi-capillary pycnometer. The weight of the sample will be measure using electronic digital balance with an accuracy of ± 0.1 mg (Model: Shimadzu AX-200). An Ubbelohde viscometer (20ml) is to be use for the viscosity measurement and efflux time is to be determined using a digital clock to within ± 0.01 s. An ultrasonic interferometer having the frequency of 3 MHz (Mittal Enterprises, New Delhi, Model: F-05) with an overall accuracy of $\pm 0.1\%$ is to be use for velocity measurement. An electronically digital operating constant temperature bath (RAAGA Industries) is to be use 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.²⁵

Theory and calculation :

From the measured values of density (ρ), ultrasonic velocity (u) and viscosity (η) we can calculate the physical parameter like 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) calculated by using following standard relation.^{2,26-28}

$$Z = \rho \cdot u \quad (1)$$

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

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

$$R = u^{1/3} v \quad (4)$$

$$W = \beta^{1/7} v \quad (5)$$

$$V_f = M_{\text{eff}} u / K \eta \quad (K=4.28 \times 10^9 \text{ is a temperature independent constant}) \quad (6)$$

(M_{eff} —effective molecular wt.of soln.

$M_{\text{eff}} = x_1 M_1 + x_2 M_2 + x_3 M_3$. 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.)

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

$$L_f = K_j \beta^{1/2} \quad (K_j = 6.0816 \times 10^4) \quad (8)$$

(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 properties like density (ρ), ultrasonic velocity (u) and viscosity (η), 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) it gives information about interactions between aqueous amino acids and glycol ether. It proved by experimental data from table no.01 to 02 and graphical representation from 01 to 06. These physical properties correlated with various concentrations 0.1 to 1.0 and at 303.15 K.

The experimental data clearly reveals that as concentration increases the parameter like density, viscosity, ultrasonic velocity, acoustical impedance, Rao's constant, free volume, increases while apparent molar volume, adiabatic compressibility, relaxation time, Wada's constant, molar volume, intermolecular free length decreases. 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 increases and hence lesser intermolecular free length, apparent molar volume, adiabatic compressibility, relaxation time, Wada's constant, molar volume. 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 it leads intermolecular interaction it shows increasing and decreasing trend of the measured parameters. The higher compressibility values it predict that the medium is loosely packed whereas the lower compressibility is an indication of maximum interaction. 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 interaction 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 interaction 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 suggest a solute-solvent interaction exist between aqueous amino acid.² In other words the increase in density may be interpreted to the structure

maker of the solvent due to H-bonding.²⁹⁻³⁰ 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 adiabatic compressibility (β) show decreasing trend with concentration which suggest the making and breaking of H-bonding.² The intermolecular free length depends upon the intermolecular attractive and repulsive forces. Eyring and Kincaid³² 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. Hence it can be concluded that there is significant interaction may be 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 system showing hydrophilic nature.

Table 1. (Aqueous Glycine and Diethylene glycol system at 303.15 K)

| X_1 | X_2 | X_3 | X | ρ | $\eta \times 10^{-3}$ | u | $z \times 10^6$ | $\beta \times 10^{-10}$ | $\tau \times 10^{-13}$ |
|--------|---------|---------|--------|-------------------|-----------------------|------------------|------------------------------------|--------------------------------|------------------------|
| | | | | kgm ⁻³ | Nsm ⁻² | ms ⁻¹ | kg m ⁻² s ⁻¹ | N ⁻¹ m ² | s |
| | | | 0.0000 | 998.0 | 0.8917 | 1503.0 | 1.4999 | 4.4355 | 5.2735 |
| 0.9611 | 0.01870 | 0.02012 | 0.1327 | 1002.1 | 0.8920 | 1506.1 | 1.5092 | 4.3998 | 5.2328 |
| 0.9377 | 0.01824 | 0.04404 | 0.2241 | 1005.0 | 0.8924 | 1510.0 | 1.5175 | 4.3639 | 5.1924 |
| 0.9099 | 0.01770 | 0.07234 | 0.3100 | 1009.2 | 0.8926 | 1513.2 | 1.5271 | 4.3274 | 5.1501 |
| 0.8753 | 0.01702 | 0.1076 | 0.4013 | 1013.1 | 0.8930 | 1517.1 | 1.5369 | 4.2886 | 5.1062 |
| 0.8303 | 0.01615 | 0.1535 | 0.5253 | 1017.2 | 0.8933 | 1520.0 | 1.5461 | 4.2550 | 5.0679 |
| 0.7752 | 0.01484 | 0.2099 | 0.6102 | 1020.1 | 0.8937 | 1524.1 | 1.5547 | 4.2201 | 5.0286 |
| 0.6915 | 0.01331 | 0.2950 | 0.7310 | 1024.0 | 0.8941 | 1527.0 | 1.5636 | 4.1881 | 4.9927 |
| 0.5707 | 0.01105 | 0.4182 | 0.8221 | 1027.0 | 0.8943 | 1532.0 | 1.5733 | 4.1486 | 4.9467 |
| 0.3792 | 0.00717 | 0.6136 | 0.9152 | 1031.1 | 0.8946 | 1536.1 | 1.5838 | 4.1101 | 4.9025 |
| | | 1.0000 | 1.0124 | 1034.2 | 0.8949 | 1539.0 | 1.5916 | 4.0824 | 4.8711 |

(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), and ultrasonic velocity (u), acoustical impedance (Z), adiabatic compressibility (β), relaxation time (τ))

| X_1 | X_2 | X_3 | X | $R (\times 10^3)$ $\text{ms}^{-1} \text{mol}^{-1}$ | W $\text{m}^3 \text{mol}^{-1}$ | V_f $\text{m}^3 \text{mol}^{-1}$ | V_m $\text{cm}^3 \text{mol}^{-1}$ | L_f \AA |
|--------|---------|---------|--------|---|-------------------------------------|---------------------------------------|--|-----------------------|
| | | | 0.0000 | 2.2816 | 9.1857 | 0.4280 | 0.1995 | 1.2808 |
| 0.9611 | 0.01870 | 0.02012 | 0.1327 | 2.2832 | 9.1751 | 0.4283 | 0.1987 | 1.2756 |
| 0.9377 | 0.01824 | 0.04404 | 0.2241 | 2.2852 | 9.1644 | 0.4286 | 0.1981 | 1.2704 |
| 0.9099 | 0.01770 | 0.07234 | 0.3100 | 2.2868 | 9.1534 | 0.4288 | 0.1973 | 1.2651 |
| 0.8753 | 0.01702 | 0.1076 | 0.4013 | 2.2887 | 9.1416 | 0.4292 | 0.1966 | 1.2594 |
| 0.8303 | 0.01615 | 0.1535 | 0.5253 | 2.2902 | 9.1314 | 0.4294 | 0.1958 | 1.2544 |
| 0.7752 | 0.01484 | 0.2099 | 0.6102 | 2.2923 | 9.1206 | 0.4297 | 0.1952 | 1.2493 |
| 0.6915 | 0.01331 | 0.2950 | 0.7310 | 2.2937 | 9.1107 | 0.4299 | 0.1945 | 1.2445 |
| 0.5707 | 0.01105 | 0.4182 | 0.8221 | 2.2962 | 9.0984 | 0.4303 | 0.1939 | 1.2387 |
| 0.3792 | 0.00717 | 0.6136 | 0.9152 | 2.2983 | 9.0863 | 0.4307 | 0.1931 | 1.2329 |
| | | 1.0000 | 1.0124 | 2.2997 | 9.0775 | 0.4309 | 0.1926 | 1.2287 |

(Rao's constant (R), Wada's constant (W), free volume (V_f), molar volume (V_m), intermolecular free length (L_f).)

The table-1 data shows relative correlation 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, molar volume, intermolecular free length decreases.

Table 2. (Aqueous L-Proline and Diethylene glycol system at 303 .15 K)

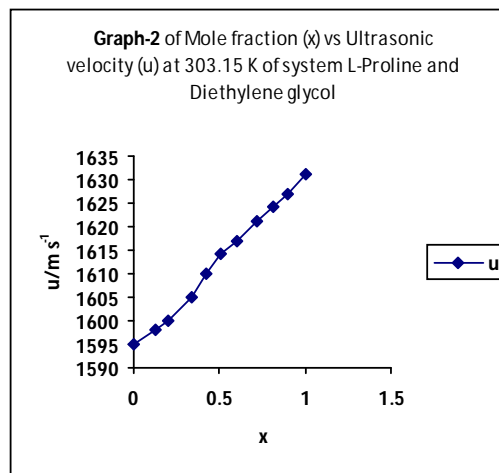
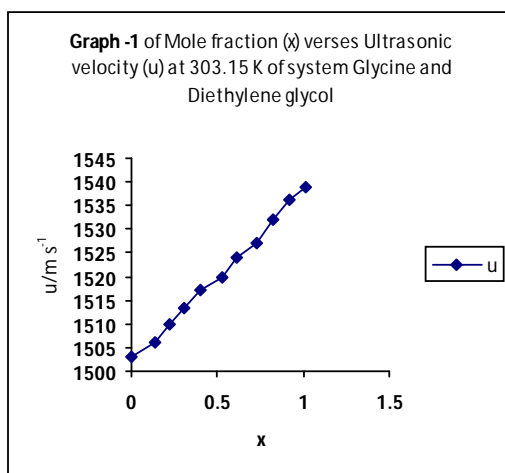
| X_1 | X_2 | X_3 | X | ρ kgm^{-3} | $\eta \times 10^{-3}$ Nsm^{-2} | u ms^{-1} | $z \times 10^6$ $\text{kg m}^{-2} \text{s}^{-1}$ | $\beta \times 10^{-10}$ $\text{N}^{-1} \text{m}^2$ | $\tau \times 10^{-13}$ s |
|--------|----------|---------|--------|-----------------------------|--|-------------------------|---|---|--------------------------------------|
| 0.9800 | 0.01993 | | 0.0000 | 1032.0 | 0.8944 | 1595.0 | 1.6460 | 3.8088 | 4.5421 |
| 0.9602 | 0.01937 | 0.01970 | 0.1251 | 1037.0 | 0.8947 | 1598.0 | 1.6571 | 3.7763 | 4.5048 |
| 0.9356 | 0.01903 | 0.04528 | 0.2010 | 1040.1 | 0.8950 | 1600.1 | 1.6642 | 3.7551 | 4.4810 |
| 0.9073 | 0.01836 | 0.07435 | 0.3401 | 1043.1 | 0.8954 | 1605.0 | 1.6741 | 3.7215 | 4.4429 |
| 0.8710 | 0.01771 | 0.1112 | 0.4214 | 1047.2 | 0.8958 | 1610.0 | 1.6859 | 3.6846 | 4.4008 |
| 0.8243 | 0.01669 | 0.1590 | 0.5100 | 1050.0 | 0.8961 | 1614.1 | 1.6948 | 3.6555 | 4.3675 |
| 0.7632 | 0.01552 | 0.2212 | 0.6041 | 1054.0 | 0.8965 | 1617.0 | 1.7043 | 3.6286 | 4.3373 |
| 0.6829 | 0.01378 | 0.3032 | 0.7210 | 1057.1 | 0.8968 | 1621.2 | 1.7137 | 3.5992 | 4.3036 |
| 0.5603 | 0.01133 | 0.4283 | 0.8102 | 1061.0 | 0.8972 | 1624.1 | 1.7231 | 3.5732 | 4.2745 |
| 0.3749 | 0.007137 | 0.6179 | 0.9013 | 1065.1 | 0.8976 | 1627.0 | 1.7329 | 3.5467 | 4.2446 |
| | | 1.0000 | 1.0014 | 1070.0 | 0.8979 | 1631.0 | 1.7451 | 3.5132 | 4.2060 |

(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))

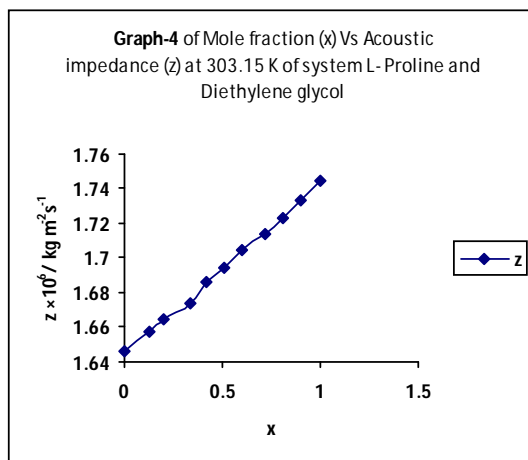
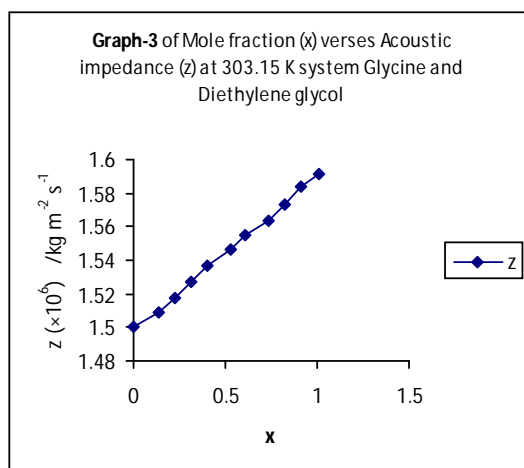
| X_1 | X_2 | X_3 | X | $R (\times 10^3)$ $\text{ms}^{-1} \text{mol}^{-1}$ | W $\text{m}^3 \text{mol}^{-1}$ | V_f $\text{m}^3 \text{mol}^{-1}$ | V_m $\text{cm}^3 \text{mol}^{-1}$ | L_f \AA° |
|--------|----------|---------|--------|---|-----------------------------------|---------------------------------------|--|-----------------------------|
| 0.9800 | 0.01993 | | 0.0000 | 2.7953 | 10.7956 | 0.4636 | 0.2318 | 1.1868 |
| 0.9602 | 0.01937 | 0.01970 | 0.1251 | 2.7971 | 10.7824 | 0.4639 | 0.2307 | 1.1818 |
| 0.9356 | 0.01903 | 0.04528 | 0.2010 | 2.7983 | 10.7738 | 0.4640 | 0.2300 | 1.1784 |
| 0.9073 | 0.01836 | 0.07435 | 0.3401 | 2.8011 | 10.7599 | 0.4644 | 0.2293 | 1.1732 |
| 0.8710 | 0.01771 | 0.1112 | 0.4214 | 2.8041 | 10.7446 | 0.4648 | 0.2284 | 1.1673 |
| 0.8243 | 0.01669 | 0.1590 | 0.5100 | 2.8064 | 10.7325 | 0.4652 | 0.2278 | 1.1676 |
| 0.7632 | 0.01552 | 0.2212 | 0.6041 | 2.8081 | 10.7211 | 0.4654 | 0.2269 | 1.1584 |
| 0.6829 | 0.01378 | 0.3032 | 0.7210 | 2.8105 | 10.7087 | 0.4657 | 0.2263 | 1.1537 |
| 0.5603 | 0.01133 | 0.4283 | 0.8102 | 2.8122 | 10.6976 | 0.4659 | 0.2254 | 1.1495 |
| 0.3749 | 0.007137 | 0.6179 | 0.9013 | 2.8139 | 10.6862 | 0.4661 | 0.2246 | 1.1453 |
| | | 1.0000 | 1.0014 | 2.8162 | 10.6718 | 0.4665 | 0.2235 | 1.13939 |

(Rao's constant (R), Wada's constant (W), free volume (V_f), molar volume (V_m), intermolecular free length (L_f)).

The table-2 data shows that 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, molar volume, intermolecular free length decreases.

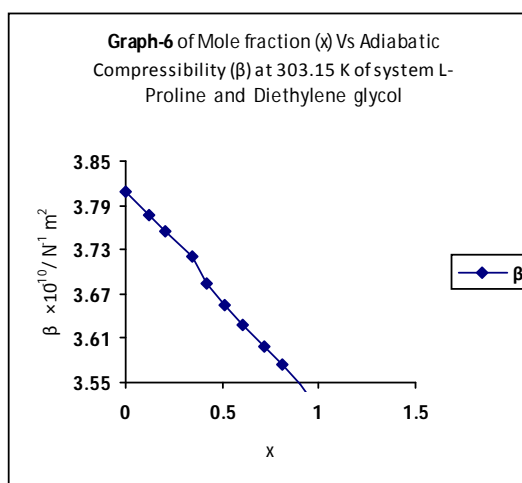
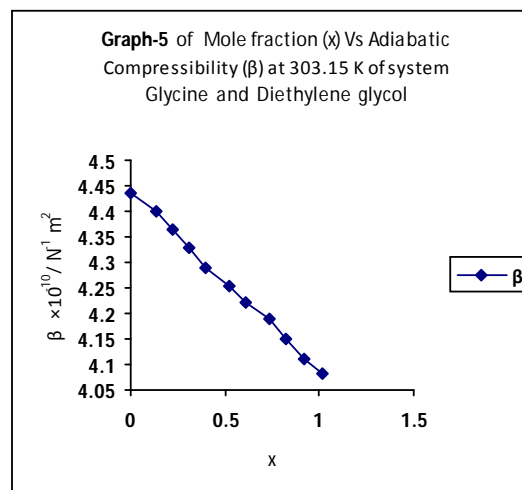


The nature of variation of ultrasonic velocity (u) with mole fraction (x) at 303.15 K is evident from table 1,2 and graphical representation of graph 1,2 shows the variation indicates increasing trends in both the systems attributed to the cohesion brought by the ionic hydration it predict the interaction between aqueous glycine with diethylene glycol and aqueous l-proline with diethylene glycol.



The correlation of acoustic impedance (z) with mole fraction (x) at 303.15 K is evident from table 1,2 and graphical representation of graph

3,4 shows the variation indicates increasing trends in both the systems it predict the interaction in present system. 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 variation of adiabatic compressibility (β) with mole fraction (x) at 303.15 K is evident from table 1,2 and graphical representation of graph 5,6 shows the variation indicates decreasing trends in both the systems it suggest the making and breaking of H-bonding. The higher compressibility values it predict that the medium is loosely packed whereas the lower compressibility is an indication of maximum interaction. The gradual decreases in adiabatic compressibility with present work suggest 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.

Conclusion

The experimental conclusion of two 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 apparent molar volume, adiabatic compressibility, relaxation time, Wada's constant, molar volume, intermolecular free length decreases. These parameter are related with intermolecular correlation of aqueous amino acid and glycol ether. The

system containing aq.amino acid and glycol ether having 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 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. It concludes that molecular interactions are confirmed. The interaction may be solute-solute or solute-solvent or solvent-solvent type.

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