Research Paper

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Excess parameters of serine in aqueous sodium chloride

PHYSICS

KEYWORDS : Serine, sodium chloride, ultrasonic velocity, excess parameters, intermolecular attraction.

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ABSTRACT

The density, viscosity and speed of sound have been measured for the systems (1M NaCl +1M serine) at different volume fraction and at different temperature 303.15,308.15 &313.15K at frequency of 2 MHz.The excess acoustic parameters such as excess ultrasonic velocity, excess adiabatic compressibility, excess acoustic impedance, excess intermolecular free length and excess relative association have been calculated for the solution. The results are interpreted in terms of molecular interactions.

Introduction

Excess thermodynamic parameters have been found to be highly useful in elucidating solute-solvent interactions in aqueous solutions and binary mixtures. Thermodynamic excess functions are found to be very sensitive towards mutual interactions between component molecules of the liquid mixture. The sign and the extent of deviation of these functions from ideality depend on the strength of interactions between unlike molecules[1-3] Excess parameter play a vital role in assessing the compactness due to molecular arrangement and the extent of molecular interactions in the liquid mixtures through charge transfer, dipole – induced dipole and dipole-dipole interactions[4], interstitial accommodation and orientation ordering, leading to more compact structure making. Derived parameters from ultrasonic velocity measurement and corresponding excess functions provide qualitative information regarding the nature and strength of interactions in liquid mixtures[6-8].

In (NaCl + serine), it may be presumed that the interactions may be taking

place as,Ionic group of serine i.e. zwitter ionic centers of serine with Na^+,Cl^- and Mg^{++} ions,NH_2 group (hydrophilic) of serine through H-bonding,CH_3-CH-OH group (hydrophobic) of serine, non polar molecules,COO^- and NH_3 or NH_2 of serine [9] and ions of solvents.These interactions compressively introduce the cohesion into solution under

investigation.

Exprimental Details

Ultrasonic velocity was measured with a single crystal interferometer (F-81, Mittal Enterprises, New Delhi) at 2MHz The interferometer was calibrated against the ultrasonic velocity of water used at T = 303.15K. The present experimental value is 1508.80 ms^{-1} which is in good agreement with literature value[10-11] 1509.55 ms^{-1}.

Accuracy in the velocity measurement was 1.0 ms^{-1}. The density measurements were performed with recalibrated specific gravity bottle with an accuracy of $2x10^{-2}$ kg m^{-3}. An average of triple measurements was taken into account. Sufficient care was taken to avoid any air bubble entrapment. Viscosity was measured with recalibrated Ostwald type viscometer. The flow of time was measured with a digital stop watch capable of registering time accurate to 0.1 s. An average of three or four sets of flow of times for each solution was taken for the purpose of calculation of viscosity. The accuracy of the viscosity measurements was 0.5 %. Accuracy in experimental temperature was maintained at 0.1K by means of thermostatic water bath.

Theory

Ultrasonic velocity (u), density (ρ) and viscosity (η) of the solutions were calculated using basic relations as follows:

Ultrasonic velocity $u = n \times \lambda$ ---------- (1)

Density $\rho = m / v$ ----------(2)

Viscosity $\eta_2 = [t_2 / t_1].[\rho_2 / \rho_1] \times \eta_1$ --- (3)

Where, n & λ are frequency and wavelength; V is the volume of the solution; η_1 & η_2 are the viscosities of the water and solutions; t_1, t_2 are time of flow of water and solution and ρ_1, ρ_2 are the densities of water and solution.

Using these data, the thermodynamic parameters such as the adiabatic compressibility (β_a), intermolecular free length (L_f), acoustic impedance (z) and relative association (R_A) were investigated for six different vol. fractions of 1M N_aCl at frequency 2 MH_z and at constant temperature 303.15,308.15 & 313.15K. From the experimental data of density (ρ), viscosity (η) and ultrasonic velocity (u),the excess parameters such as u^E, βa^E, z^E, Lf^E, and RAE have been calculated using the following equations [12-15] .

Excess ultrasonic velocity $u^E = u_{mix} - [(1- x) u_+ + x u_2]$ ---------- (4)

Excess adiabatic compressibility $\beta_a^E = \beta_{amix} - [(1- x) \beta_{a1} + x \beta_{a2}]$ ---------- (5)

Excess acoustic impedance $z^E = z_{mix} - [(1- x) z_1 + x z_2]$ ---------- (6)

Excess intermolecular free length $L_f^E = L_{fmix} - [(1- x) L_f 1 + x L_{f2}]$ ---------- (7)

Excess relative association $R_A^E = R_{Amix} - [(1- x) R_{A1} + x R_{A2}]$ ---------- (8)

Where, x- represents vol. fraction of the component and subscript 1 and 2 stands for components 1 & 2.

Results and Discussion

Using these experimental and computed data, excess parameters such as excess ultrasonic velocity (u^E), excess adiabatic compressibility (βa^E), excess acoustic impedance (z^E), excess intermolecular free length (Lf^E) and excess relative association (RAE)

have been computed. The values of excess parameters have been presented in Table – 2. The graph plotted of excess parameters versus vol. fraction (x) for liquid system as shown in Figure.1 to 5.

In the (1M NaCl+ 1M Serine)system from Table 1,the values of density,viscosity and ultrasonic velocity increase with increase of molal concentraction of amino acid.And the same.expect ultrasonic velocity decreases with rise in temperature.The ultrasonic velocity (u) for amino acid electrolytes solutions at 2MHz frequency and at different temperatures have been determined using relation (1) and presented in Tables 1&Table-2 thermo dynamical excess parameters for the system (1M NaCl + 1M Serine), the variations in ultrasonic velocity in liquid mixtures depend on concentration (x) of solutes and temperatures. Ultrasonic velocity (u) is related to, intermolecular free length. As the free length decreases due to the increase in concentrations of solutes, the ultrasonic velocity has to increase. The experimental results support the above statement in four liquid systems. Consequently, ultrasonic velocity of system increases depending on the structural properties of solutes. The solute that increases the ultrasonic velocity is structure maker.

From Tables-1 & 2 ultrasonic velocity increases with increase with increase in concentrations of solute (1M serine) in liquid system investigated such as (1M NaCl + 1M serine). When NaCl is dissolved in solution, the sodium ion (Na+) has a structures breaking effect, would disrupt the water structure16,17. This makes the liquid medium less compressible and hence the ultrasonic velocity increases above that of pure value.

The values of excess ultrasonic velocity(uE) have been calculated using the standard relation (4) and are presented in Tables 2 . From Table 2 thermo dynamical excess parameters for the system (1M NaCl + 1M Serine), and Fig.1it is clear that the values of (uE) are positive at the beginning but becomes negative thereafter by increasing volume fractions of 1M serine in the liquid mixture. The values of excess velocity decreasing. More negative values of uE in case of (1M NaCl+1M serine) indicates that the interaction between 1M NaCl and 1M serine is more stronger. Graphs shown in Fig.2 for (1M NaCl+1M serine) at different temperature and various volume fractions, excess values of (uE) are less positive at x-0.0 then become negative with increasing volume fraction.

Increase in negative values of (uE) with x-0.3 (Fig-1) is indicative of the increasing strength of interaction between component molecules of the mixtures. This supports our view that the interaction between component molecules in liquid mixtures is strong18. Fig.2 , shows that (uE) values are large negative for (1M NaCl + 1M serine). Thus interactions between the molecules of system (1M NaCl + 1M serine) are weaker.

The variations in excess adiabatic compressibility (βaE) with volume fractions at different temperatures are presented in Tables-2 and have been calculated by slandered relation(5). From Fig.3 it is observed that the values of βaE are negative at the lower volume fraction up to x-0.4 whereas the sign inversion of the β aE values changes by increasing volume fraction x-1.0. The curves show that the positive values of excess compressibility reaches maximum at x=1.0 volume fraction of 1M serine. From Table 2 thermo dynamical excess parameters for the system (1M NaCl + 1M Serine), the values of excess compressibility changes from negative to positive by increasing volume fractions of aqueous solutions of serine in 1M NaCl .

The values of βaE decreases19 with increase in temperatures which indicates that as the temperature of the system is raised, the system tends to attain ideal behavior in which the values of βa E should be zero.This means that the system is temperature sensitive and the interaction between the component molecules decreases with rise of temperature. The negative value of βaE, suggest significant interactions between the component molecules in the mixture, forming donor-acceptor complex between electrolytes and amino acid molecules. As a result there is contraction in volume, resulting in negative values of βaE, with. The positive values of βaE, for the system suggest the presence of weak interaction between unlike molecules. The size of component molecules almost no equal, it seems that their molecules do not pack well into each other structures. This results in expansion in volume, and hence positive βaE values.The negative value of βaE suggests significant interaction between component molecules in the mixture forming donor-acceptor complex between amino acids and electrolytes. As a result there is contraction in volume resulting negative values of βaEwith volume fraction (x).

Excess acoustic impedance (zE) has been calculated using relation (6) and calculated values of zE are presented in Tables 2 From Table, it is clear that the values of zE are positive at the beginning but becomes negative thereafter by increasing volume fractions of 1M serine in the liquid mixtures.

Graphs shown in Fig .3 for (1M NaCl + 1M serine) at different temperature and various volume fractions, excess values of zE are less positive at x – 0.4 then becomes negative with increasing volume fraction. zE has more positive values (with minimum at x-0-8) over entire range of volume fraction except x=1.0. Increase in positive values of zE with x-0.4 Fig.3 is indicative of the decreasing strength of interactions between component molecules of the mixture as suggested by Tiwari et al. This supports our view that the interaction of the component molecules in liquid mixtures is weak18. Fig- 8 show that zE values are small positive for (1M NaCl + 1M serine)

The changes in excess intermolecular free length (LfE) have been calculated with the help of equation (7).The values of LfE are given in the Tables – 2 thermo dynamical excess parameters for the system (1M NaCl + 1M Serine),The plot of (LfE) versus vol. fraction (x) and 303.15, 308.15 & 313.15K are shown in Fig.4 LfE values are negative at the beginning then become positive with increasing volume fraction (x) for all the systems at all temperatures suggesting strong specific interactions between amino acids and electrolytes molecules. Fig .4 ,shows variation in LfE at 303.15, 308.15, and 313.15K. It is seen that LfE values are negative at lower volume fraction of 1M NaCl . The sign of LfE play a vital role in assessing the compactness due to molecular arrangement and the extent of molecular interactions in the liquid mixtures through charge transfer, dipole- induced dipole and dipole – dipole interactions20 interstitial accommodation and orientation ordering21 leading to more compact structure making.

Negative L_f^E in the present investigation is an indication of strong interactions in the liquid mixtures, as well as interstitial accommodation of sodium chloride into the serine . This trend suggests that hetero association and homo association of molecules decreases with electrolytes.

The excess value of L_f^E being negative indicates strong interaction in the electrolytes – amino acids solutions. However, the excess value in free length shows positive values and the changes are very small. The negative value indicates that interactions between electrolytes (salt) and amino acid are not very strong. The positive L_f^E arises due to breaking of H- bonds in the self associated amino acids. Again the values of L_f^E are negative for the system NaCl suggests that the strong interactions occur between electrolytes and serine.

The variation of excess relative association function(R_A^E) with volume fraction (x) is mention in Tables- 2 thermo dynamical

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excess parameters for the system (1M NaCl + 1M Serine), and graphically depicted in Fig .5 shows that R_A^E is more positive for the system (1M NaCl +1Mserine). At beginning values R_A^E is positive for liquid mixtures as the volume fraction increases up to x= 0.4 as per Tables. The negative value of R_A^E suggests significant interactions between the component molecules in the mixture, forming donor – acceptor complex between amino acid and electrolytes molecules. As a result there is contraction in volume, resulting in negative values of R_A^E with x. The positive values of R_A^E for the system suggest the presence of weak interaction between unlike molecules.

Table-1: Variation of thermodynamic parameters at different volume fraction (x) and different temperatures for the system (1M NaCl+1M Serine) at 2MHz.

Vol.fra (x)	u ms^{-1}	ρ kg m^{-3}	η $Nm^{-2}s$
303.15K			
0.0	1554.50	1056	1.0428
0.2	1561.70	1058	1.0507
0.4	1568.00	1060	1.0578
0.6	1570.04	1062	1.0605
0.8	1575.10	1061	1.0710
1.0	1586.08	1066	1.010
308.15K			
0.0	1568.00	1054	0.9478
0.2	1571.70	1055	0.9561
0.4	1571.00	1058	0.9541
0.6	1579.08	1060	0.9691
0.8	1581.00	1062	0.9853
1.0	1588.07	1064	0.9911
313.15K			
0.0	1572.88	1052	0.9227
0.2	1587.04	1053	0.9440
0.4	1582.07	1055	0.9681
0.6	1584.88	1058	0.9802
0.8	1586	1060	0.9825
1.0	1588.04	1063	0.9909

Where u, ultrasonic velocity; ρ, density of the solution ; η,viscosity of solution;

Table-2: Variation of Excess parameters at different volume fraction (x) and different temperatures for the system (1M NaCl+1MSerine) at 2 MHz .

u^E ms^{-1}	$\beta^E x10^{-1}$ Nm^{-2}	$z^E x10^6$ A^0	L_f^E	R_A^E
303.15K				
44.4000	-0.51260	0.13784	-0.02467	0.05316
-6.65456	-0.07836	0.02787	-0.00240	0.02372
-3.07928	-0.06213	0.01178	-0.00167	0.01640
-75.7444	0.43432	-0.13766	0.02564	-0.01719
-108.680	0.59783	-0.18526	0.03484	-0.01968
-128.256	0.89628	-0.25161	0.04331	-0.03554
308.15k				
45.9000	-0.48350	0.13970	-0.02501	0.04984
2.91784	-0.10514	0.06438	-0.00560	0.00255
-6.45059	-0.02651	0.01798	-0.00141	-0.00927
-70.3463	0.41574	-0.12859	0.02312	-0.07558
-108.425	0.59106	-0.18907	0.03341	-0.09639
-134.448	0.73295	-0.25713	0.04219	-0.12868
42.8800	-0.46400	0.15521	-0.02426	0.05070
3.55472	-1.11487	0.09395	-0.00658	0.02734
-7.61371	-0.02801	0.09561	-0.00151	0.01922
-70.0156	0.40859	-0.03331	0.02293	-0.01595
-105.118	0.56701	-0.06133	0.03220	-0.01425
-179.305	0.88390	-0.14817	0.05124	-0.02317

Where, u^E = Excess ultrasonic velocity; βa^E= Excess ad. compressibility; z^E=Excess acoustic impedance; L_f^E=Excess intermolecular free length; R_A^E = Excess relative association.

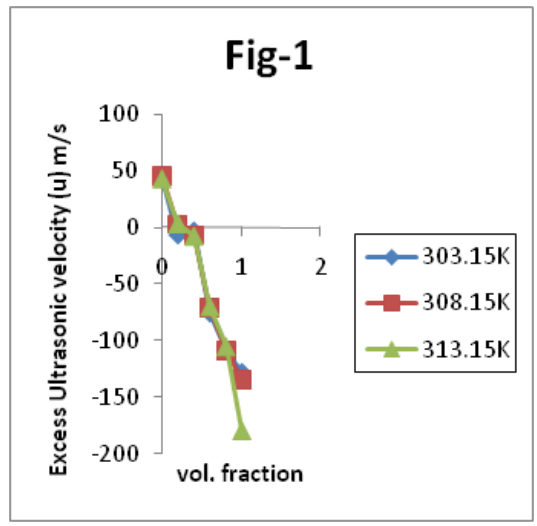

Fig. 1 –Plot of excess ultrasonic velocity (u^E) against volume fraction (x) of system(1M NaCl + 1M serine) at $2MH_z$ and 303.15, 308.15 and 3013.15K temperatures.

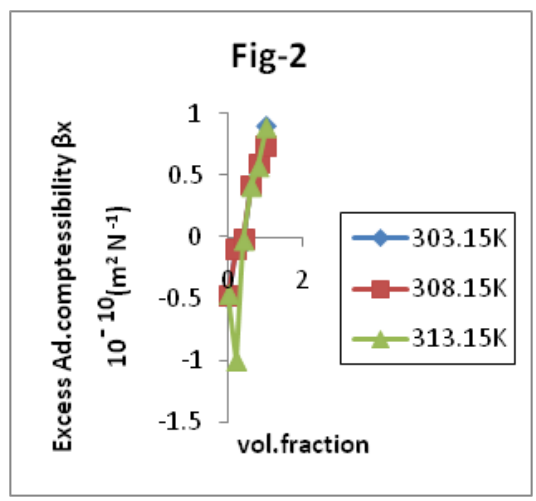

Fig. 2- Plot of excess adiabatic compressibility (β_a^E) against volume fraction (x) of system (1M NaCl + 1M serine) at $2MH_z$ and 303.15, 308.15 and 3013.15K temperatures.

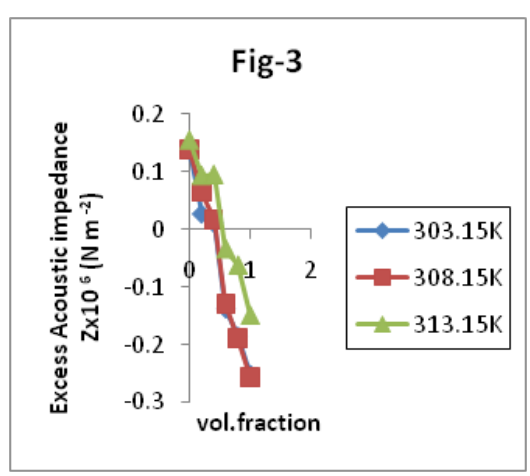

Fig. 3–Plot of excess acoustic impedance (z^E) against volume fraction (x) of system(1M NaCl + 1M serine) at $2MH_z$ and 303.15, 308.15 and 3013.15K temperatures.

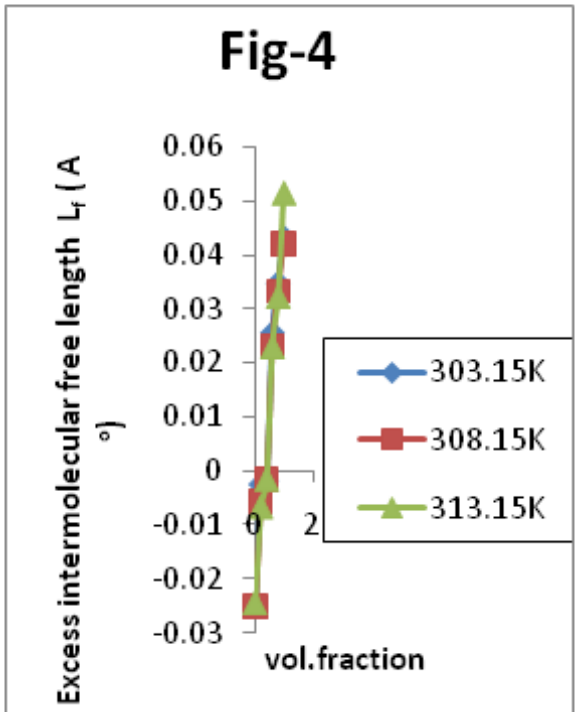

Fig.4- Plot of excess intermolecular free length (L_f^E) against volume fraction (x) of system (1M NaCl + 1M serine) at $2MH_z$ and 303.15, 308.15, 3013.15K temperatures.

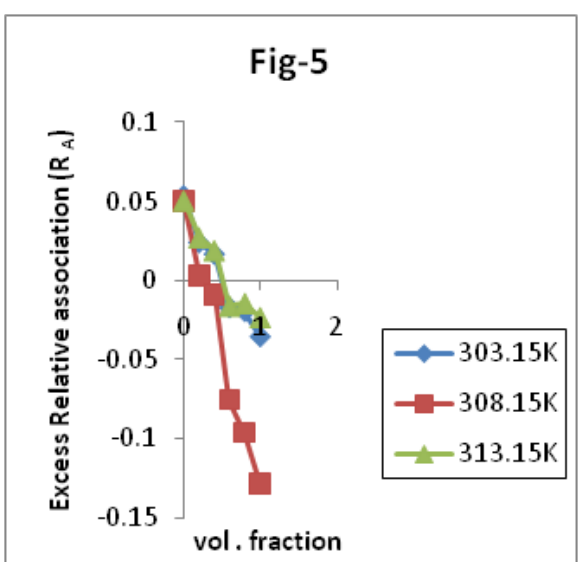

Fig5–Plot of excess relative association (R_A^E) against volume fraction (x) of system(1M NaCl+1M serine) at $2MH_z$ and 303.15, 308.15 and 3013.15K temperatures.

Conclusion

It may be concluded that ultrasonic velocity of system increases depending on the structural properties of solutes. It is well known that solutes causing electrostriction lead to decrease in the compressibility of the solution. Hydrophilic solutes often show negative compressibility, due to ordering that is induced by them in water structure. The solute that increases the ultrasonic velocity is of structure maker (SM). It has been observed that intermolecular free length decreases linearly on increasing concentrations of solutes in the systems. The excess parameters such as excess ultrasonic velocity (u^E); excess adiabatic compressibility (β_a^E); excess acoustic impedance (z^E); excess intermolecular free length (L_f^E) and excess relative association (R_A^E) have been studied in this investigation. These excess thermodynamic parameters threw more light on the molecular interactions such as hydrogen bonding, ion – ion, ion – solvent, solute – solvent interactions in aqueous solutions and binary mixtures.

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