STUDIES ON MOLECULAR INTERACTION OF L-SERINE IN MAGNESIUM CHLORIDE – WATER MIXTURE AT VARIOUS TEMPERATURES.

N.Sundaramurthy[1st] , S.Rajalakshmi[2nd]

[1]Department of Physics,Annamalai University,Annamalai Nagar.
[1st]Post Graduate and Research Department of Physics, Thiru Kolanjiappar Government Arts College, Vriddhachalam, 606001.
[2nd]Department of Physics, University College of Engineering Panruti, Anna University.

Abstract : Densities and ultrasonic velocities of L-Serine in aqueous $MgCl_2$ (0.08 M) solutions have been measured at various temperature. From these experimental data adiabatic compressibility, apparent molar volume, apparent molar adiabatic compressibility, limiting apparent molar volume and limiting apparent molar adiabatic compressibility and their constants were calculated for the ternary systems. The data have been interpreted in terms of solute–solute and solute–solvent interactions. These results show that various interactions operating in these systems.

Keywords: Amino acid, Electrolyte, Adiabatic compressibility, Apparent molar volume, Apparent molar adiabatic compressibility.

I.Introduction:

Amino acids and peptides have been taken up as modal compounds for understanding the behavior of more complex protein molecules in solutions. Amino acids in aqueous solution are ionized and can act as acids or bases. Knowledge of acids-base property of amino acids is extremely important in understanding many properties of proteins (Badrayani and Kumar,2003a). Ultrasonic and thermodynamic properties of these model compounds (amino acid) in aqueous electrolytes media provide information of solute–solvent and solute–solute interactions (Bai and Yan,2003,Ali et al,2005a,Akthar,2004). Metal ions have been reported (Badrayani and Kumar,2002 Badrayani and Kumar,2003bAli et al,2005b) to play an important role in biological system and the presence of the magnesium amino acids complexes in human serum enhances the uptake of Magnesium. It is very important for the normal functioning of cells, nerves, muscles, bones, and the heart. Usually, a well-balanced diet provides normal blood levels of magnesium. Therefore, knowledge of water–amino acid interaction and the effect of inorganic ions on such interaction are necessary to understand several biological processes occurring in living organisms. There has been an increased interest in physicochemical properties of amino acids in aqueous and aqueous electrolytes media (Banipal and Singh,2000, Yan et al,2002). Amino acids have zwitterion and are the constituents of the most important class of biopolymers, i.e. proteins. Derangement of water and electrolyte balance in living systems causes a wide variety of health problems. Ultrasonic velocity measurements have been successfully employed to detect and assess weak and strong molecular interactions.

The density and ultrasonic velocity and its derived parameter are sensitive to structural changes that occur in solutions and to any interactions between solvent and solute . The adiabatic compressibility studies of amino acids in salts solutions are few (Nithiyanantham and Palaniappan,2008,Natarajan et al,1990).In the present paper, we report that densities, and ultrasonic velocities of L-Serine (0.0 – 0.5 M) in aqueous $MgCl_2$ (0.08 M) were measured at different temperatures. From these experimental data, a number of thermodynamic parameters namely, adiabatic compressibility (β), apparent molar volume(φ_v), apparent molar adiabatic compressibility(φ_k), limiting apparent molar volume (φ_v^0),and limiting apparent molar adiabatic compressibility(**φ_K^0**) have been calculated. These parameters were utilized to study various interactions taking place in the solutions of electrolyte ($MgCl_2$) and the amino acid (L-Serine).

II.MATERIALS AND METHODS:

L-serine (Sigma Chemicals Co.) and Magnesium chloride are obtained from sd Fine Chemicals, India, which are used as such without further purification. Water used in the experiment was deionised, distilled and degassed prior to making solutions. Solutions of aqueous Magnesium chloride (0.8 $mol.dm^{-3}$) were prepared by volume and used on the day they were prepared. . Aqueous solutions of $MgCl_2$ (0.00 and 0.05 M) were prepared and these were used as solvents to prepare the L.Serine solutions on mass on the molarity concentration scale with precision electronic digital balance (Model: SHIMADZU AX-200). The density was determined using a specific gravity bottle by relative measurement method with an accuracy of ± 0.01 kgm^{-3}. An ultrasonic interferometer having the frequency of 2 MHz (MITTAL ENTERPRISES, New Delhi, Model: F-81) with an overall accuracy of ± 0.1% has been used for velocity measurement. An electronic digital operated constant temperature bath (Raaga Industries, Model: ULTRA COLD CHAMBER-437) has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desired temperature. The accuracy in the temperature measurement is ± 0.1 K.

III.RESULTS AND DISCUSSION:

The densities, viscosity and ultrasonic velocities of the $MgCl_2$ and their ternary mixtures with L-serine as a third component were determined at 298.15,303.15,313.15 and 323.15K and are recorded in Table 1 .

Molality ($mol.Kg^{-1}$)	DENSITY $\rho(kg/m^3)$				VISCOSITY $\eta(\times10^{-3} NSm^{-2})$				VELOCITY U/ms^{-1}			
	Temperature (K)											
	298.15	303.15	313.15	323.15	298.15	303.15	313.15	323.15	298.15	303.15	313.2	323.15
0	1015.6	1014.3	1013.3	1011.1	0.9572	0.8554	0.7233	0.7187	1519.8	1526.7	1537.6	1549.6
0.1	1018.9	1017.5	1015.2	1014.2	0.9784	0.8733	0.7811	0.7273	1525.1	1534.2	1549.2	1561.6
0.2	1022.2	1020.7	1018.3	1016.8	0.9896	0.8832	0.7989	0.7335	1530.4	1541.7	1560.8	1573.6
0.3	1025.5	1023.9	1021.9	1019.4	0.9898	0.8931	0.8067	0.7467	1535.7	1549.2	1572.4	1585.6
0.4	1028.8	1027.1	1024.5	1022.0	0.9928	0.9193	0.8245	0.7629	1541.5	1556.7	1584.3	1597.6
0.5	1032.2	1030.3	1027.0	1024.5	1.0903	0.9229	0.8423	0.7901	1546.3	1564.2	1595.6	1609.6

Table-1: Values of density (ρ), viscosity (η) and ultrasonic velocity (U) of amino acid in aqueous Magnesium chloride at various temperatures

The values of velocity and density increase with increase in concentration of amino acids in all the ternary systems under investigation, which appear to be due to hydrophobic properties of solutes i.e. H-bond forming the variation of ultrasonic velocity with the concentration of serine can be shown to depend upon the concentration derivations of the density and adiabatic compressibility of the system investigated. This makes positive, showing that velocity increases with the concentration of serine in the systems serine $MgCl_2$ + water which is in good agreement with the results reported for adenosine mono,di and tri phosphates + dixane– H_2O (Rodriguez et al,2003).

The adiabatic compressibility of the serine + $MgCl_2$ + water mixture was determined at 298.15, 303.15, 313.15 and 323.15K from the density and velocity data. The adiabatic (compressibility were calculated by this relation

$$\beta=1/u^2\rho \quad \text{-------1}$$

The observed values of the adiabatic compressibility, (β) Table 2 are found to decrease with the concentration of serine in the ternary systems. This clearly suggested that the strength of interaction (hydration of the serine molecules) in the systems decreases with increasing concentration of electrolyte in the solution. The compressibility behavior of serine molecules in the present systems can be explained by considering the strong electrostrictive compression of the solvent produced by NH_3 and COO ends of the serine dipolar molecules (Pal and Kumar,2005). The decrease in adiabatic compressibility is attributed to the influence of the electrostatic field of ions ($NH3^+$ and COO-) on the surrounding solvent molecules (Mg^{2+}) called electrostriction.

Molality	**L-Serine**											
(mol.Kg^{-1})	**adiabatic compressibility**				**Change in adiabatic compressibility**				**Relative change in adiabatic compressibility**			
	(β)				(−Δβ)				($-\Delta\beta/\beta_0$)			
	Temperature (K)											
	298.15	**303.15**	**313.15**	**323.15**	**298.15**	**303.15**	**313.15**	**323.2**	**298.15**	**303.15**	**313.2**	**323.15**
0	4.3970	4.3520	4.2860	4.2110	…	…	…	…	…	…	…	…
0.1	4.3810	4.3230	4.2300	4.1590	0.8830	0.8728	0.8570	0.9040	2.0543	2.0574	2.0542	2.2044
0.2	4.3640	4.2940	4.1800	4.1060	1.3875	1.4111	1.3890	1.3420	3.2282	3.3262	3.3294	3.2707
0.3	4.3480	4.2660	4.1330	4.0550	1.8880	1.9347	1.9117	1.7730	4.3925	4.5604	4.5820	4.3214
0.4	4.3330	4.2380	4.0830	4.0040	2.3767	2.4646	2.4251	2.1980	5.5296	5.8096	5.8126	5.3567
0.5	4.3170	4.2110	4.0340	3.9540	2.8604	2.9701	2.9295	2.7220	6.6549	7.0011	7.0218	6.6349

Table-2: Values of adiabatic compressibility, Change in adiabatic compressibility and Relative change in adiabatic compressibility of amino acid in aqueous Magnesium chloride at various temperatures

Amino acids molecules in the neutral solution exist in the dipolar form and thus have stronger interaction with the surrounding water molecules. The increasing electrostrictive compression of water around the molecules results in a large decrease in the compressibility of the solutions. The interaction between the solute and the water molecules present in the solvent can be termed as hydration. (Franka and Wen ,1957).

The following observation has been made on φ_K and φ_V (Table-3) of the amino acid in aqueous Magnesium chloride solutions at 298.15, 303.15, 313.15 and 323.15K

1 . The values of φ_K and φ_V are all negative over the entire range of the molarity.

2. The negative values of φ_K and φ_V increase with the increase in concentration of Serine, but it is found to decrease with increasing the temperature.

Molality m (mol.Kg^{-1})	**Apparent molal compressibility $-\varphi_k$($\times 10^{-8}$ m^2 N^{-1})**				**Apparent molal volume $-\varphi_v$($\times$m^2 mol^{-1})**			
	Temperature (K)							
	298.15	**303.15**	**313.15**	**323.15**	**298.15**	**303.15**	**313.15**	**323.15**
0.1	10.183	10.039	10.112	10.293	11.1612	11.279	11.2934	11.3711
0.2	8.2011	8.274	8.1462	8.5678	11.4252	11.475	11.5396	11.5951
0.3	7.5277	7.6435	7.6226	7.8266	11.4596	11.524	11.6142	11.6364
0.4	7.1553	7.339	7.4929	7.5942	11.4737	11.533	11.6291	11.6571
0.5	6.9141	7.1991	7.2199	7.5259	11.4986	11.556	11.6462	11.672

Table-3: Values of apparent molar compressibility (φ_K), and apparent molar volume (φ_V) of amino acid in aqueous Magnesium chloride at various temperatures.

The values of S_v of amino acids are found to be less negative suggesting strong solute–solute interactions. The values of S_v indicating the solute–solvent interactions are greater than the solute–solute interactions. Table 4(A,B) shows the less negative values of **(φ_k^0)** which indicates strong solute–solvent interactions. The apparent molar adiabatic compressibility of serine as a function of $MgCl_2$ + water solutions. The **φ_k^0** and φ_v^0 values can also be explained on the basis of co-sphere overlap model(Gurney,1953) in terms of solute-co-solute interactions. According to this model, ion-ion and ion-hydrophilic group interactions contribute positively, whereas ion-non-polar group interactions contribute negatively to the φ_k^0 and φ_v^0 values.

where φ_k^0 is the limiting apparent molar compressibility It provides information regarding solute–solvent interaction. The calculated values of φ_k^0 and S_K are also included in Table 4 along with the values of φ_v^0 and S_v. Appreciable negative values of φ_k^0 for the systems strengthen our view that strong solute–solvent interaction.

The above observation clearly suggests that the negative values of φ_k^0 in the systems indicate the presence of ion-solvent interactions. The increases in φ_V^0 is due to strong ion-ion interaction and vice-versa. The Positive values of φ_V^0 indicate electrostrictive solvation of ions (owaga et al,1954,Wadi and Goyal,1992).

Amino Acid	$-\varphi_k^0$($\times 10^{-8}$ m^2 N^{-1})				S_K / ($\times 10^{-8}$ N^{-1} m^{-1} mol^{-1})			
	Temperature (K)							
	298.15	303.15	313.15	323.15	298.15	303.15	313.15	323.15
L-Serine	1.3348	1.2176	1.198	1.2898	8.2897	7.4372	7.313	8.6999

Table 4A

Amino Acid	φ_v^0($\times m^3$ mol^{-1})				S_V / (N^{-1} m^{-1} mol^{-1})			
	Temperature (K)							
	298.15	303.15	313.15	323.15	298.15	303.15	313.15	323.15
L-Serine	11.580	11.180	11.320	11.490	7.157	-3.235	-3.853	-3.680

Table 4B

Table-4 A, B Values of limiting apparent molar compressibility, limiting apparent molar volume, and their constants S_K and S_v of amino acid in aqueous Magnesium chloride at various temperatures.

Conclusion:

The result of the present investigation volumetric and compressibility L-serine in aqueous Magnesium chloride at various temperature were obtained using density, viscosity and ultrasonic velocity data and the results have been used to study the existence of ion-solvent interactions. From the φ_k^0 and φ_v^0 , it can be concluded that L-serine possesses strong ion-solvent interaction.

Reference:

1. Badarayani R, Kumar A, "Densities and speed of sound of glycine in concentrated aqueous NaBr, KCl, KBr and $MgCl_2$ at T= 298.15 K", J. chem. thermodynamics.2003; 35:897-908

2. Amalendu Pal, Suresh Kumar, "Volumetric studies of some amino acids in binary aqueous solutions of $Mgcl_2.6H_2O$ at 288.15, and 308.15 K,"J. chem. sci, 2005;117: 267-273.

3. Bai, T, B. Yan, "Viscosity B-coefficients and activation parameters for viscous flow of a solution of heptanedioic acid in aqueous sucrose solution" Carbohydr. Res, 2003; 338: 2921-27.

4. Anwar Ali, Hyder S, Nain A.K, “Intermolecular and ion solvent interactions of sodium iodide and potassium iodide in dimethyl formamide + 1-propanol mixtures at 303 K”, J. Pure & Appl. Ultrason., 1999; 21: 127-132 .

5. Badarayani R., Satpute D.B., Kumar A.,”Effect of NaBr, KBr and MgCl2 on viscosities of aqueous glycine and L-alanine solutions at 298.15 K”, J. chem. Eng. data.,2005; 50, 1083-1086.

6. Badarayani, R. ,A. Kumar, “Effect of temperature on the volumetric properties of the L-alanine(1) + KCl (2) + H_2O (3) system”. J. Chem. Eng. Data, 2003; 48: 664-668.

7. Ali A., Hyder S. and Akhtar Y, “Viscometric studies of α-amino acid in aqueous NaCl and MgCl2 at 303 K”, Ind. J. Phys,2005; 79: No. 2, 157-160.

8. Banipal T.S, Singh G. , Lark B.S,”Partial molal volumes of transfer of some amino acids from water to aqueous 1,4-dioxane solutions at 298.15K”, Indian J. Chem,2000; 39(A): 1011-1018.

9. Mishra A.P,Gautam S,” Viscometric and volumetric studies of some transition metal chlorides in glycine water solution”, Ind. J. Chemistry, 2001; 40(A): 100-104

10. Dhanalakshmi, Jasmine Vasantharani E, “Analysis of apparent molal volume and apparent molal compressibility of quaternary ammonium salt in non-aqueous medium”, J. Pure & Appl. Ultrason,1999;21: 79-82

11. Nithiyanantham.S ,Palaniappan L, “Acoustical studies on some disaccharides (sucrose, lactose, maltose) in aqueous media at room temperature”, Metals Mate. Proces,2008; 20:203-208

12. Natarajan M, Wadi R.K , Gaur H.C, “Apparent molar volumes and viscosities of some -and -amino acids in aqueous ammonium chloride solutions at 298.15K”, J. Chem. Eng. Data,1990;35: 87-93.

13. Rodriguez H, Soto A, Arce A,Khoshbarchi M.K. Apparent molar volume, isentropic compressibility, refractive index and viscosity of DL alanine in aqueous NaCl solutions, J. Solution Chem.,(2003);32:53-63.

14. Pal A , Kumar S, “Volumetric and ultrasonic studies of some amino acids in binary aqueous solutions of $MgCl_2 6H_2O$ at 298.15 K”, J. Mol. Liq.2005;121: 148-155.

15. Frank.H.S, W.Y.Wen, “Ion-solvent interaction. Structural aspects of ion-solvent interaction in aqueous solutions: A suggested picture of water structure”. Disc. Faraday Soc, 1957;24:133-140.

16. Kestin J, M. Sokolov , W.A. Wakeham, “Viscosity of liquid water in the range -8 °C to 150 °C”. J. Phys. Chem. Ref. Data, 1978; 941-948.

17. Gurney R W, (McGraw-Hill, New York). 1953
.

18. Wadi, R.K, R.K. Goyal, “Densities, viscosities and application of transition-state theory for water+potassium thiocyanate+amino acid solutions at 288.15-308.15 K”. J. Chem. Eng. Data,1992; 37: 377-386.