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Ultrasonic and thermodynamic studies of glycine in aqueous electrolytes solutions at 303 K

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Abstract Densities and ultrasonic velocities of glycine (0.01–0.09 M) in aqueous NaCl and MgCl₂ (0.02 and 0.06 M) solutions have been measured at 303 K. From these experimental data adiabatic compressibility K_s , apparent molar volume, ϕ_v , apparent molar adiabatic compressibility, ϕK_s , partial molar volume ϕ_v^0 and partial molar adiabatic compressibility, $\phi^0 K_s$ at infinite dilution were calculated for all the ternary systems. The data have been interpreted in terms of solute–solvent and solute–solvent interactions. These results show that dipole–dipole and ion–solvent interaction are strong in glycine–aqueous MgCl₂ than in glycine–aqueous NaCl.

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1. Introduction

In continuation of our earlier work (Akhtar, 2007) on the study of interactions between L-proline and L-glutamine in electrolytes (Cu II nitrate and Ni II chloride) in aqueous medium at 308 K, we present in this paper, the study of glycine in aqueous NaCl and MgCl₂ at 303 K. Ultrasonic and thermodynamic properties

of these model compounds (amino acid) in aqueous electrolytes media provide information of solute–solvent and solute–solute interactions (Rai and Yan, 2003; Ali et al., 2005a; Akhtar, 2004; Badaryani, 2002). Metal ions have been reported (Akhtar, 2007; Badaryani et al., 2003; Ali et al., 2005b; Banipal and Singh, 2000; Yan et al., 2002) to play an important role in biological system and the presence of the copper amino acids complexes in human serum enhances the uptake of copper by liver tissue. Nickel, an integral component of enzyme urease may be involved in the action of hydrogenase. In physiological media such as blood, membranes, and cellulose fluids, the dipolar character of amino acids (in the presence of ions such as Na⁺, K⁺, Mg²⁺ and Cl[−] dissolved in body water) has an important bearing on their biological functions. Therefore, a knowledge of water–amino acid interaction and the effect of inorganic ions on such interaction is necessary to understand several biological processes occurring in living organisms. Very recently, we have made systematic effort to investigate the volumetric, viscometric and thermodynamic properties of L-alanine, D-serine, DL-threonine, L-histidine, glycine and glycylglycine in water and in aqueous concentrated

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electrolytes solution and l-serine and l-threonine in aqueous sodium and magnesium acetate solutions at 298.15 K. There has been an increased interest in physicochemical properties of amino acids in aqueous and aqueous electrolytes media (Yan et al., 2004; Pinho, 2008). Amino acids have zwitter-ion 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.

In the present paper, we report that densities, ρ , and ultrasonic velocities, u , of ternary systems of glycine (0.10–9.0 M) in aqueous NaCl/MgCl₂ (0.02 and 0.06 M) were measured at 303 K. From these experimental data, a number of thermodynamic parameters namely, adiabatic compressibility K_s , apparent molar volume, ϕ_v , apparent molar adiabatic compressibility, ϕK_s , partial molar volume ϕ_v^0 and partial molar adiabatic compressibility ϕK_s^0 at infinite dilution respectively have been calculated. These parameters were utilized to study various interactions taking place in the solutions of electrolytes (NaCl and MgCl₂) and the amino acid (glycine).

2. Experimental

2.1. Chemicals and preparation

Glycine (Sigma Chemicals Co.), NaCl and MgCl₂ (A R grade) were of highest commercially available purity and were used as such without further purification, after drying over calcium chloride in a desiccator for more than 48 h. Aqueous solutions of NaCl and MgCl₂ (0.02 and 0.06 M) were prepared and these were used as solvents to prepare the glycine solutions on mass basis covering the whole composition range. All the solutions were prepared in a dry box and stored in special air tight bottles. The weighing was done on an Afcoset ER-120A electronic balance with a precision of ± 0.1 mg. The densities of solvents (aq. NaCl and aq. MgCl₂) and ternary mixture (glycine + aq. NaCl/aq. MgCl₂) were measured using a single-capillary pycnometer (made of Borosil glass) of bulb capacity of 8×10^{-6} m³. The marks of the stems were calibrated using double distilled water at 303 K. The pycnometer was kept for about 30 min in a thermostatic water bath so that the thermal fluctuation in density was minimized. The ultrasonic velocities in solutions were measured using a single crystal variable path interferometer at 3 MHz. The temperature of the test solutions was maintained at 303 ± 0.2 K in an electronically controlled thermostatic water bath. The velocity and density data were found to be accurate within $\pm 0.01\%$ and $\pm 0.02\%$, respectively.

3. Results and discussion

The densities and ultrasonic velocities of the NaCl, MgCl₂ and their ternary mixtures with glycine as a third component were determined at 303 K and are recorded in Table 1. The values of u and ρ 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 glycine (du/dc) can be shown to depend upon the concentration derivations of the density and adiabatic compressibility of the system investigated. Thus in the relation:

Table 1 Densities (ρ) and ultrasonic velocity (u) of glycine + aqueous NaCl and glycine + aqueous MgCl₂ at 303 K.

C (mol ^l)	0.02 M		0.06 M	
	ρ (kg m ³)	u (ms ⁻¹)	ρ (kg m ³)	u (ms ⁻¹)
<i>Glycine + aqueous NaCl</i>				
0.00	1020.6	1513.5	1003.8	1509.4
0.10	1021.3	1515.1	1004.6	1512.0
0.20	1024.1	1517.3	1005.1	1514.1
0.30	1028.9	1552.6	1007.3	1522.3
0.40	1029.4	1560.3	1009.1	1524.4
0.50	1031.2	1645.9	1011.8	1537.3
0.60	1032.9	1683.3	1019.1	1543.2
0.70	1035.7	1724.2	1020.6	1545.9
0.80	1038.1	1765.3	1020.9	1550.6
0.90	1041.3	1783.5	1024.7	1557.4
<i>Glycine + aqueous MgCl₂</i>				
0.00	998.7	1512.0	1006.2	1511.6
0.10	1004.0	1521.9	1006.4	1512.3
0.20	1010.0	1525.3	1014.3	1525.7
0.30	1013.4	1530.4	1015.7	1525.9
0.40	1017.2	1538.6	1016.7	1526.4
0.50	1024.9	1545.4	1017.5	1527.0
0.60	1027.1	1574.0	1019.8	1535.1
0.70	1034.2	1594.2	1020.9	1546.7
0.80	1035.6	1686.0	1024.9	1549.7
0.90	1038.5	1733.1	1025.3	1553.1

$$du/dc = -u/2[1/\rho(dp/dc) + (1/K_s)(dK_s/dc)] \quad (1)$$

The quantity $(1/\rho)(dp/dc)$ is positive while $(1/K_s)(dK_s/dc)$ is negative and the net value is negative. This makes du/dc positive, showing that u increases with the concentration of glycine in both the systems glycine + NaCl + water and glycine MgCl₂ + water which is in good agreement with the results reported for adenosine mono-, di- and tri-phosphates + dioxane-H₂O (Mishra and Gautum, 2001).

3.1. Adiabatic compressibility

The adiabatic compressibility of the Gly + NaCl + water and Gly + MgCl₂ + water mixture was determined at 303 K from the density and velocity data. The adiabatic compressibilities were calculated by this relation

$$K_s = 1/u2\rho \quad (2)$$

The observed values of the adiabatic compressibility, K_s Table 2 are found to decrease with the concentration of glycine in all the ternary systems. However, the decrease in K_s is more marked in 0.02 M electrolyte solution and become less so as the 0.06 M concentration of the electrolyte in the solution. This clearly suggested that the strength of interaction (hydration of the glycine molecules) in both the systems decreases with increasing concentration of electrolyte in the solution (Yu et al., 2002). The compressibility behavior of glycine molecules in the present systems can be explained by considering the strong electrostrictive compression of the solvent produced by NH₃⁺ and COO⁻ ends of the glycine dipolar molecules (Ogawa et al., 1984). As the concentration of electrolyte in solution increases, the interaction between NH₃⁺ and Cl⁻ and between COO⁻ and Na⁺/Mg⁺² become increasingly strong, there by, reducing the electrostrictive effect of NH₃⁺ and COO⁻ ends of glycine molecules. Consequently,

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