WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.074
Volume 7, Issue 4, 1066-1075. Research Article ISSN 2277– 7105

TRANSFER VOLUMES OF GLYCINE FROM WATER TO AQUEOUS ELECTROLYTE AND NON-ELECTROLYTE SOLUTIONS AT 298.15 K

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Article Received on
24 Dec. 2017,
Revised on 13 Jan. 2018,
Accepted on 03 Feb. 2018,
DOI: 10.20959/wjpr20184-11064

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ABSTRACT

Partial molar volumes $\varphi^0{}_v$) of glycine (c=0.02-0.22 mol·dm^{-3}) in aqueous electrolyte solutions (NaCl and KCl, c=0.15, 0.45 and 0.60 mol·dm^{-3}) and non-electrolyte solutions (sucrose, c=0.15, 0.45 and 0.60 mol·dm^{-3}) were determined at 298.15 K. Partial molar volume of transfer ($\Delta_{tr}\varphi^0{}_v$) of glycine from aqueous to aqueous electrolyte and non-electrolyte solutions has been calculated and interpreted in terms of different interactions in studied solutions.

KEYWORDS: Density, Apparent molar volume, Ion–hydrophilic interactions, Hydrophilic–hydrophilic group interactions.

INTRODUCTION

Most biochemical processes take place in aqueous solutions and all the biological systems are aqueous solutions of salts, proteins, carbohydrates and lipids.[1] Number of workers has studied aqueous glycine system and hydration structure of glycine in different environments.[2-6] Densities, partial molar volumes and heat capacities of glycine in aqueous magnesium chloride solutions at different temperatures have been studied by B. S. Lark *et al*[7], transfer volumes of glycine, from water to 1,2- butanediol-water mixtures at 298.15 K were studied by L. Xu *et al*[8] and influence of hydrotropic agents on the solute-solvent interactions in aqueous solutions of glycine at different temperatures were studied by S. Pattnaik *et al.*[9] Viscosity behavior of α-amino acids in acetate salt solutions at 303.15 to 323.15 K was studied by J. A. Siddique *et al.*[10] Extensive studies of solute-solute and solute-solvent interactions have been carried out by many workers.[11-17]

Interactions of glycine in aqueous electrolytes and sucrose solution plays a vital role in understanding the nature of action of bioactive molecules or the thermodynamic behavior of biochemical processes in the body system.[18] Important information regarding ion-ion and ion-solvent interactions in solutions can be obtained from partial molar volumes of solution.[19-21] Structure making and breaking properties of solutes can be understood form the physicochemical investigations of solutions.[22]

Studies of volumetric properties and molecular interaction of glycine with electrolytes and sucrose solutions are interesting due to the existence of interactions between them and to understand the effect of these co-solutes on volumetric and viscometric behaviour of glycine. The ion–ion, zwitterion–ion, zwitterion–water dipole, and ion–water dipole interactions in these systems are interesting to study. In continuation with our earlier studies[23-29], here, in view of physicochemical applications and research interests, the effect of electrolytes/ionic salts (NaCl and KCl) and non-electrolyte/sugar (sucrose) on volumetric behaviour of aqueous glycine solutions has been studied.

MATERIALS AND METHODS

Glycine (*sd fine*, AR Grade, purity>99%) was used. NaCl, KCl (Qualigens, >99.5) and sucrose (*sd fine*) solids were used as received. The HPLC grade deionized distilled water obtained from Millipore prefiltration kit (Direct-Q^{TM} system series) was used for preparation of solutions. Solutions of glycine having different concentrations were prepared in distilled water in calibrated volumetric flasks by dissolving accurately weighed glycine in different media. All the glassware used during experiments was of Borosil make and calibrated before use. Measurement of density was carried out using three different single capillary pycnometers and average values were considered for the calculation of density of solution. Weighing was done on electronic balance.

RESULTS AND DISCUSSION

The density data of ternary systems containing glycine in aqueous salts and sucrose solutions are reported in Table 1. It has been observed from density data that the densities of solutions increased with concentration of glycine in each system of aqueous 0.15, 0.45 and 0.60 $mol \cdot dm^{-3}$ NaCl, KCl and sucrose. Further the densities of glycine in aqueous salts and sucrose solutions increase with concentration of salts and sucrose which may be attributed to enhanced structure of solvent due to added glycine in NaCl, KCl and sucrose solutions. Variation in the density of studied solutions with concentration indicates changes in the structural arrangements and existence of molecular interactions between the components of the system at 298.15 K and atmospheric pressure.

Table 1: Molar concentrations (*c*), densities (ρ) and apparent molar volumes (φ_V) of glycine in aqueous NaCl/KCl/Sucrose solutions at 298.15 K.

***c* (Gly)**	ρ	φ_V	ρ	φ_V	ρ	φ_V
	0.151 mol·dm^{-3} NaCl		**0.151 mol·dm^{-3} KCl**		**0.156 mol·dm^{-3} sucrose**	
0.02	1.0038	47.96	1.0046	47.70	1.0165	44.35
0.06	1.0050	46.29	1.0057	46.20	1.0177	44.22
0.10	1.0062	45.92	1.0069	45.86	1.0190	43.98
0.14	1.0076	44.44	1.0083	44.39	1.0202	43.72
0.18	1.0088	44.09	1.0096	44.06	1.0215	43.65
0.22	1.0101	43.85	1.0110	43.00	1.0227	43.46
	0.455 mol·dm^{-3} NaCl		0.457 mol·dm^{-3} KCl		0.502 mol·dm^{-3} sucrose	
0.02	1.0162	49.94	1.0182	51.65	1.0505	46.65
0.06	1.0173	48.29	1.0192	50.29	1.0516	46.57
0.10	1.0185	46.59	1.0203	48.22	1.0527	46.44
0.14	1.0197	45.84	1.0216	46.68	1.0538	46.35
0.18	1.0211	44.66	1.0231	44.83	1.0550	46.14
0.22	1.0223	44.29	1.0243	44.42	1.0561	45.81
	0.608 mol·dm^{-3} NaCl		0.612 mol·dm^{-3} KCl		0.698 mol·dm^{-3} sucrose	
0.02	1.0223	50.77	1.0247	56.02	1.0658	47.39
0.06	1.0233	48.77	1.0256	53.08	1.0669	47.14
0.10	1.0245	47.28	1.0268	49.86	1.0679	46.90
0.14	1.0257	46.62	1.0280	47.83	1.0690	46.76
0.18	1.0270	45.74	1.0294	46.19	1.0701	46.58
0.22	1.0281	45.56	1.0308	45.13	1.0712	46.41

*Foot note: c=mol·dm^{-3}; ρ g·cm φ_V =cm^3·mol^{-1}.

The apparent molar volume (φ_V) of glycine in aqueous NaCl, KCl and sucrose solutions were calculated from the density of solvent, density of solution, molality of glycine and molar mass of glycine using following Equation:

$$\varphi_v = \frac{M_2}{\rho} + \frac{1000}{c\rho\rho_0}(\rho_0 - \rho) \qquad (1)$$

Where, ρ_0= density of pure solvent/solution in which experimental solutions were prepared (g·cm^{-3}), ρ density of experimental solution (g·cm^{-3}), M_2= molar mass of solute (g·mol^{-1}) and c= concentration of solution (mol·dm^{-3}). The calculated φ_V values are reported in Table 1. The values of glycine in aqueous solutions of salts and sucrose are higher than the values in water. It is seen that φ_V values of glycine decreased with increase in concentration of glycine increased with increase in concentrations of NaCl, KCl and sucrose for given glycine concentration. An increase in φ_V with electrolyte and sucrose concentration is a result of increased interaction between polar ends of glycine and ions of the electrolytes or polar groups of sucrose which shields the polar terminal groups of glycine[30] and increased solute-solvent interactions.

The φ_v data of glycine was fitted to the Massons linear relation, $\varphi_v = \varphi^0_v + S_v \times \sqrt{c}$,[31,23] and from the plots of φ_v vs. $\sqrt{c}$, the apparent molar volume at infinite dilution (partial molar volume, φ^0_v) of glycine in these aqueous systems was determined (Figure 1-3) as intercept and S_v, the experimental slope was determined as slope. The φ^0_v and S_v values are reported in Table 2.

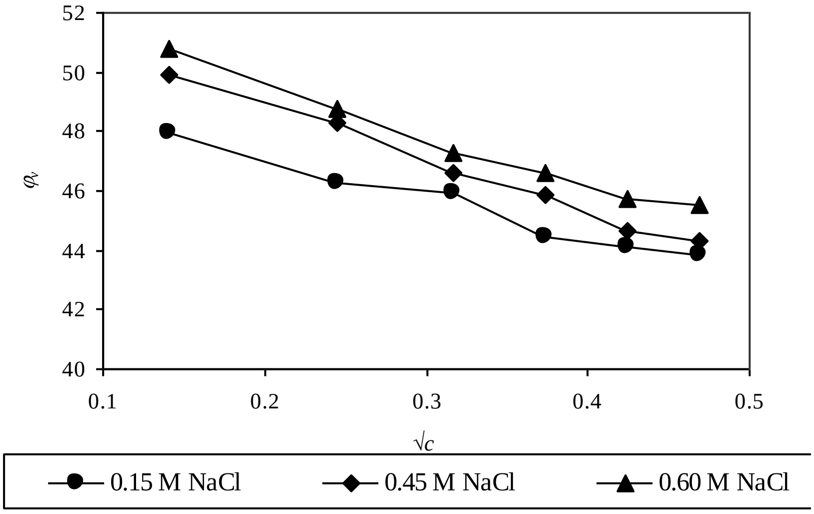

Figure 1. Graphical determination of φ^0_v and S_v for glycine in aqueous NaCl solutions from φ_v vs. $\sqrt{c}$ plot using Masson's relation.

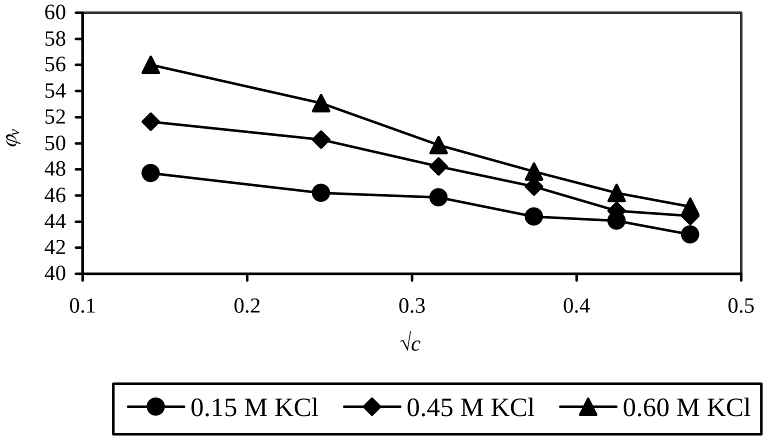

Figure 2: Graphical determination of φ^0_v and S_v for glycine in aqueous KCl solutions from φ_v vs. $\sqrt{c}$ plot using Masson's relation.

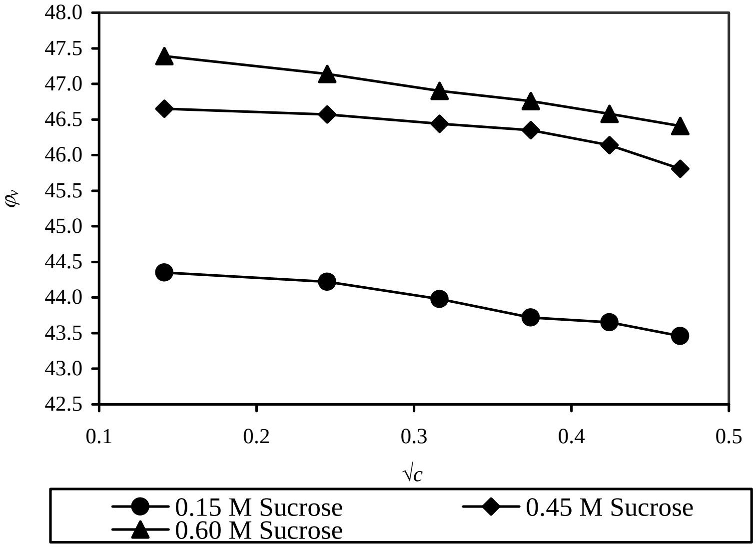

Figure 3: Graphical determination of φ^{0}_{v} and S_{v} for glycine in aqueous sucrose solutions from φ_{v} vs. $\sqrt{c}$ plot using Masson's relation.

Table 2: Partial molar volumes ($\square^{\square}_{\text{v}}$), experimental slope ($S_{\text{v}}$) and volumes transfer of glycine in aqueous NaCl/KCl/sucrose solutions at 298.15 K.

c (mol·kg^{-1})	φ^{0}_{v} (cm^{3}·mol$^{\square\square}$)	φ^{0}_{v} and $\Delta_{\text{tr}}\varphi^{0}_{\text{v}}$ (cm^{3}·mol$^{\square\square}$)	S_{v} (cm^{2}·dm$^{1/2}$·mol$^{-3/2}$)
NaCl			
0.60	52.83	9.67	-16.36
0.45	52.49	9.33	-17.93
0.15	49.68	6.52	-12.95
KCl			
0.60	61.05	17.89	-34.60
0.45	55.51	12.35	-23.85
0.15	49.76	6.60	-13.87
Sucrose			
0.60	47.84	4.68	-2.98
0.45	47.10	3.94	-2.35
0.15	44.82	1.66	-2.82

The φ^{0}_{v} for glycine in water obtained in present work=43.16 cm^{3}·mol$^{\square\square}$.

The partial molar volume (φ^{0}_{v}) reflects solute-solvent interaction and magnitude of the slope (S_{v}) reflects solute-solute interaction.[32] The φ^{0}_{v} increased with increase in the concentration of salts and sucrose which may be attributed to increase in the solvation of glycine at higher concentration of salts and sucrose. The observed positive values of φ^{0}_{v} indicate existence of solute-solvent interactions in all the solutions and presence of strong ion-solvent interactions in solution due to solvation of ions.

Further, the values of φ^0_{v} increased with increase in the concentration of salt and sucrose due to disruption of side group hydration by charged end.[33] The S_{v} values represent volumetric and energetic effects for the solute molecule and sign of S_{v} values can be related with the nature of interaction between the solvated solute molecules.[34] The graphical parameter S_{v} has negative values for all the studied systems due to weak solute-solute interactions.

In order to understand interactions between solute and co-solute, the partial molar volume of transfer (standard transfer volume of glycine, φ^0_{v} $^{\text{and}}$ $\Delta_{\mathrm{tr}}\varphi^0_{\mathrm{v}}$) at infinite dilution from pure water to aqueous salts/sucrose solutions are studied. The $\square^{\square}_{\mathrm{v}}$ value obtained for glycine in water is 43.14 $\mathrm{cm}^{3}\cdot\mathrm{mol}^{-1}$. The φ^0_{v} $^{\text{and}}$ $\Delta_{\mathrm{tr}}\varphi^0_{\mathrm{v}}$ values were calculated and reported in Table 2. Variation in the φ^0_{v} $^{\text{and}}$ $\Delta_{\mathrm{tr}}\varphi^0_{\mathrm{v}}$ with salt concentration is presented in Figure 4. It is seen that φ^0_{v} $^{\text{and}}$ $\Delta_{\mathrm{tr}}\varphi^0_{\mathrm{v}}$ values are positive for all the systems which is attributed to decrease in volume of shrinkage because of direct electrostatic interactions between salts/sucrose and charged centers of glycine which leads to the electrostriction of water.

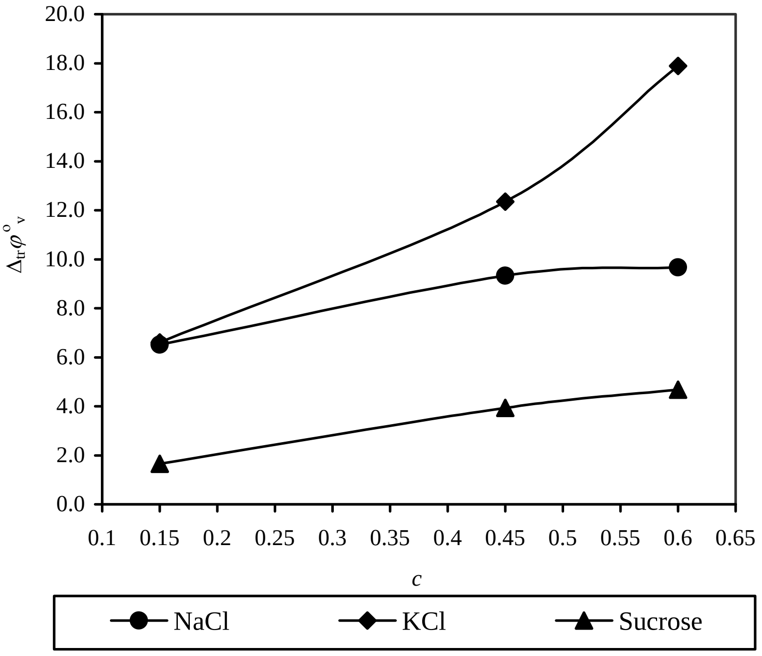

Figure 4. Variation in the $\Delta_{\mathrm{tr}}\varphi^0_{\mathrm{v}}$ with *c*oncentration of salts and sucrose at 298.15 K.

The positive values of $\Delta_{\mathrm{tr}}\varphi^0_{\mathrm{v}}$ also indicate dominating ion-hydrophilic and hydrophilic-hydrophilic interactions. This also suggests existence of ion-hydrophilic or ion-polar interactions. Glycine gets less hydrated in presence of salts and sucrose as ions in salts (through solvation) and sucrose molecules (through hydrogen bonding) takes water molecule to hydrate and glycine will leave with less water molecules (overall enhancement of water structure). Therefore, hydration number of glycine decreases on addition of salts and sucrose and further decreases with concentration of salts and sucrose due to existence of solute-co-solute interactions. Dominating hydrophilic-hydrophilic or ion-hydrophilic interactions are observed in present systems and these interactions strengthen with increase in concentration of salts and sucrose. The terminal zwitter ionic groups of glycine ($–NH_3^+$ and $–COO^-$) are hydrated in electrostatic manner and the electrostriction of $–NH_3^+$ group is greater than $–COO^-$.[30] The increase of φ^0_v and $\Delta_{tr}\varphi^0_v$ suggests that electrostriction effect is decreased in salts + water and sucrose + water than in pure water which brings about increase in the volume of solvent.[32] Due to molecular interactions, around each solute molecule there is a region of water where the properties of these water molecules differ from those of bulk water.

CONCLUSION

Densities of glycine + aqueous-{NaCl/KCl/sucrose} solutions at 298.15 K have been measured. Apparent molar volumes (φ_v), partial molar volumes (φ^0_v) and partial molar volumes of transfer ($\Delta_{tr}\varphi^0_v$) of glycine at infinite dilution from pure water to aqueous NaCl/KCl/sucrose solutions were calculated. It is concluded from the $\Delta_{tr}\varphi^0_v$ values that, the ion–hydrophilic and hydrophilic–hydrophilic group interactions are predominant over hydrophilic–hydrophobic group interactions. Magnitude of $\Delta_{tr}\varphi^0_{v\ v}$ indicates the more interactions between glycine and sucrose compared to glycine and salts, whereas, the order of electrostriction of water are more in salts than in sucrose solution. The hydrophilic–ionic group interactions are weak in glycine + sucrose solution and are strongest in glycine + KCl solution. Further, increase in the infinite dilution partial molar volume is due to dehydration of zwitterionic center of amino acids which is because of hydrophilic-ionic group interaction between the ion (from dissociation of salts) and water molecules. The increase of φ_v and $\Delta_{tr}\varphi^0_v$ suggests that electrostriction effect is decreased in salts + water and sucrose + water than in pure water which brings about increase in the volume of solvent.

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