



## Study of Solute-solute and Solute-solvent Interaction of Glycerin and Dextrose in Buffer Solutions at Different Temperature by Using Volumetric and Acoustic Methods

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### Author's contribution

The sole author designed, analyzed and interpreted and prepared the manuscript.

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### ABSTRACT

Densities and Ultrasonic velocities of glycerin and dextrose in Na<sub>2</sub>CO<sub>3</sub> and NaHCO<sub>3</sub> buffer solutions have been determined experimentally at 308 and 313K. From these experimental results the adiabatic compressibility K<sub>s</sub>, acoustic impedance Z, intermolecular free length L<sub>f</sub>, relative association R<sub>A</sub>, available volume V<sub>a</sub> and hydration number H<sub>n</sub> have been calculated. The results are interpreted in terms of solute-solute and solute-solvent interactions in these ternary systems. It has been observed that there exist solute-solvent interaction and complex formation between in these ternary systems.

*Keywords: Glycerin; dextrose; adiabatic compressibility; acoustic impedance; intermolecular free length; relative association; available volume and hydration number.*

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## 1. INTRODUCTION

The study of thermodynamic properties of carbohydrates in aqueous and non-aqueous solvent is an important step for understanding their behavior biological fluids containing different ionic species. Also, it can provide useful information regarding conformational stability and interaction in the ternary system. Ultrasonic technique has been found to be more accurate and comprehensive in understanding solute-solvent interactions. To understand the role played by the biological molecules in living organism [1-3]. Frank et al. [4] and Kaulgud [5] have studied the thermodynamic properties of several carbohydrates like ribose, galactose, monosaccharides and disaccharides in aqueous solutions. Amino acids have zwitter-ion and are the constituents of the most important class of biopolymers, i.e. Proteins Disarrangement water and electrolyte balance in living systems cause a wide variety of health problems. In physiological media such as blood, membranes, cellulose fluids etc., the dipolar character of amino acids (in presence of ions such as  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{+2}$  and  $\text{Cl}^-$  etc., dissolved in body water) has an important bearing on their biological functions. Carbohydrates located at cell surfaces are important receptors for the bioactive structures of enzymes, hormones, viruses, antibodies etc. The electrolyte –carbohydrates and protein - carbohydrates interactions are important for immunology, biosynthesis pharmacology, medicine and cosmetic industry. The complex conformational and configurationally factors determining the structure of carbohydrates in aqueous electrolytes solutions [6-9].

Recently, we have made systematic effort to investigate densities, ( $\rho$ ) and ultrasonic velocities, ( $u$ ) of ternary systems of D(+) glucose with mixed solvent of aqueous NaCl, KCl,  $\text{MgCl}_2$  and  $\text{CaCl}_2$  solutions at 303 K [10]. This increase could be attributed to the interactions of the ions of the NaCl, KCl,  $\text{MgCl}_2$  and  $\text{CaCl}_2$ , causing the transfer of hydrated water molecule to the bulk state.

In the present paper, we report densities and ultrasonic velocities of glycerin and dextrose in  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  buffer solutions have been determined experimentally at 308 and 313 K. From these experimental results the adiabatic compressibility  $K_s$ , acoustic impedance  $Z$ , intermolecular free length  $L_f$ , relative association  $R_A$ , available volume  $V_a$  and hydration number  $H_n$  have been calculated. These parameters were

utilized to study various interactions taking place in the solutions of these ternary systems were measured at 308 and 313 K.

## 2. EXPERIMENTAL

### 2.1 Chemicals and Preparation

Glycerin and dextrose (99.6% purity),  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  (99.8% purity) were procured from E Merck Germany and S d Fine Ltd. The ultrasonic velocities and densities of the Glycerin and dextrose in buffer solution solutions at various concentrations as well as in triple distilled de-ionized water were measured experimentally. The triple distilled water was used to make aqueous solvent of  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  and these were used as solvent to prepared glycerin and dextrose solutions. All the solutions were prepared by mass in dry box and were stored in special air-tight bottles and kept in dark to avoid photochemical degradation. The weighing was done on an electronic balance (model: GR-202R, and Japan) with a precision of  $\pm 0.01$  mg.

### 2.2 Measurement of Density and Ultrasonic Velocity

The densities were measured with a single capillary pycnometer (made of Borosil glass) of bulb capacity of  $8 \times 10^{-6} \text{m}^3$ . The marks of the stems were calibrated using double distilled water at 308 and 313 K. The pycnometer was kept for about 30 minutes 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 3MHz. The temperature of the test solutions was maintained at 308 and 313K  $\pm 0.02\%$  K in an electronically controlled thermostatic water bath. The velocity and density data were found to be accurate with in  $\pm 0.10\%$  and  $\pm 0.01\%$  respectively.

## 3. RESULTS AND DISCUSSION

The densities and ultrasonic velocities of the glycerin and dextrose (0.30, 0.60, 0.90, 1.2 and 1.5) M with mixed solvent of aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  (0.5) M were determined at 308 and 313 K are recorded in Table 1. The values of density and velocity positively increase and linearly (According to Pearson's r coefficient is a measure of the linear correlations between two variables X and Y giving a value between +1 and -1 inclusive where +1 is total positive and -1 is

total negative) with increase in concentration of all the ternary systems under investigation, [11] which appear to be due to hydrophobic properties of solutes i.e. H-bond forming. Solutes may occupy the interstitial spaces in solvent or get solvated forming new weaker bonds. The rise of temperature the ion-solvent interactions are weak of the systems due to the presence of weak intermolecular forces and thermal dispersion forces. It was suggested that what is experimentally observed for any systems reflect the compromise between the tendency for the ions and to interact with each other and inclination of the solutes to associate with the solvent. The change in structure of solvent or solution as a result of H- bond formation leads to decrease in intermolecular free length [12]. The variation of ultrasonic velocity with the concentration of glycerin and dextrose, ( $du/dc$ ) can be shown to depend upon the concentration derivations of the density and adiabatic compressibility of the system investigated.

Thus, in the relation:

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

The quantity  $(1/\rho)(dp/dc)$  is negative which indicates change in structure of solution as a result of H- bond formation leads to decrease in intermolecular free length and ion - solvent interactions are strong. while  $(1/K_s)(d K_s /dc)$  is positive and the net value is negative. This makes  $du/dc$  positive, showing that  $u$  increases with the concentration of the ternary systems.

### 3.1 Adiabatic Compressibility

The adiabatic compressibility of the glycerin + aqueous  $\text{Na}_2\text{CO}_3 + \text{NaHCO}_3$  and dextrose + aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  were determined at 308 and 313 K from the density and velocity data. The adiabatic compressibility was calculated by this relation

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

The per usual of Table 2 exhibits the values of the adiabatic compressibility,  $K_s$  Table 1 is found to be decrease with the concentration of solute (glycerin and dextrose) in all the ternary systems. Such a decrease in adiabatic compressibility observed in the ternary systems clearly confirms the conclusion drawn from the ultrasonic velocity data. It is well known fact that when a solute dissolves in a solvent. Some of the solvent ions ( $\text{Na}^+$ ,  $\text{HCO}_3^-$  and  $\text{CO}_3^{2-}$ ) are attach to the

molecules of glycerin and dextrose because of solute-solvent interactions. Since the solvent molecules are oriented in ionic field (i.e. electrostatic field of ions). The solvent molecules are more compactly packed in the primary solvation shells. This is the reason, why solvent is compressed by the introduction of the ions. Thus the electrostatic field of the ions causes the compression of the medium giving rise to phenomenon called 'Electrostriction'. Since the water molecules are compressed, they do not respond to a further application of pressure. So the solutions become harder to compress. This will lead to the decrease in compressibility values. This may further ascribed that such a decrease in adiabatic compressibility,  $K_s$  is attributed to the influence of the electrostatic field of the ions ( $\text{Na}^+$ ,  $\text{HCO}_3^-$  and  $\text{CO}_3^{2-}$ ) on the accompanying molecules. It may be inferred that the weakening of hydrogen bond strength formed by the solute and solvent molecules and maximum complex formation may also be the reason for decrease in compressibility. The decrease in density and increase in velocity with temperature indicates decrease in intermolecular forces due to increase in thermal energy of the system which causes increase in volume expansion and hence increase in free path length. Thus is in accordance with the view proposed by others [13,14].

### 3.2 Intermolecular Free Length

The Intermolecular Free Length,  $L_f$  were calculated from measured density data of glycerin + aqueous  $\text{Na}_2\text{CO}_3 + \text{NaHCO}_3$  and dextrose + aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  solution at different molarities and at 308 and 313 K using the following equation:

$$L_f = K \cdot K_s^{1/2} \quad (3)$$

Where  $K$  values are different for different were taken from the Jacobson relation [15]. The decrease in intermolecular free length with increase in concentration of the solute, but it increases with temperature in all the systems are shown in Table 2. This indicates that there is a significant interaction between solute and solvent molecules, suggesting the structure promoting behavior on the addition of solute. It is attributed to the influence of the electrostatic field of the ions ( $\text{Na}^+$ ,  $\text{HCO}_3^-$  and  $\text{CO}_3^{2-}$ ) on the surrounding solvent molecules. The increase in temperature however makes the free length to increase, as expected due to thermal expansion of liquids.

### 3.3 Acoustic Impedance

The values of acoustic impedance,  $Z$  of these ternary systems (glycerin + aqueous  $\text{Na}_2\text{CO}_3 + \text{NaHCO}_3$  and dextrose + aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$ ) were calculated by the following relation and are reported in Table 3.

$$Z = u \cdot \rho \quad (4)$$

The values of  $Z$  increase with increase in molarities of electrolytes which indicates solute-solvent interaction are present and they behave as structure makers are shown in Table 3. The specific acoustic impedance of the medium for the particular type of wave being propagated and through it. The transmission of acoustic wave from one medium to another is important for transmission phenomenon in fluids. It may also correlate with ionic size  $\text{Na}^+$ ,  $\text{HCO}_3^-$  and  $\text{CO}_3^{2-}$  of ions. The behavior of acoustic impedance can be explained on the basis of lyophilic interaction between solute (glycerin and dextrose) and solvent (aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$ ) molecules, which maximum complex ion formation and become responsible for the propagation of ultrasonic wave.

### 3.4 Relative Association

The relative association  $R_A$  was calculated by using to the following standard equation [16].

$$R_A = (\rho / \rho^0)(u^0/u)^{1/3} \quad (5)$$

The derived values of  $R_A$  are summarized in Table 3. Table 3 shows that the values of  $R_A$  are increase with increase in concentration and temperature of these ternary systems which indicates ion-solvent interactions are present. The increase in temperature however makes the free length to increase, as expected due to the thermal expansion of the volume. The values of  $R_A$  are less in presence of glycerin system than those of dextrose system. A mutual comparison of these ternary systems shows the values of  $R_A$  are larger in case of dextrose than in glycerin. There are strong hydration co sphere around them therefore, Solute - solvent interaction will be much more than that of glycerin which is in good agreement with the results reported in glucose – alcohol – water mixture [17].

### 3.5 Available Volume

The available volume,  $V_a$  is calculated using the following relation:

$$V_a = V_T (1 - u/u_\infty) \quad (6)$$

Where  $u_\infty$  is the limiting velocity and is taken as  $1600 \text{ ms}^{-1}$ . The perusal of Table 4 reveals that the  $V_a$  values are positive of these ternary systems which indicate the presence solute-solvent interactions. These trends of  $V_a$  values are due to their hydration behavior [18] which compromise that due to reduction of the electrostriction terminals, whereas it decreases

**Table 1. Densities ( $\rho$ ) and ultrasonic velocity ( $u$ ) of glycerin + aqueous  $\text{Na}_2\text{CO}_3 + \text{NaHCO}_3$  and dextrose + aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  solutions at 308 and 313 K**

M (moldm <sup>-3</sup> )	$\rho(\text{kg m}^{-3})$	$u(\text{ms}^{-1})$			
		$\rho(\text{kg m}^{-3})$	$u(\text{ms}^{-1})$		
<b>Glycerin+aqueous <math>\text{Na}_2\text{CO}_3 + \text{NaHCO}_3(0.5 \text{ M})</math></b>					
		<b>308 K</b>	<b>313 K</b>		
0.00	1071.9	1627	1069.3	1635	
0.30	1075.4	1641	1073.4	1647	
0.60	1080.6	1646	1078.2	1652	
0.90	1085.1	1655	1082.3	1661	
1.20	1088.0	1663	1086.0	1666	
1.50	1091.0	1670	1090.1	1676	
<b>Dextrose+aqueous <math>\text{Na}_2\text{CO}_3 + \text{NaHCO}_3(0.5 \text{ M})</math></b>					
		<b>308 K</b>	<b>313 K</b>		
0.00	1071.9	1627	1069.3	1635	
0.30	1081.3	1650	1088.0	1655	
0.60	1110.6	1663	1107.2	1677	
0.90	1131.0	1683	1127.3	1686	
1.20	1150.0	1693	1147.0	1703	
1.50	1174.0	1710	1157.1	1715	

**Table 2. Adiabatic compressibility ( $K_s$ ) and free length ( $L_f$ ) of glycerin + aqueous  $\text{Na}_2\text{CO}_3$  +  $\text{NaHCO}_3$  and dextrose + aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  solutions at 308 and 313 K**

M (mol dm <sup>-3</sup> )	$K_s 10^{-10}$ (m <sup>2</sup> N <sup>-2</sup> )	$L_f 10^{-10}$ (m)	$K_s 10^{-10}$ (m <sup>2</sup> N <sup>-2</sup> )	$L_f 10^{-10}$ (m)
		<b>308 K</b>	<b>313 K</b>	
0.00	3.5242	119.39	3.4985	120.06
0.30	3.4532	118.18	3.4344	118.95
0.60	3.4157	117.54	3.3984	118.33
0.90	3.3646	116.66	3.3490	117.47
1.20	3.3234	115.94	3.3176	116.92
1.50	3.2866	115.30	3.2657	115.99
<b>Dextrose+aqueous <math>\text{Na}_2\text{CO}_3</math>+<math>\text{NaHCO}_3</math>(0.5 M)</b>				
		<b>308 K</b>	<b>313 K</b>	
0.00	3.5242	119.39	3.4984	120.06
0.30	3.3969	117.22	3.3556	117.59
0.60	3.2558	114.76	3.2116	115.03
0.90	3.2944	112.36	3.1206	113.39
1.20	3.0338	110.78	3.0061	111.29
1.50	2.9130	108.55	2.9383	110.03

**Table 3. Relative association ( $R_A$ ) and acoustic impedance ( $Z$ ) of glycerin + aqueous  $\text{Na}_2\text{CO}_3$  +  $\text{NaHCO}_3$  and dextrose + aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  solutions at 308 and 313 K**

M (mol dm <sup>-3</sup> )	$R_A$	$Z 10^4$ (Kg m <sup>-2</sup> s <sup>-1</sup> )	$R_A$	$Z 10^4$ (Kg m <sup>-2</sup> s <sup>-1</sup> )
		<b>308 K</b>	<b>313 K</b>	
0.00	-	174.44	-	174.83
0.30	1.0014	176.47	1.0015	176.78
0.60	1.0049	177.86	1.0051	178.12
0.90	1.0065	179.58	1.0069	179.77
1.20	1.0089	180.93	1.0099	180.92
1.50	1.0109	182.19	1.0129	182.70
<b>Dextrose+aqueous <math>\text{Na}_2\text{CO}_3</math>+<math>\text{NaHCO}_3</math>(0.5 M)</b>				
		<b>308 K</b>	<b>313 K</b>	
0.00	-	174.39	-	174.83
0.30	1.0139	162.19	1.0151	180.06
0.60	1.0299	184.69	1.0309	185.68
0.90	1.0544	190.35	1.0299	190.06
1.20	1.0638	194.69	1.0644	195.33
1.50	1.0730	200.75	1.0738	198.44

due to disruption of a side group hydration by that of charge end. The hydrophilic interaction ionic interaction between OH groups of glycerin and dextrose with  $\text{Na}^+$ ,  $\text{HCO}_3^-$  and  $\text{CO}_3^{2-}$  ions of sodium carbonate and sodium bicarbonate. The observed positive values of  $V_a$  suggest that the hydrophilic –hydrophilic group of interactions is dominate in theses ternary systems. The  $V_a$  values increase with increase in concentration of glycerin and dextrose solutions. This is due to greater hydrophilic –ionic groups and hydrophilic-hydrophilic group interactions with increased concentration of carbohydrates. The increase in  $V_a$  values with increase in temperature for theses

ternary systems, resulting in the expansion of the solution.

### 3.6 Hydration Number

The values of hydration number  $H_n$  of these ternary systems were calculated by the following relation and are reported in Table 4.

$$H_n = (n_1/n_2) (1 - K_s/K_s) \quad (7)$$

Further it is observed that the values of  $H_n$  decrease with increase of temperature which indicates solute-solvent interaction are weak.

**Table 4. Available volume ( $V_a$ ) and Hydration number ( $H_n$ ) of glycerin + aqueous  $\text{Na}_2\text{CO}_3$  +  $\text{NaHCO}_3$  and dextrose + aqueous  $\text{Na}_2\text{CO}_3$  and  $\text{NaHCO}_3$  solutions at 308 and 313 K**

M (mol dm <sup>-3</sup> )	$V_a 10^{-6}(\text{m}^3 \text{mol}^{-1})$		$H_n$	
	<b>Glycerin+aqueous <math>\text{Na}_2\text{CO}_3</math>+<math>\text{NaHCO}_3</math>(0.5 M)</b>			
	308 K		313 K	
0.00	18.420	-	18.554	-
0.30	18.890	3.8	19.011	3.7
0.60	19.170	2.7	19.294	2.6
0.90	19.476	2.6	19.565	2.5
1.20	19.998	2.3	20.390	2.2
1.50	20.892	2.3	20.562	2.2
	<b>Dextrose+aqueous <math>\text{Na}_2\text{CO}_3</math>+<math>\text{NaHCO}_3</math>(0.5 M)</b>			
	308 K		313 K	
0.00	18.420	-	18.554	-
0.30	18.801	7.5	19.019	7.4
0.60	19.085	6.9	19.363	7.0
0.90	20.898	5.5	19.955	5.3
1.20	21.653	5.0	21.811	4.8
1.50	21.838	4.8	22.015	4.9

The interaction between the solute and the water molecules in the solvent is term as hydration. The positive values of hydration number of indicate an appreciable salvation of solutes. This is added support for the structure promoting nature of solute as well as the presence of appreciable dipole-dipole interaction between solute and water molecules. The hydration number increases non-linearly which indicates molecular interaction between solute-solvent molecules.

#### 4. CONCLUSION

The volume and compressibility data have been used to study of solute –solute and solute-solvent interaction in these ternary systems. It can be concluded that the existence of solute-solvent interaction is in the order of dextrose>glycerin. This suggests greater number of –OH group in dextrose than glycerin, greater association taking place and strong structure maker than glycerin. Further, with rise of temperature the ion-solvent interactions are weak of the systems due to the presence of weak intermolecular forces and thermal dispersion forces. The best accuracy measurement in these ternary systems at 308 K than 313 K.

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#### COMPETING INTERESTS

Author has declared that no competing interests exist.

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