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SOLUTE-SOLUTE AND SOLUTE-SOLVENT INTERACTIONS STUDIES OF SACCHARIDES IN AQUEOUS SODIUM BUTYRATE SOLUTION AT 308K TEMPERATURES

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Abstract:

Density and viscosity of D (+) galactose and D (+) lactose mono hydrates in aqueous solution of sodium butyrate solutions have been determined experimentally at 308 K. The results obtained from density and viscosity measurement have been used to calculate the, apparent molal volume ϕ_v , partial molal volume ϕ_v^0 , transfer volume $\Delta\phi_{tr}^0$ at infinite dilution, A and B coefficient and S_v experimental slope. The results are interpreted in terms of solute-co- solute and solute-solvent interactions in these systems. It has been observed that there exist strong solute-solvent and solute-solute interactions and complex formation between in these ternary systems. The properties of the D (+) galactose and D (+) lactose mono hydrates in aqueous solution of sodium butyrate solutions are discussed in terms of the structure making and hydrogen bonding effect.

Keywords: D(+) Galactose; D(+) Lactose Mono Hydrates; Sodium Butyrate; Apparent Molal Volume Φ_v ; Partial Molal Volume Φ_v^0 ; Transfer Volume $\Delta\Phi_{tr}^0$ At Infinite Dilution; A And B Coefficient And S_v Experimental Slope.

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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. Volumetric 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 [1-7]. The physicochemical studies of interaction between saccharides in aqueous and inmixed aqueous medium, play an important role in biological and industrial process. We present in this paper, D (+) galactose and D (+) lactose mono hydrates in aqueous solution of sodium butyrate the study of interaction between them at 308 K. The hydration behavior of saccharides has been found to be related to number of configuration of hydroxyl group. Saccharides and their derivatives are very important chemicals in life processes. Interactions of saccharides are very important in exploring the stability of polysaccharides in biological systems as well as in the chemical industries of saccharides in biological systems as well as in the chemical

industry of saccharides. It is an essential component for maintaining cell viability, a natural cell-protecting agent, as well as an energy reservoir in many organisms.[8] The solute-solvent interaction has great importance in biological chemistry, surface chemistry, environmental chemistry and geochemistry. Aqueous solutions of sodium butyrate are biologically and chemically important and these are widely used in biological applications. It can promote growth of beneficial bacteria and inhibit the growth of harmful bacteria in the gastrointestinal tract. It is an energy source of differentiation [9].

Very recently, we have made systematic effort to investigate the ultrasonic and volumetric properties of glycerin and dextrose in Na_2CO_3 and NaHCO_3 buffer solutions and amino acids in concentrated electrolytic solution (10-12). The thermodynamic parameters were utilized to study of various interactions taking place in the solutions of these ternary systems at 308 and 313K. It was found that solute-solvent interaction and complex formation between in these ternary systems. It was found that NaCl and MgCl_2 increase the apparent molar volume and decrease the adiabatic compressibility of amino acids. This increase could be attributed to the interactions of the ions of the NaCl and MgCl_2 electrolytes and zwitter-ion head group of amino acids, causing the transfer of hydrated water molecule to the bulk state. Structural interactions of ionic solutes with electrolytes solvent are important in many fields of chemistry and biochemistry.

In the present paper, we report densities, ρ and *viscosity*, η of D(+) galactose and D(+) lactose mono hydrate (0.00, 0.02,0.03,0.05,0.07 & 0.08)M in aqueous solution of sodium butyrate(0.00,0.03,0.05,0.08 & 0.10) M solutions have been determined experimentally at 308K. From these experimental data a number of thermodynamic parameters namely, apparent molalvolume ϕ_v partial molalvolume ϕ_v^0 , transfer molalvolume, $\Delta\phi_{tr}^0$ at infinite dilution and experimental slopes $S_{v,A}$ and B coefficients respectively have been calculated. These parameters were utilized to study various interactions taking place in the solutions of D(+) galactose and D(+) lactose mono hydrates in aqueous solution of sodium butyrate the study of interaction between them at 308 K.

2. Experimental

2.1. Chemical and Preparation

Sodium butyrate (99.5% purity), D(+)galactose andD(+) lactosemono hydrates (99.8% purity) were procured from Merck and S d Fine Ltd. They were used as such without further purification, after drying over calcium chloride in desiccators for more than 48 hours. The viscosities and densities of D(+) galactose and D(+) lactose mono hydrates in aqueous solution of sodium butyrate solution at various concentrations as well as in double distilled de-ionized water were measured experimentally at 308 K. Aqueous solutions of sodium butyrate(0.00,0.03, 0.05, 0.08 & 0.10) M were prepared and these were used as solvents to prepare sodium butyrate solutions on mass basis covering the whole composition range. All the solutions were prepared by mass in dry box and were stored in special air-tight bottles and kept in dark to avoid photo chemical degradation. The weighing was done on an Afcoset ER-120A electronic balance with an accuracy ± 0.1 mg.

2.2. Measurement of Density and Viscosity

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 308K. The pycnometer was kept for about 30 minutes in a thermostatic water bath so that the thermal fluctuation in density was minimized. The viscosity measurements were carried out by Ostwald's viscometer which was first calibrated with double distilled water. The viscometer was allowed to stand in an electronically controlled thermostatic water bath for 30 minutes to minimize the thermal fluctuation. The time of fall was recorded with a stop watch of least count 0.1 s. At least three time recorded were obtained, and the average value was used as the experimental flow time. Poiseuille's equation was employed to calculate the viscosity of the D(+) galactose and D(+) lactose mono hydrates + sodium butyrate + water solutions.

$$\eta = \frac{\pi r^4 h g \rho}{8 l V t} = \rho \beta t \quad (1)$$

Here ρ is the density of the solutions, h the height of the column in the viscometer, g is the acceleration due to gravity, r is the radius of the capillary, l the length capillary and t is the time of fall of the solution of volume V . The term h, g, r, l and V are constant for a given viscometer therefore these have been replaced by single term β . The temperature of the water bath was maintained at 30°C. The viscosity and density data were found to be accurate within $\pm 0.1 \%$ and $\pm 0.01\%$ respectively.

3. Results and Discussion

The density, ρ and viscosity, η of D(+) galactose and D(+) lactose mono hydrate (0.00, 0.02, 0.03, 0.05, 0.07 & 0.08)M in aqueous solution of sodium butyrate (0.00, 0.03, 0.05, 0.08 & 0.10) M solutions have been determined experimentally at 308K and are presented in Table -1. It is observed from Table 1 that densities ρ and viscosities η for all the ternary systems increase with increase in molalities of aqueous sodium butyrate solution. The values of ρ and η increase with increase in concentration of sodium butyrate in all the ternary systems under investigation, which appear to be due to hydrophobic properties of solutes i.e. H-bond forming. This increasing behavior shows strong interactions may be attributed to the cohesion brought by the hydroxyl group of saccharides in aqueous sodium butyrate mixtures solutions. This may be attributed to the formation of clusters by the sodium butyrate and strong intermolecular forces in the solute. The changes in structure of solvent or solution as a result of H-bond formation lead to decrease in intermolecular free length (13). Solute may occupy the interstitial spaces in solvent or get solvated forming new weaker bonds.

The viscosity data were used to calculate the relative viscosity using Jones- Dole equation [14]

$$\eta_{rel} = \eta / \eta_o = [1 + AC^{1/2} + BC] \quad (2)$$

Where, η and η_o viscosities of the solutions and solvent respectively. B , is the Jones- Dole coefficient (14), an empirical constant, and is measure of ion-solvent interaction. Its values depend

on the size and shape of the solute particles. The A is the Falkenhagen coefficient (15) which indicates ion-pair electrostatic interactions. They were obtained by a least square treatment as the intercepts and slopes of the linear plots of $\eta / \eta_0 - 1/m^{1/2}$ versus $m^{1/2}$ and their values are given in Table -3.

The viscosity, η , of dilute solution of non-electrolytes is represented by

$$\eta = \eta_0(1+BC) \quad (3)$$

For a dilute solution of unsolvated spherical colloidal suspension, has derived by Einstein relation

$$\eta_{rel} = 1 + 2.5\phi \quad (4)$$

Where ϕ is the volume fraction of the solute(16) . If this equation is valid or amino acids, Eq. (3) becomes

$$\eta_{rel} = 1 + 0.0025 V_h C \quad (5)$$

Where V_h is the hydrodynamic volume. Since $AC^{1/2}$ term in Eq. 2 can be assumed to be negligible in a dilute solution, the following relation holds

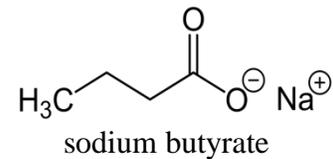
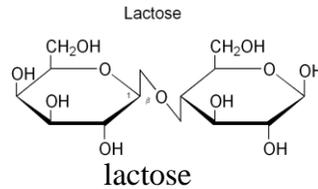
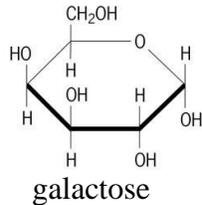
$$B = 0.0025V_h \quad (6)$$

Hakinet.al (17) may be assumed that the partial molar volume at infinite dilution of the unsolvated solute particle in a continuum solvent. The more B values in the mixed solvent might mean a more hydrodynamic volume in the mixed solvent.

A perusal of Table -3 shows that the values of A and B coefficients are large positive for all the ternary systems and these values are increase with increase in concentration of sodium butyrate an these ternary systems under investigation, thereby suggesting the solute-solute interactions and solute-solvent interactions are strong. The B coefficients measures the size and shape of the solute particles as well as the structural effects, induced by solute solvent interactions [18]. The magnitude of B is in the order:

D(+) lactose > D(+) galactose

A mutual comparison of the D(+) galactose and D(+) lactose shows that values of A and B are larger in case of D(+) lactose than D(+) galactose. Sodium butyrate of the solvent ions (Na^+) are attach to the molecules of D(+) galactose and D(+) lactose because of solute-solvent interactions. Since the solvent molecules are oriented in ionic field (i.e. electrostatic field of ions ($-CH_2OH$ and $CHOH$)). 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 that the solutions become harder to compress.



Thus, the trends and magnitude of the viscosity various parameters obtained from viscosity measurement reported in this paper. The studies suggest that solute- solvent and solute-solute interactions are stronger in D(+) lactose. The extent of interactions and structure making ability is greater in case of D(+) lactose.

The apparent molal volume, ϕ_v were calculated from measured density data of D(+) galactose and D(+) lactose mono hydrate in aqueous solution of sodium butyrate solutions have been determined experimentally at 308K using the following equation :

$$\phi_v = [1000 (\rho^0 - \rho) / m\rho \rho^0] + M/\rho \quad (7)$$

Where M is the molecular mass of the solutes, ρ^0 and ρ are densities of solvent and solution. The calculated values of ϕ_v of these ternary systems are given in Table 2. In these cases where molality dependence of ϕ_v , having definite trend points, The ϕ_v values increase due to reduction in the electrostriction effect at terminals, whereas it decreases due to disruption of side group hydration by that of the charged end.

The partial molal volume at infinite dilution ϕ_v^0 was calculated by taking an average data points. The linear variation is obtained by least square fitting to the following equation.

$$\Phi_v = \phi_v^0 + S_v m^{1/2} \quad (8)$$

The intercept ϕ_v^0 which is the partial molar volume at infinite dilution and the experimental slope, S_v which is considered to be volumetric pair wise coefficient. The derived values ϕ_v^0 of along with S_v are summarized in Table 3. Table 3 shows that the values of ϕ_v^0 are positive of these ternary systems which indicates ion-solvent interactions are strong. The values of ϕ_v^0 are less in presence of D(+) galactose than those of D(+) lactose mono hydrate. A mutual comparison of these saccharides shows the values of ϕ_v^0 are larger in case of D(+) lactose mono hydrate than in D(+) galactose. In these ternary systems the following types interactions are possible among solutes (saccharide) and co-solute (sodium butyrate):

- 1) Hydrophilic- ionic interactions between hydrophilic sites (-OH, -C=O and -O) of the saccharides and the ions (Na^+ / CH_3COO^-) of the co-solute.
- 2) Hydrophobic -ionic interactions between the hydrophobic parts of the saccharide molecules and the ions of the co-solute.

The transfer molar volume, $\Delta\phi_{tr}^0$ of each saccharides from water to aqueous sodium butyrate solutions have been calculated by the following equations:

$$\Delta\phi_{tr}^0 = \Delta\phi^0(\text{inaqueous sodium butyrate solutions}) - \Delta\phi_v^0(\text{in water}) \quad (9)$$

According to the co-sphere overlap model [19 &20], first types of interactions contribute positively whereas the later type of interactions makes negative contributions of $\Delta\phi_{tr}^0$ values. The significant positive transfer molar volume, $\Delta\phi_{tr}^0$ at infinite dilution (Table-3) observed for saccharides studied that the hydrophilic ionic interactions predominate over the hydrophilic –ionic interactions and increase in values with concentration of sodium butyrate which indicates the strengthening of the hydrophilic –ionic interactions over the entire range of concentrations.

Table- 1: Densities (ρ) and viscosities (η) of D (+) galactose and D (+) lactose mono hydrate solutions at 308K

C (mol.dm ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)
D(+) galactosemono hydrate+ aqueous + sodium butyrate					
	0.00 M	0.03	0.05	0.08M	0.10
0.00	995.7	1006.8	1022.6	1025.0	1032.1
0.02	1012.6	1019.2	1027.2	1029.9	1045.0
0.03	1016.2	1022.5	1030.7	1040.2	1053.0
0.05	1020.3	1028.4	1028.4	1041.1	1056.0
0.07	1029.1	1036.2	1048.2	1050.2	1059.1
0.08	1032.5	1043.5	1056.6	1058.2	1065.2
C (mol.dm ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)	ρ (kg m ⁻³)
D(+) lactosemono hydrate + aqueous + sodium butyrate					
	0.00 M	0.03	0.05	0.08M	0.10
0.00	995.7	1006.8	1022.6	1025.0	1032.1
0.02	1009.6	1016.2	1032.2	1039.1	1047.5
0.03	1010.2	1018.5	1038.0	1058.2	1063.5
0.05	1012.5	1018.4	1051.4	1077.4	1082.5
0.07	1015.8	1022.2	1057.2	1079.5	1086.8
0.08	1017.5	1024.6	1058.1	1080.2	1087.6
D(+)galactosemono hydrate + aqueous + sodium butyrate					
C	$(\text{mol.dm}^{-3})\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})$			$\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})$	$\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})$
	0.00 M	0.03	0.05	0.08M	0.10
0.00	0.7976	0.8160	0.8724	0.8890	1.0467
0.02	0.8197	0.8320	0.8967	0.9099	1.1966
0.03	0.8230	0.8449	0.9216	0.9482	1.2216
0.05	0.8287	0.8500	0.9322	0.9530	1.3112
0.07	0.8290	0.8539	0.9542	0.9722	1.3310
0.08	0.8398	0.8707	0.9735	0.9870	1.3540
D(+)lactosemono hydrate + aqueous + sodium butyrate					
C	$(\text{mol.dm}^{-3})\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})$			$\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})$	$\eta(\times 10^{-3}\text{Nm}^{-2}\text{s})$
	0.00 M	0.03	0.05	0.08M	0.10
0.00	0.7976	0.8160	0.8724	0.8890	1.0467
0.02	0.8283	0.8388	0.9042	1.0289	1.1448
0.03	0.8295	0.8573	0.9217	1.1892	1.2628
0.05	0.8375	0.8791	0.9620	1.2763	1.2971

0.07	0.8489	0.8926	0.9780	1.3134	1.3221
0.08	0.8522	0.9002	0.9881	1.3234	1.6592

Table 2: Apparent molar volume (ϕ_v) of D (+) galactose and D(+) lactose mono hydrate solutions at 308K

C(mol.dm ⁻³)	$\phi_v(10^{-3}m^3/mol)$	$\phi_v(10^{-3}m^3/mol)$	$\phi_v(10^{-3}m^3/mol)$	$\phi_v(10^{-3}m^3/mol)$	$\phi_v(10^{-3}m^3/mol)$
D(+) galactose+ aqueous + sodium butyrate					
	0.00 M	0.03	0.05	0.08M	0.10
0.02	845.22	546.20	317.01	244.21	563.52
0.03	654.96	502.16	275.42	452.90	438.56
0.05	565.31	489.42	312.75	388.04	380.62
0.07	515.72	399.72	322.05	383.02	366.49
0.08	503.34	417.92	354.70	377.51	356.49
D(+) lactosemono hydrate + aqueous + sodium butyrate					
	0.00 M	0.03	0.05	0.08M	0.10
0.02	983.62	655.52	398.81	666.15	677.82
0.03	549.81	572.81	340.22	772.32	698.21
0.05	559.01	425.26	434.22	780.74	725.11
0.07	515.72	872.36	442.56	785.69	669.70
0.08	514.92	485.84	417.81	639.49	539.92

Table 3: Falkenhagen coefficient, (A), Jones Dole coefficient, (B), partial molal volume ϕ_0v , experimental slope (Sv) and transfer molal volume at infinite dilution of D (+) galactose and D(+) lactose mono hydrate solutions at 308K

C (mol I ⁻¹)	A (dm ^{3/2} mol ^{-1/2})	B ϕ_v^0 (dm ³ mol ⁻¹)	(10 ⁻³ m ³ /mol)S _v	$\Delta\phi_{tr}^0$ (10 ⁻³ m ³ mol ⁻¹)	
D(+) galactose					
0.00	0.1162	0.3286	1035.1	1946.4	-
0.03	0.0135	0.8099	599.2	642.4	452.3
0.05	0.0198	1.0472	123.2	1907.2	930.6
0.08	0.1083	1.1994	202.5	751.8	850.2
0.10	0.6427	1.2986	586.0	578.2	448.1
D(+)Lactose					
0.00	0.1249	0.3986	1224.1	2447.4	-
0.03	0.0467	0.9843	709.2	892.4	562.3
0.05	0.0918	1.5750	689.2	647.2	430.6
0.08	0.0942	2.3940	869.5	751.8	450.2
0.10	0.0998	3.2860	996.0	578.2	448.9

4. Conclusion

The volumetric studies have been used to the solute –solute and solute-solvent interaction in these ternary systems. It can be concluded that the existence of molecular interaction is in the order of D(+)Lactose >D(+) galactose. This suggests D(+)Lactose in aqueous sodium butyrate solution is strong structure maker than D(+)galactose in aqueous sodium butyrate solution. The transfer molar

volume, $\Delta\phi_{tr}^0$ and $\Delta\phi_v^0$ suggest the predominance of hydrophilic –ionic interactions over hydrophobic –ionic interactions. These parameters reflect that the solute-co solute interactions are dominating over solute-solvent interactions for the saccharides in aqueous sodium butyrate solutions.

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