

To Study Solvation of Polyols with 5% Ethanol-Water at Room Temperature

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ABSTRACT

Density (ρ) and viscosity(η) of Mannitol and Sorbitol have been measured in 5% Ethanol-Water solvent system in the concentration range 0.05-0.5M at room temperature 298K for the density data, apparent molar volume (Φ_v) and partial molar volume (Φ_v^0) were worked out. The viscosity coefficient B and A constants and Stauding Constant (k_n) were calculated from the viscosity data by using Jones-Dole and Stauding equation. From viscosity coefficient constant B and partial molar volume, solvation number (B/Φ_v^0) of Mannitol and Sorbitol were worked out. From these parameters, results were associated with solute-solute, solute-solvent and solvent-solvent interactions.

Keywords : Polyols, Apparent Molar Volume, Partial Molar Volume, Association Number.

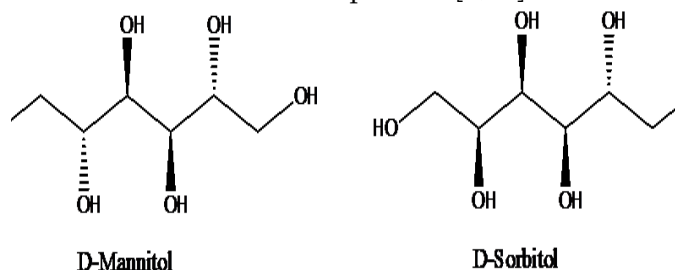
I. INTRODUCTION

Solvation is one of the important intermolecular interactions. It is responsible to maintain the secondary structure of biomolecules and expressing biological and medicinal process of cellular systems [1]. Polyols (mannitol and sorbitol) are used as ingredient in products like cosmetics, health care products and pharmaceuticals [2]. Volumetric behavior of polyols gives useful information for solvation process [3, 4]. Apparent Molar Volume and Partial Molar Volume of polyols in solution are used to study solute-solvent interaction [5,6].

Polyols and carbohydrates are most important class of biomolecules and show their different biological functions such as structure and defensive metabolic recognition, receptor affinity and selectivity [7].

The molecular interactions of dilute as well as concentrated solutions of sugars in water play an important role in expressing biophysical and

medicinal processes of cellular systems. The viscometric behavior of electrolytes and non-electrolytes give useful information for intermolecular interactions in the solution [8,9]. Sorbitol is white crystalline powder, 6-C sugar soluble in water, it is also called Glucitol. Sorbitol is a substitute of sugar which is about 60% the sweetness of sucrose. Mannitol is a 6-Carbon sugar derived from dextrose. It has been used to treat human brain for more than 30 years. The complication of mannitol therapy is fluid and electrolyte imbalance. Hence its interaction studies with the solvent become important. [8,10].



D-Mannitol

D-Sorbitol

II. METHODS AND MATERIAL

Mannitol and Sorbitol used in this work is analytical grade with purity of > 99% was procured from SHIMADZU. Ethanol used in this work is of AR grade from CSS with 99.9% purity. Double distilled water used for the preparation of solutions. The molar aqueous solution of solute was prepared by using digital electronic balance (Model-AJO20, aiwa) with an accuracy of ± 0.1 mg.

Densities (ρ) and viscosities (η) of aqueous solutions of Mannitol and Sorbitol in 5% Ethanol-Water were measured by using specific gravity bottle by relative measurement method with accuracy of ±0.1 kg.m⁻³ and an Ostwald's viscometer was used for the measurement of viscosity of liquid mixtures with an accuracy of 0.0001 Nsm². The viscometer was calibrated before used. Time flow of water and Mannitol and Sorbitol in 5% Ethanol-Water solutions were measured respectively.

OBSERVATION TABLE:

Table 1: Apparent molar volume and partial molar volume and S_v for Mannitol and Sorbitol at 298K at different concentrations

Concentration(mol /dm ³)	\sqrt{C}	Apparent Molar Volume (Φ_v) (m ³ mol ⁻¹)	
		Mannitol	Sorbitol
0.05	0.2236	165.54	162.47
0.1	0.3162	164.55	161.09
0.15	0.3873	162.20	156.12
0.20	0.4472	156.04	151.24
0.25	0.5	150.91	146.43
0.3	0.5477	148.84	144.79
0.35	0.5916	143.92	140.75
0.4	0.6324	141.99	138.25
0.45	0.6708	136.92	134.32
0.5	0.7071	133.67	131.63
Partial molar volume (Φ_v^0) (m ³ mol ⁻¹)		192.975	172.862
S_v (m ³ Kg ^{-1/2} mol ^{-1/2})		-82.186	-51.840

Table 2: Relative Viscosity ($\frac{\eta}{\eta_0}$) for Mannitol and Sorbitol at 298K at various concentrations.

Concentration (mol/dm ³)	\sqrt{C}	Relative Viscosity ($\frac{\eta}{\eta_0}$)	
		Mannitol	Sorbitol
0.05	0.2236	1.05629	1.0607
0.1	0.3162	1.05968	1.06387
0.15	0.3873	1.07255	1.06967
0.20	0.4472	1.08713	1.07854
0.25	0.5	1.0981	1.09212
0.3	0.5477	1.12079	1.1288
0.35	0.5916	1.1522	1.1535
0.4	0.6324	1.1902	1.1866
0.45	0.6708	1.2255	1.2287
0.5	0.7071	1.2526	1.2841

Table 3: Values of parameters of *Staurding, Jone Dole equation* and association number for Mannitol and Sorbitol at 298K.

Compound	$\left(\frac{\eta}{\eta_0 - 1}\right)$ versus C	$\left(\frac{\eta}{\eta_0 - 1}\right)$ versus \sqrt{C}	B x 10 ³ / Φ ⁰
Mannitol	$k\eta = 0.5649 \text{ dm}^3 \text{ mol}^{-1}$	B = 0.52 dm ³ mol ⁻¹ A = -0.081 dm ^{3/2} mol ^{-1/2}	2.69
Sorbitol	$k\eta = 0.4958 \text{ dm}^3 \text{ mol}^{-1}$	B = 0.61 dm ³ mol ⁻¹ A = -0.180 dm ^{3/2} mol ^{-1/2}	3.52

III. RESULTS AND DISCUSSION

Density and viscosity of mannitol and sorbitol were measured at room temperature at various concentrations ranging from 0.05-0.5M. Apparent Molar Volume can be calculated using density data by using the equation below [11].

$$\Phi_v = \frac{M}{\rho_0} - 1000 \frac{(\rho - \rho_0)}{C \rho_0} \quad \dots \dots \dots \quad \dots \dots \dots \quad \dots \dots \dots \quad (1)$$

Where, Φ_v = Apparent molar volume, C = Molarity, ρ = density of solvent, ρ₀=density of solvent and M= Molar mass of Mannitol and Sorbitol.

Volume changed due to addition of solute into solvent is called apparent molar volume. Apparent molar volume at infinite dilution, the solvent-solvent interaction is predominant known as partial molar volume [12]. The smaller values of apparent molar volumes result in strong interactions of solute-solvent molecules [13]. As the concentration increases, the interactions between solute-solute increased whereas those of solute-solvent decreases. This is because the electrostatic interaction between the solute molecules increases. The apparent molar volume data can be expressed with Messon's relation given below least square fit method [14,15].

$$\Phi_v = \Phi_v^0 + S_v C \quad \text{--- eqn (2)}$$

Where, Φ_v^0 is partial molar volume, it talks about the solute-solvent interactions. The values of Φ_v^0 for mannitol and sorbitol are given in Table 1, which shows positive Φ_v^0 values for both mannitol and sorbitol indicating positive interactions between solute and solvent molecules. Also, greater Φ_v^0 value for mannitol indicates stronger solute-solvent interactions in mannitol as compared to sorbitol.

Negative values of S_v obtained for mannitol and sorbitol indicates breaking of water-ethanol structure due to mannitol and sorbitol. [16] This means that, mannitol and sorbitol interact strongly with water-ethanol molecules than water interacts with itself. This results in breaking of hydrogen bonds within water molecules. The value is greater for sorbitol as compared to mannitol which indicates mannitol interacts strongly with solvent system.

Relative viscosity of mannitol and sorbitol were calculated at room temperature considering solutes as monomer units of polymer system. The polymer species follows *Staurding equation* given below [17]

$$\frac{(\eta - \eta_0)}{\eta_0} = kn Cn \quad \text{--- eqn (3)}$$

Where, η is viscosity of solution, η_0 is viscosity of pure solvent, k is constant for given solute in a given solvent, C is molar concentration of solute and n is the number of monomer units in polymer. The observed

values of relative viscosity for mannitol and sorbitol at 298K are given in Table 2.

Observed data were examined to study the agreement of viscosity with *Staurding equation*. As a result, relative viscosity values were plotted as a function of different concentrations at room temperature for mannitol and sorbitol which showed linearity.

Structure breaking and making properties of solute can also be studied by considering *Jone-Dole equation* given below [18]

$$\frac{\eta}{\eta_0} = 1 + A + B\sqrt{C} \quad \text{--- eqn (4)}$$

Where, $\frac{\eta}{\eta_0}$ is the relative viscosity, C is molar concentration of solute, A and B are constants for studied solute.

Coefficient A talks about the contribution for interionic electrostatic forces and coefficient B specifies chaos produced by ions in electrolyte and solutes in non-electrolytes in solvent structure [19].

Therefore, $\left(\frac{\eta}{\eta_0-1}\right)/\sqrt{C}$ values plotted against \sqrt{C} shows linearity for mannitol and sorbitol with slope B and intercept A . The value of both the constant are reported in Table 3. The *Jone-Dole equation* is more useful for ionic solute as coefficient A gives idea about ion-ion interaction. But, in case of Mannitol and Sorbitol, being non-electrolyte covalent compounds, the values of coefficient A are found to be very small. This is because, the interionic interaction is weak in case of non-electrolytes. The very small values of intercept A may be due to non-covalent interactions like hydrogen bonding, van der waals forces, etc.

Viscosity coefficient B indicates solvation of solute and its environment [20] which depends on the solute-solvent interactions and on the relative sizes [21]. Larger and positive value of viscosity coefficient B indicates structure making property of solute with the solvent [22]. From Table 3, we can observe the positive values of B for both mannitol and sorbitol which shows their structure making ability, but the larger value is observed for sorbitol which means

structure making ability for sorbitol is greater than mannitol.

IV. CONCLUSION

The observed values for constant kz for mannitol and sorbitol are in close agreement with the values of coefficient B. The values of $B / \Phi V$ indicates the solvation of solute. Its values show important significance [23]. If the value is greater than 2.5, greater would be the association [24]. From Table 3, we can observe the values >2.5 for mannitol and sorbitol indicating their strong association with ethanol-water solvent system. The value is much greater than 2.5 in case of sorbitol showing greater association with solvent system.

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