

Volume 12, Issue 8, 149-159.

**Conference** Article

ISSN 2277-7105

# THERMODYNAMIC BEHAVIOUR OF ANTIBACTERIAL SULPHOSALICYLIC DRUG IN AQUEOUS SOLUTION OF MANNOSE SOLUTIONS THROUGH DENSITY, REFRACTIVE INDEX AND UTRAACOUSTIC PROPERTIES

J. N. Chormalle<sup>1</sup>, S. N. Gundale<sup>2</sup>, A. V. Pawde<sup>3</sup>, Rahul Jadhav<sup>4</sup> and A. D. Arsule<sup>5</sup>\*

<sup>1</sup>School of Chemical Sciences, Swami Ramanand Teerth Marathwada University, Nanded -431 606 (MS) India.

<sup>2</sup>Department of Chemistry Mahatma Jyotiba Fule Jr. College, Hingoli-431702 (MS) India.
 <sup>3</sup>Department of Chemistry, Adarsh College, Hingoli-431513 (MS) India.
 <sup>4</sup>Department of Chemistry, Dayanand Science College, Latur-413512 (MS) India.

<sup>5</sup>Assistant Professor Deptt. of Chemistry Madhavrao Patil College, Palam Dist; Parabhani

(MS).

Article Received on 04 April 2023,

Revised on 25 April 2023, Accepted on 15 May 2023 DOI: 10.20959/wjpr20238-28158

\*Corresponding Author A. D. Arsule Assistant Professor Deptt. of Chemistry Madhavrao Patil College, Palam Dist; Parabhani (MS).

# ABSTRACT

Density, refractive index and ultrasonic velocity of sulphosalicylic acid with concentration range (0.02, 0.04, 0.06, 0.08 and 0.1) mole·kg<sup>-1</sup> in aqueous (0.025, 0.050 and 0.100) mol·kg<sup>-1</sup> solutions of d-mannose have been measured at T= 303.15 K. The effects of concentration of dmannose on different thermodynamic properties such as density, refractive index and ultrasonic velocity have been calculated. Derived thermodynamic properties such as apparent molar volume ( $V_{2,\phi}$ ), partial molar volume ( $V_{2,\phi}^o$ ), isentropic compressibility ( $K_s$ ), apparent molar isentropic compressibility ( $\kappa_{s,2,\phi}$ ), partial molar compressibility

 $(\kappa_{s,2,\phi}^0)$  specific acoustic impedance (z) and atomic polarization  $(P_a)$ 

are calculated by using measured properties. These properties have been explored in terms of molecular interaction between solute and cosolute

**KEYWORDS:** Thermodynamic properties, molecular interaction, antiracial drug, drug solution.

### **INTRODUCTION**

Sulpha/Sulfonamides drugs which are used against the infection caused by several Gram negative and Gram positive bacteria such as fungi, bacteria and cretin protozoan.<sup>[1-3]</sup> In addition, these types of molecules have shown different kind of activities such as diuretic, hypoglycemic and antitumoral effects.<sup>[4]</sup> Sulphosalicylic acid (Fig.1) is used in urine tests to determine urine protein content.



Figure 1: Structure of Sulphosalicylic acid.

Thermophysical properties of solutions with different composition and temperatures provide useful information concerning solute-solute and solute-solvent interaction in solutions and effect of cosolute on drug–solvent interactions.<sup>[5-7]</sup> Water is universal solvent and most of biochemical reaction occurs in aqueous medium. Drug–water interactions and their temperature dependence play a vital role in finding the drug action across the biological membrane.<sup>[8]</sup> Solvation behaviour of biologically important drug molecules in solution has significant role to understand the activity of drug in living system. Drug-solvent, drug-drug and drug-cosolute interactions can be altered by additives such as salt, carbohydrate, amino acid, ionic liquid, surfactant and different solvent. Moreover, drug–solvent interactions also differ with concentration and temperature of solution.<sup>[9-12]</sup> All living organism, carbohydrates located at cell surface, are importance as receptors for the biologically active structures of enzymes, antibodies, hormones and viruses etc. D-mannose (Fig. 2) is monomer sugar unit of aldohexose series of carbohydrate and associated with hereditary disorders of glycosylation.<sup>[13]</sup> It is present in glycoconjugates of protein and used to synthesis of mammalian glycoprotein<sup>[14]</sup>, distributed throughout the body.<sup>[15]</sup>



Figure 2: Structure of D-mannose.

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Present article, we have measured density (p), ultrasonic velocity (u) and refractive index (n) of (0.02, 0.04, 0.06, 0.08 and 0.1) mole·kg<sup>-1</sup> sulphosalicylic acid drug in (0.025, 0.050 and 0.100) mol·kg<sup>-1</sup> D-mannose solutions have been performed at temperature 30<sup>o</sup>C. Using the experimental data we have been calculated the different derived physical parameters. The results are interpreted in terms of ion-ion/hydrophilic, ion-hydrophobic interactions and structure breaking/making tendency of sulphosalicylic acid drug in D-mannose solutions. According to literature survey, density and ultrasonic sulphosalicylic acid in aqueous D-mannose at this concentration are not reported.

## **MATERIALS AND METHODS**

Sulphosalicylic acid (Thermo Fischer Scientific India Pvt. Ltd. with Minimum assay 99%) and D-mannose (Thermo Fischer Scientific India Pvt. Ltd. with Minimum assay 99%) was used for the experiment. Double distilled water was used for the preparation of all solutions. Solutions were prepared and keep in airtight stopper bottles. Density measurements were performed using single capillary pycnometer having bulb capacity 10 cm<sup>3</sup> volume. Pycnometer was calibrated at experimental temperature using tripe distilled water. Weighing was done on single pan electronic balance ( $\pm 0.0001g$ ).

Ultrasonic velocity (*u*) was measured using thermostatically controlled ultrasonic interferometer (Model-F05, Mittal, 2 ±0.0001 MHz). Refractive index measurements were performed on thermostatically controlled Cyber LAB-Cyber Abbe refractometer (Amkette Analytics, ±0.0002, 1.3000 to 1.7000). Refractometer was calibrated using standard specimen (*n*=1.5167). Averages of three readings of density and refractive index are reported.

#### Theoretical

From experimental density of solution (p), refractive index (n) and ultrasonic velocity (u) and acoustical properties like apparent molar volume ( $V_{2,\phi}$ ), isentropic compressibility ( $K_s$ ), apparent molar isentropic compressibility ( $\kappa_{s,2,\phi}$ ), specific acoustic impedance (z) and atomic polarization ( $P_a$ ) are calculated using following equations (1-8)

$$V_{2,\phi} = \frac{M_2}{\rho} + \frac{1000}{m\rho\rho_0} (\rho_0 - \rho)$$
(1)

$$V_{2,\phi} = V_{2,\phi}^o + S_v c^{1/2} \tag{2}$$

$$\Delta_{t} V_{2,\phi}^{o} = V_{2,\phi}^{o}(aq.solution) - V_{2,\phi}^{o}(H_{2}O)$$
(3)

$$\kappa_s = \frac{1}{u^2 \rho} \tag{4}$$

$$\kappa_{s,2,\phi} = \frac{1000(\kappa_s \rho_o - \kappa_o \rho)}{m \rho \rho_o} + \frac{M \times \kappa_s}{\rho}$$
(5)

$$\kappa_{S,2,\phi} = \kappa_{S,2,\phi}^0 + S_k c^{1/2}$$
(6)

$$\Delta_t \kappa^0_{S,2,\phi} = \kappa^0_{S,2,\phi}(aq.solutions) - \kappa^0_{S,2,\phi}(H_2O)$$
(7)

$$Z = u\rho \tag{8}$$

Where,

 $V_{2,\phi}$  = apparent molar volume  $p_0$  = density of solvent in which solutions are prepared (g·cm<sup>-3</sup>)  $p \square \square$  density of experimental solution (g·cm<sup>-3</sup>)  $M_2$ = molar mass of solute (drug) and c= molar concentration of solution (mol·dm<sup>-3</sup>). m= molal concentration of drug solution,  $V_{2,\phi}^o$  = limiting infinite dilution apparent molal volume and  $S_v$ = experimental slope which represents solute-solute interactions.  $\Delta_i V_{2,\phi}^o$  = Partial molar volume of transfer,  $V_{2,\phi}^o$  (Aq. solution) = Partial molar volume in aqueous-alcoholic solution and  $V_{2,\phi}^o$  (H<sub>2</sub>O) = Partial molar volume in water. The  $\kappa_{s,2,\phi}^0$ , and experimental slope  $S_k$  are interpreted in terms of solute-solvent and solute-solute interactions respectively.

## **RESULTS AND DISCUSSION**

# **Volumetric properties**

The experimental density values of sulphosalicylic acid (SSA) drug at different concentrations in aqueous D-mannose solutions at 30<sup>o</sup>C are presented in figure 3. Density of studied system increases with increase in the sulphosalicylic acid concentration due to shrinkage in the volume and association which suggested effective solute-solute/solvent interactions in solution. Apparent molar volumues ( $V_{2\phi}$ ) of SSA solutions were calculated from the density data using equation (1). Apparent molar volumes are positive and increases with drug concentration in each system which suggested that strong solute-solvent interactions between sulphosalicylic acid drug and D-mannose.

The partial molar volume  $(V_{2\phi}^{o})$  of solute was calculated from Massons equation (2).  $V_{2\phi}^{o}$  is apparent molar volume at infinite dilution and useful tool for measure the solute-solvent interactions, whereas, the experimental slope  $(S_V)$  provides the quantitative estimation of the solute-solute interactions. The partial molar volumes of studied system are listed in Table 2. The positive values of  $V_{2,\phi}^o$  was obtained for the SSA in aqueous D-mannose solution and increases with an increasing in the concentration of SSA as well as D-mannose and observed  $V_{2,\phi}^o$  values suggested that hydrophilic-hydrophilic interactions are dominant than hydrophobic-hydrophobic interactions. The positive  $S_V$  values of SSA in aqueous D-mannose solution, which signifies that, the strong solute-solute interactions between hydrophilic part of SSA and hydrophilic groups of D-mannose. The partial molar volume transfer ( $\Delta_t V_{2,\phi}^o$ ) has been calculated by using equation (3). The  $\Delta_t V_{2,\phi}^o$  values are shown in Table 2 for system containing SSA in aqueous D-mannose solution. According to the co-sphere overlap model, an overlap of co-sphere of two ionic species cause increase in volume, whereas overlap of hydrophobic-hydrophobic groups results in the volume decrease. Positive  $4V_{2,\phi}^o$  values and increase with an increasing in the concentration of D-mannose indicates that strong hydrophilic interactions of solute and cosolute because these contain polar and hydrophilic groups.

### **Acoustic properties**

Experimental ultrasonic velocity and related acoustic properties of solutions are useful to understand the solute-solute, solute-solvent interaction and solvation behavior of solution. The values of ultrasonic velocity for studied system at  $30^{\circ}$ C which is shown in figure 5. Ultrasonic velocity of solution increases with increasing concentration of sulphosalicylic acid as well as aqueous D-mannose solution at  $30^{\circ}$ C. The isentropic compressibility ( $K_s$ ) of SSA in 0.025, 0.050 and 0.10 mol·kg<sup>-1</sup> aqueous D-mannose solution at 30<sup>o</sup>C calculated from ultrasonic velocity data by using equation (4). The graphical representation of  $K_s$  of the SSA in aqueous D-mannose solutions at  $30^{\circ}$ C is reported in figure 7. The values  $K_s$  decrease with increase in concentration of sulphosalicylic acid as well as the concentration of aqueous Dmannose solution at  $30^{\circ}$ C. The K<sub>s</sub> values decrease with increase the concentration of Dmannose solution may indicate that the hydrophilic-hydrophilic and hydrophilic-hydrophobic interaction occurs. The apparent molar isentropic compressibility  $\kappa_{s,2,\phi}$  of SSA solutions was calculated from the density and ultrasonic velocity data using equation (5). They are negative and increases with drug concentration in each system. The negative values of  $\kappa_{s,2,\phi}^0$  are attributed to the strong drug-solvent interactions in the solution. The magnitude of the  $\kappa_{s_2,\phi}^0$ value is a measure of solute-solvent interactions, at infinite dilution there is no significance

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solute-solute interaction. The  $S_k$  values (experimental slopes) obtained from the plots of concentration dependence of  $\kappa_{S,2,\phi}^0$  are found to be positive which suggests that their existence of hydrophilic-hydrophilic interactions along with the solute-solvent interactions.  $\Delta_t \kappa_{S,2,\phi}^0$  values are reported in Table 3. Negative  $\Delta_t \kappa_{S,2,\phi}^0$  values observed and increase with increasing in the concentration of solute from Table 3 which indicates that ion/hydrophilic-hydrophilic interactions.



Figure 3: Variation in the density of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C.



Figure 4: Variation in the refractive index of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C.



Figure 5: Variation in the ultrasonic velocity of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C.



Figure 6: Variation in the apparent molar volume of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C.



Figure 7: Variation in the isentropic compressibility of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C



Figure 8: Plots of specific acoustic impedance with concentration of Sulphosalicylic acid + aqueous D-mannose at 30°.



Figure 9: Variation in the atomic polarization of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C.



Figure 10: Variation in the apparent molar isentropic compressibility of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C.

Table 1: The  $n_D^0$  and constant *K* obtained from plot of  $n_D$  vs. *c* of solutions containing Sulphosalicylic acid + aqueous D-mannose at 303.15 K.

System	$n^0_{\rm D}$	K	$R^2$
Water	1.3307	0.0320	0.9961
0.025M aq. D-mannose	1.3332	0.046	0.9851
0.050M aq. D-mannose	1.3341	0.050	0.9929
0.100 M aq. D-mannose	1.3349	0.050	0.9952

Foot Note: K,=dm<sup>3</sup>·mol<sup>-1</sup>.

Table 2: The  $V_{2,\phi}^{o}$ ,  $S_{v}$  and  $\Delta V_{2,\phi}^{o}$  values of solutions containing Sulphosalicylic acid +

# aqueous D-mannose at 303.15 K.

$V^{o}_{2,\phi}$	$S_{v}$	$\Delta V^o_{2,\phi}$
156.77	15.59	0.00
160.23	8.52	3.46
160.87	9.36	4.10
161.57	8.39	4.80
	$\frac{V^o_{2,\phi}}{156.77}\\ 160.23\\ 160.87\\ 161.57$	$\begin{array}{c c} V^o_{2,\phi} & {\pmb{S}}_{\pmb{v}} \\ \hline 156.77 & 15.59 \\ \hline 160.23 & 8.52 \\ \hline 160.87 & 9.36 \\ \hline 161.57 & 8.39 \\ \hline \end{array}$

Foot Note:  $V_{2,\phi}^{o} = \operatorname{cm}^{3} \cdot \operatorname{mol}^{-1}$ ,  $S_{v} = \operatorname{cm}^{3} \cdot \operatorname{mol}^{-3/2} \cdot \operatorname{kg}^{1/2}$ .

Table 3: The  $\kappa_{S,2,\phi}^0$ ,  $S_k$  and  $\Delta_t \kappa_{S,2,\phi}^0$  values of solutions containing Sulphosalicylic acid + aqueous D-mannose at 30°C.

System	$\kappa^0_{S,2,\phi}$	Sk	$\Delta_t \kappa^0_{S,2,\phi}$	
Water	-5.76	1.56	0.00	
0.025M aq. D-mannose	-5.21	0.99	-0.55	
0.050M aq. D-mannose	-4.77	1.16	-0.99	
0.100 M aq. D-mannose	-4.46	1.05	-1.30	
$-14$ $3$ $-1^{-1}$ D $-1$ C $10^{-14}$ $3$ $-1^{-3/2}$ L $-1/2$ D $-1$				

Footnote:  $\kappa_{s,2,\phi}^{0} = \times 10^{-14} \text{ m}^{3} \cdot \text{mol}^{-1} \cdot \text{Pa}^{-1}, S_{k} = \times 10^{-14} \text{ m}^{3} \cdot \text{mol}^{-3/2} \cdot \text{kg}^{1/2} \cdot \text{Pa}^{-1}.$ 

The specific acoustic impedance (*Z*) was calculated by using equation 8, the graphical representation of specific acoustic impendence with concentration of SSA in aqueous D-mannose solution at  $30^{\circ}$ C in figure 8. The value of *Z* increases with increasing the concentration of SSA as well as the concentration aqueous D-mannose.

# **Refractive Indices**

The graphical representation of refractive indices with Sulphosalicylic acid concentration in aqueous D-mannose solutions is presented in Figure 4. Refractive indices increase with the concentration of SSA as well as aqueous D-mannose solution. The increasing trends of n which indicate that the increasing compactness of solution due increasing the interaction between solute and solvent. Atomic polarization of sulphosalicylic acid in different

concentration of aqueous D-mannose solution at  $30^{\circ}$ C has been calculated by using the equation 9 which are shown in figure 9. The values  $P_a$  of studied system increase with an increasing concentration of sulphosalicylic acid and aqueous D-mannose solution.

# CONCLUSION

- Experimental density, refractive index and ultrasonic velocity measurement for Sulphosalicylic acid in aqueous D-mannose solution at constant temperature have been studied.
- The apparent molar volume, compressibility and transfer properties have been computed from experimental properties.
- > The positive  $V_{2,\phi}^{o}$  values suggested the existence of solute-solvent interactions.
- > The positive  $(\Delta_{V_{2,\phi}^o})$  values indicate that hydrophilic-hydrophilic interactions overcome hydrophobic-hydrophobic interactions in the solution.
- > The negative  $\Delta_t \kappa_{S,2,\phi}^0$  values were observed for the studied solutions. The refractive index data shows linear dependence over the drug concentration at constant temperatures, which is well in accordance with the data obtained from volumetric and acoustical study.

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