



Evaluation of Acoustical Parameters of Aqueous Solution of 5-Sulphosalicylic Acid

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Abstract

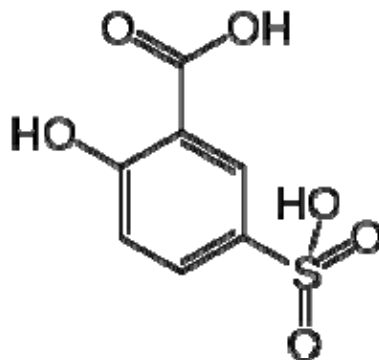
The ultrasonic studies are extensively used in the conformational analysis of organic molecules. These are also used for the determination of molecular interactions in the liquids which provide valuable information about the behavior of liquids and solutions. In the present work, attempts have been made to investigate the behavior of 5-sulphosalicylic acid in water at various concentrations and also at different temperatures. The ultrasonic velocity, viscosity and density are measured experimentally. In order to get more information on the nature and strength of molecular interaction, we have calculated the other related acoustical parameters such as adiabatic compressibility, intermolecular free length, Rao's constant, Wada's constant, free length, relaxation time and acoustical impedance. The non linear variation of these derived acoustical parameters with different concentration of the solute is explained on the basis of structural changes occurring in a solution.

Keywords: Ultrasonic waves, Molecular Interaction, Intermolecular free length, Rao's constant(R), and Wada's constant(W).

Introduction:-

Ultrasonic studies in the aqueous solutions of various drugs yield information about the nature of molecular interactions as observed by various researchers¹⁻¹⁰. In many industrial applications, liquid mixtures rather than single component liquid system, are used in processing and product formulations¹¹⁻¹². Liquid mixtures consisting of polar and non-polar components are of considerable importance in petrochemical, pharmaceutical and dye industries.

A commercial use of salicylic acid and its derivatives like 5-sulphosalicylic acid are widely used to synthesize different antibiotic drugs. An exhaustive survey of literature reveals that studies on the use of acoustic and volumetric properties and their excess functions in order to understand molecular interactions in binary liquid mixtures of 5-sulphosalicylic acid and water have not been studied so far. Hence adiabatic compressibility, molar free volume, intermolecular free length, relaxation time and other parameters have been calculated at three temperatures at an interval of 5⁰C for 298K, 303K and 308K. Sound velocity, viscosity and density are measured at 4MHz frequency and different ultrasonic parameters have been calculated with a view to investigate the exact nature of the molecular interactions.¹³⁻¹⁴



2-Hydroxy-5-Sulpho-Benzoic Acid

Experimental Section:

Materials:-

Analytical Range (AR) 5-sulphosalicylic acid is used in the present work. The solutions were prepared by using double distilled water as a solvent. The concentration range selected 5-sulpho salicylic acid is 0.1M, 0.01M and 0.001M.

Methods:-

All the weighing was done on digital electronic balance Model - CB/CA/CT-Series Contech having accuracy ± 0.0001 g. The sound speed was measured by using ultrasonic multifrequency Interferometer (Model-M-83) supplied by Mittal Enterprises, New Delhi operating at 4 MHz frequency with an accuracy of ± 2 m/s. The viscosities (η) of solution and solvent were determined by using Ostwald's viscometer by calibrating with double distilled water. The densities (d_s) of the solutions were measured accurately using digital densitometer (Model - DMA-35, Anton Paar). The experimentation is carried out at three different temperatures viz. 298K, 303K and 308K so as to study the comparative interactions¹⁵⁻¹⁶.

Results And Discussion:

The experimentally measured values of density, viscosity and sound speed of solutions of sodium salicylate in water at 298K, 303K and 308K are given in **Table 1**.

The acoustical parameters were calculated from v , η and d values using standard formulae, and given in **Table 2-4**.

- | | | | |
|--------------------------------|---|----------------------------------------------------------------------------|----------|
| 1) Adiabatic Compressibility | - | $\beta = 1/v^2 d_s$ | ...(1) |
| 2) Intermolecular free length | - | $L_f = K \sqrt{\beta_s}$ | ...(2) |
| 3) Specific acoustic impedance | - | $Z = v_s \cdot d_s$ | ...(3) |
| 4) Rao's Constant | - | $R = (M_{eff}/d_s) \times v^{1/3}$ | ...(4) |
| 5) Wada's Constant | - | $W = (M_{eff}/d_s) \times \beta^{-1/7}$ | ...(5) |
| 6) Relative Association | - | $R_A = d_s / d_o [v_o / v_s]^{1/3}$ | ...(7) |
| 7) Relaxation time | - | $\tau = 4/3 \beta \times \eta$ | ...(8) |
| 8) Free Volume | - | $V_f = M_{eff} \times v_s / k \times \eta$ |(9) |
| | | $k = 4.28 \times 10^9$, Temperature Independent Constant for all liquids. | |
| 9) Equivalent Conductance | - | $\lambda = Kc[1000/N]$ |(10) |



Table 1: Density, Velocity and Viscosity at 298, 303, 308 K (At Frequency-4MHz)

Sr.No.	Temperature (^o K)	Concentration (M)	Density (d _s) (Kg/m ³)	Velocity (v _s) (m/s)	Viscosity (□) X 10 ⁻⁰⁴ (Pa.S.) or Kg m ⁻¹ s ⁻¹
1	298	0.1	1007.2	4004.40	9.59
2		0.01	0999.7	4647.80	9.13
3		0.001	0998.0	5503.18	8.86
4	303	0.1	1006.9	3903.12	8.85
5		0.01	0998.8	4460.23	8.49
6		0.001	0997.7	5350.18	8.18
7	308	0.1	1006.3	3802.10	8.08
8		0.01	0998.3	4380.03	7.86
9		0.001	0997.3	5120.06	7.64

Table 2 Adiabatic Compressibility, Acoustic impedance and Free length at 298, 303, 3080 K.

Sr. No.	Temperature (^o K)	Concentration (M)	Adiabatic Compressibility (β _s x 10 ⁻¹¹)Pa ⁻¹	Acoustic Impedance Z (Kgm ⁻² S ⁻¹)	Free length Lf X 10 ⁻¹¹ m
1	298	0.1	6.19	4033232	1.55
2		0.01	4.63	4646406	1.34
3		0.001	3.31	5492174	1.13
4	303	0.1	6.52	3930052	1.6
5		0.01	5.03	4454878	1.4
6		0.001	3.5	5337875	1.17
7	308	0.1	6.87	3826053	1.66
8		0.01	5.22	4372584	1.45
9		0.001	3.82	5106236	1.24

Table 3 : Relative association, apparent molar compressibility and relaxation time.

Sr. No.	Temperature (^o K)	Concentration (M)	Relative Association (R _A)	Relaxation Time τ X 10 ⁻¹⁴
1	298	0.1	1.113129	7.92
2		0.01	1.051307	5.64
3		0.001	0.992053	3.91
4	303	0.1	1.143218	7.69
5		0.01	1.084691	5.69
6		0.001	1.019742	3.82
7	308	0.1	1.177727	7.41
8		0.01	1.114535	5.47
9		0.001	1.056961	3.9



Table 4 : Rao’s Constant, Wada’s Constant, Free volume and Equivalent conductance.

Sr. No.	Temperature (°K)	Concentration (M)	Rao’s Constant (R)×10 ⁻³	Wada’s Constant (W)×10 ⁻³	Free Volume (Vf) ×10 ⁻²	λ=Kc*(1000/N) mhos eq.
1	298	0.1	1.58	2.85	3.05	347
2		0.01	1.66	2.99	4.09	531
3		0.001	1.76	3.13	5.49	1300
4	303	0.1	1.56	2.83	3.30	388
5		0.01	1.64	2.95	4.28	601
6		0.001	1.75	3.11	5.94	1420
7	308	0.1	1.55	2.81	3.64	411
8		0.01	1.63	2.94	4.67	654
9		0.001	1.72	3.07	6.15	1630

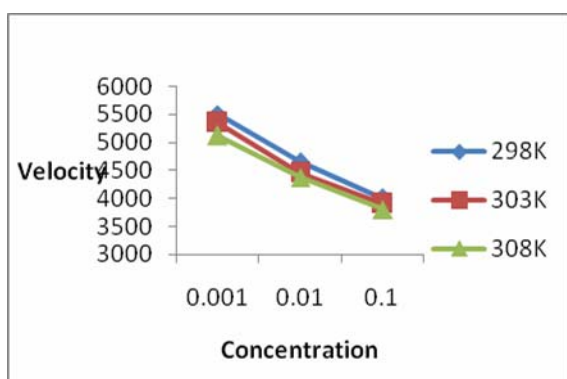


Fig-1. Ultrasonic velocity Vs Conc.

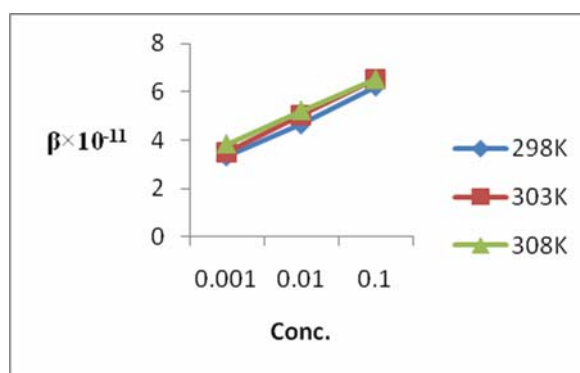


Fig-2. Adiabatic comp. Vs Conc.

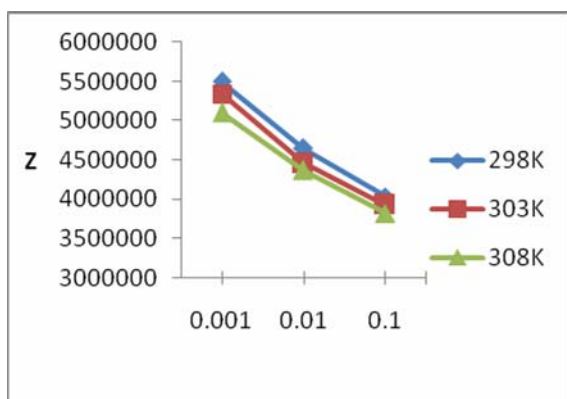


Fig-3. Acoustiv Impedance Vs Conc.

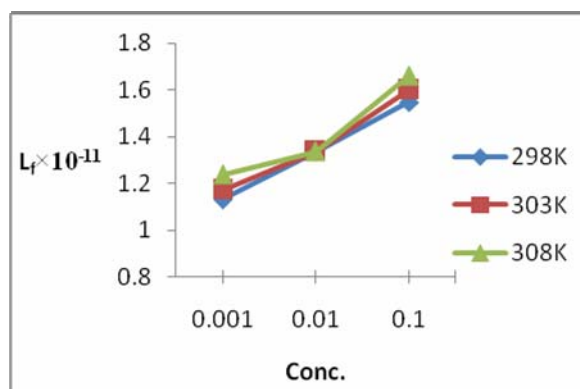


Fig-4. Free Length Vs Conc.

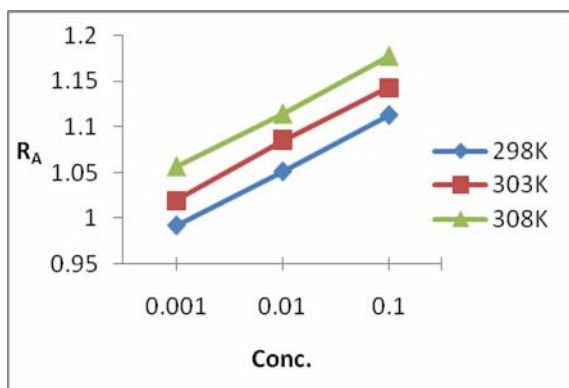


Fig-5. Relative association Vs Conc.

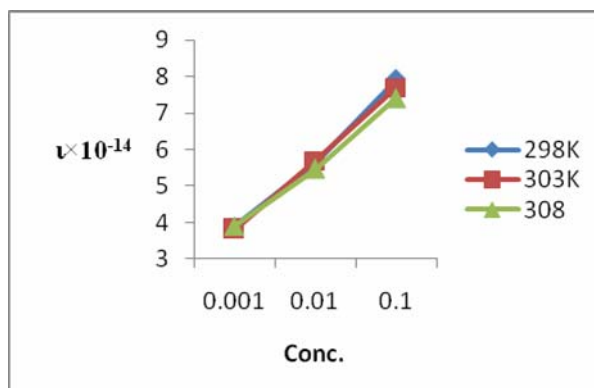


Fig-6. Relaxation time Vs Conc.

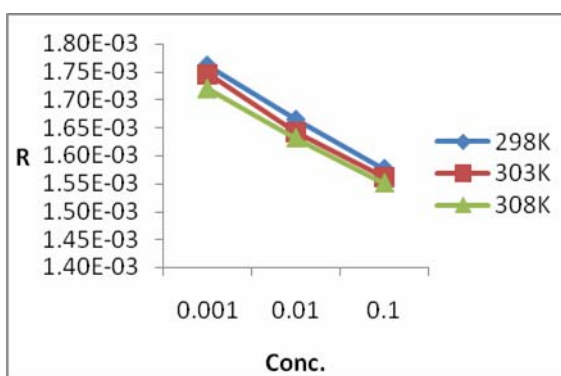


Fig-7. Rao's Constant Vs Conc.

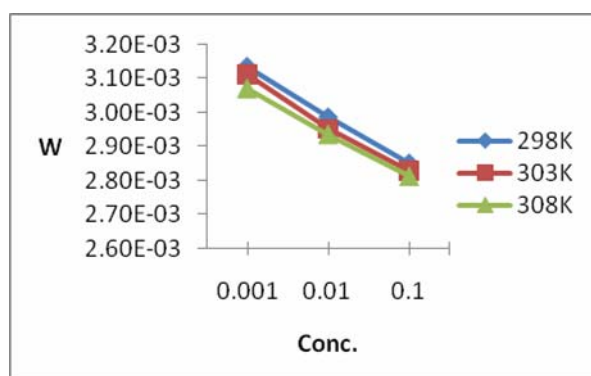


Fig-8. Wada's Constant Vs Conc.

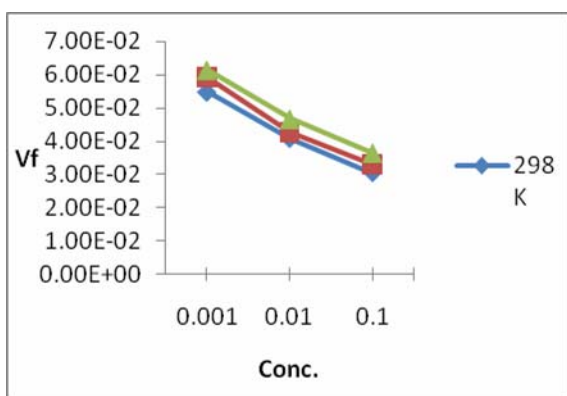


Fig-9. Free Volume Vs Conc.

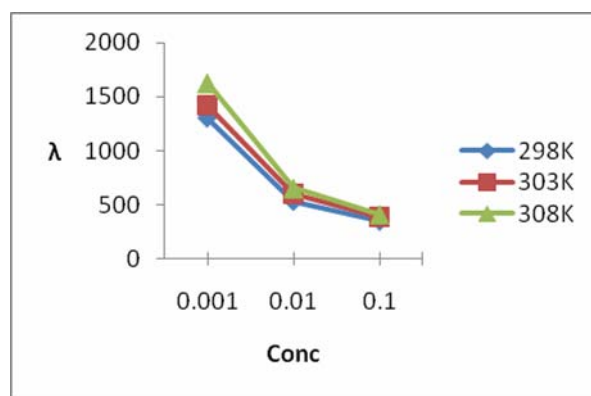


Fig-10. Equi. Conductance Vs Conc.

The variation in ultrasonic velocity in any solution generally indicates molecular association in it. It is seen from the **Table 1 and Fig. 1** that the ultrasonic velocity decreases with increase in concentration. This is due to the formation of more hydrogen bonds with increase in concentration as a result of solute-solvent interactions¹⁷. It is also observed from **Table 1** that the density increases with an increase in the concentration of the solution. This may be attributed to the shrinkage in the volume which in turn is due to the presence of the solute. In other words, the increase in density may be interpreted due to the enhanced structure of the solvent mixture due to added drug¹⁸. It is further seen from the **Table 1** that



viscosity values increase with increase in concentration of 5-sulpho salicylic acid. When solute is dissolved in a solvent, some of the solvent molecules are attached to the solute as a result of solute-solvent interaction and the viscosity of solution increases. Generally the increase in viscosity of the solution on addition of solute indicates the structure making aspect of solutes¹⁹. The viscosity values of the solutions decreases with an increase in temperature. The increase in temperature may have caused the increase in the kinetic energy of molecules and ion present in the solution, which in turn, decreases the solute-solvent interactions²⁰.

Free volume is generally expressed as the effective volume in which the centre of molecule can move when all the other molecules are held fixed at their mean position. **Table 4 and Fig. 9** show that free volume decreases with increase in concentration of 5-sulphosalicylic acid. The addition of solute in the solution enhances the structural arrangement of the system. The decrease in free volume indicates the decrease in the entropy of the system. This also confirms that the free volume of a molecule at a given temperature and pressure depends upon the internal pressure of the liquid in which it is immersed, as suggested by Hirschfelder and co-workers²¹⁻²².

Table 2 shows the variation of adiabatic compressibility with concentration at different temperatures. The decrease in adiabatic compressibility show there is a significant molecular interaction at higher concentration. The trend in intermolecular free length with concentration (**Fig. 4**) is similar to the trend in adiabatic compressibility. The increase in free length signifies weak molecular interaction and decrease in length signifies specific interaction. The increase in free length with increase in velocity indicates the presence of significant interactions between solute and solvent molecules due to which the structural arrangement in the neighborhood of constituent ions are considerably affected. The values of intermolecular free length at different concentrations and at different temperatures are represented in **Table 2**. The variation of Rao's constant and Wada's constant with molar solutions of 5-sulphosalicylic acid in water are represented in Table-4. From the **Table 4 and Fig. 7 and 8**, it is observed that non linear variation of Rao's constant and Wada's constant indicates significant molecular interactions between molecules. The equivalent conductance values are found to be decreasing for increase in concentration while increasing for increase in the temperature as expected. These values are given in **Table 4** and shown in **Fig. 10**. Acoustical impedance (z) shows a trend similar to ultrasonic velocity (**Table 2**) at 298K, 303K and 308K, acoustic impedance increases (**Fig. 3**). This increase in acoustic impedance shows that the molecular interactions in these solutions are associative²³.

Acoustical relaxation time (τ) is found to decrease with increase in temperature and varies with concentration shown in **Table 3**. A comparative study of adiabatic compressibility and acoustical relaxation time indicate that the variations in acoustical relaxation time are mainly due to the changes in the viscosity of the solution due to both concentration and temperature (**Fig. 6**).



Relative association (R_A) (Table 3 and Fig. 5) shows a general increase with increase in temperature. It is found to be nearly equal to unity and variations in its values indicates molecular interactions.

Conclusion:-

Thermodynamical parameters like free volume, intermolecular free length, adiabatic compressibility etc were estimated for 5-sulphosalicylic acid in aqueous media at three different temperatures and related to the strength of interactions between solute and solvent molecules. Further the solute (drug) acts as a structure maker in the solvent complimenting the results obtained from partial molar volumes (V^0_ϕ), viscosity coefficients which were reported in details²⁴.

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