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Research Article

Identification of molecular-interactions using ultrasonic studies of sodium-2-hydroxy benzoate solutions

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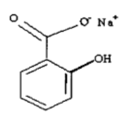
Abstract

The molecular interaction behavior of analgesic and antipyretic drug Sodium 2-hydroxy benzoic acid with particular emphasize on its intermolecular interaction was studied using ultrasonic technique at 4 MHz frequency at three different concentrations 0.1M, 0.01M, 0.001M. Ultrasonic velocity, viscosity, and density were measured at three different temperatures 298K, 303K and 308K. Different interaction parameters like adiabatic compressibility, Intermolecular free length, Specific acoustic impedance, Rao's Constant, Wada's Constant, Apparent Molar Compressibility, Relative Association, Relaxation time, Free Volume etc have been calculated using the experimental values of density, viscosity and ultrasonic velocity of aqueous solution of sodium 2-hydroxy benzoic acid. Results are interpreted in terms of solute-solvent interactions. The ultrasonic velocity, adiabatic compressibility, free length and viscosity with concentration for all the systems vary regularly without showing any maxima or minima and thereby corroborating the nonexistence of any complex formation. In these systems, the magnitude of the excess acoustical parameters values inferred the solute-solvent interactions in the system. This interaction may be due to rupture of hydrogen bonds via dissociation or dilution that occurs between the water molecules.
Keywords: Ultrasonic Velocity, Adiabatic compressibility, Apparent Molar Compressibility, free volume, Relaxation time

1. Introduction

The propagation of ultrasonic waves in liquid is a tool used by researcher to probe into the properties of liquids[1-3]. One can study the physical and chemical behavior of solutions and their molecular interaction by measuring the density, viscosity and ultrasonic velocity. Measurement of these parameters with respect to different concentration and temperature will help to determine the acoustic parameters such as adiabatic compressibility, intermolecular free length, specific acoustic impedance, Rao′s constant, Wada′s constant. The free volume is the average volume in which the centre of the molecule can move inside, enclosed by its neighbors. The free volume plays an important role in the propagation of ultrasonic waves in the liquid mixtures[4].

It is found in the literature survey that ultrasonic study of liquid mixtures is highly useful in understanding the nature of molecular interaction[5]. Ultrasonic studies in aqueous solutions of various drugs yield information about the nature of molecular interactions as observed by several researchers[6]. In the present paper, solution of sodium salt of salicylic acid is used to study by passing ultrasound waves in the solution at 4 MHz frequency. Salicylic acid derivatives are widely used in the medicinal field. Sodium salicylate is used in medicine as an analgesic and antipyretic. It is also acts as non steroidal anti inflammatory drug (NSAID) and induces apoptosis in cancer cells[7] and also necrosis[8]. It is also a potential replacement for aspirin for people sensitive to it.



Sodium 2-hydroxybenzoate,

Density, viscosity and ultrasonic velocity were measured for 0.1M, 0.01M and 0.001M Sodium salicylate solution prepared by using distilled water as a solvent. The said measurements were taken at 298K, 303K and 308K. The acoustic and thermodynamic parameters are determined for the sodium salt of 2-Hydroxy benzoic acid and their molecular interactions are discussed in the paper.

2. Materials and Methods

2.1 Materials: Analytical Range (AR) sodium salicylate is used in the present work. The solution was prepared by using double distilled water as a solvent. The concentration range selected for sodium salicylate is 0.1M, 0.01M and 0.001M.

2.2 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 ±2m/s. The viscosities (**η**) of solution and solvent were determined by using Ostwald's viscometer by calibrating with double distilled water. The densities (ds) 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 interactions.

3. Statistical Methods: 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 ρ values using standard formulae.

3.1 Adiabatic Compressibility - $\beta = 1/v^2 d_S$ **…(1)**

3.2 Intermolecular free length - $L_f = K\sqrt{\beta_S}$ **…(2)**

3.3 Specific acoustic impedance - $Z = v_s . d_S$ **…(3)**

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3.4 Rao's Constant - $R = (M_{eff}/d_S) \times v^{1/3}$ …(4)

3.5 Wada's Constant - $W = (M_{eff}/d_S) \times \beta^{-1/7}$ …(5)

3.6 Apparent Molar Compressibility - $\Phi_K = [1000 (\beta S\ d_O - \beta_O\ d_S) / m\ d_S\ d_O] + (\beta_S M / d_S)$ …(6)

3.7 Relative Association - $R_A = d_S / d_O [v_o / v_s]^{1/3}$ …(7)

3.8 Relaxation time - $\tau = 4/3\ \beta \times \eta$ …(8)

3.9 Free Volume - $Vf = M_{eff} \times v_s / k \times \eta$ ….(9)

$k = 4.28 \times 10^9$,
Temperature Independent Constant for all liquids.

3.10 Equivalent Conductance - $\lambda = Kc[1000/N]$ ….(10)

The symbols have their usual meaning.

4. Results and Discussion

From **Table 1** and **Fig. 1** it is observed that there is increase in sound speed which is attributed to the formation of hydrogen bonds between sodium salicylate and water[9]. When the ultrasonic energy passes through the medium, part of the energy is used in the weakening of or breaking of O-H---O bonds. Therefore it is very likely that during the compression cycle of ultrasonic wave, hydrogen atoms are pushed closer resulting in a partially irreversible weakening or breaking of hydrogen bonds due to the absorption of energy. The increase in absorption is a characteristic feature of the solutions in which association due to molecular interactions is present[10].

Density is a measure of solvent-solvent and ion solvent interactions. Decrease in density with concentration indicates the decrease of solvent-solvent and solute- solvent interactions. The decrease in density with concentration is due to the shrinkage in the volume, which in turn is due to the presence of solute molecules. In other words, decrease in density is due to structure maker property of the solvent due to added solute.

The values in **Table 2** and **Fig. 2** show the trend of linear increase of specific acoustic impedance with concentration at a given temperature, this is due to increase in the strength of intermolecular attraction. Free length is the distance between the surfaces of the neighboring molecules and variation in free length with concentration and temperature is similar to that of adiabatic compressibility[11] as shown in **Table 2** and **Fig. 4.**

The relative association depends on either the breaking up of solvent molecules or solvation of ions that are present. In the present case relative association decreases which is due to the breaking up of molecule in the solution which also indicates prominent solute-solvent interaction (**Table -3 and fig.5**). Acoustic relaxation time (**τ**) **(Fig.7)** is found to decrease with increase in temperature and varies with changes in concentration. A comparative study of adiabatic compressibility (**Fig. 3** and **Fig. 7**) and acoustical relaxation time indicates that the variations in acoustical relaxation time are mainly due to the changes in the viscosity of the solutions due to both concentration and temperature. The values of acoustical parameters calculated are shown in **table 2 to 4.**

The values of apparent molar compressibility (Φ_K) increase with decrease in concentration **(Table-3 and fig.6)** at the temperature studied which indicates occurrence of solute-solvent interaction.

Properties like Rao's constant and Wada's constant (**Table-4, Fig. 8 and 9**) also show that the values increase with temperature and decrease with decrease of concentration of aqueous solution of sodium salicylate. The linear decrease with concentration in both constants shows the presence of solute-solvent interactions. Linear decrease in R and W suggests the existence of weak interaction.

Free volume is the effective volume in which the centre of a molecule can move when all other molecules are held fixed at their mean positions. **Table 4 and Fig.10** Shows that, free volume increases with decrease in concentration of sodium salicylate. The increase in free volume indicates the increase in entropy of the system.

From the data of **Table 4 and Fig. 11** it is seen that equivalent conductance increases with increase in dilution which indicates that there are free ions responsible for the conductance in the solution.

5. Conclusion

Thermodynamic parameters like free volume, intermolecular free length, adiabatic compressibility etc. were estimated for solution of sodium salt of 2-hydroxy benzoic acid in aqueous media at three different temperatures. The ultrasonic velocity, adiabatic compressibility, free length and viscosity with concentration for all the systems vary regularly without showing any maxima or minima and thereby corroborating the nonexistence of any complex formation. In these systems, the magnitude of the excess acoustical parameters values inferred the solute-solvent interactions in the system. This interaction may be due to rupture of hydrogen bonds via dissociation or dilution that occurs between the water molecules.

Table No. 1. Density, Velocity and Viscosity at 298, 303, 308 K. (At Frequency-4MHz)

Sr. No.	Temperature (^{0} K.)	Concentration (M)	Density(d_S) (Kg/m^3)	Velocity(v_s) (m/s)	Viscosity(η) (Pa.S.) or $Kg\ m^{-1}\ s^{-1} \times 10^{-3}$
1	298	0.1	997	5106.4	1.01334
2		0.01	981.67	5337.6	0.9786
3		0.001	968.5	5520.16	0.9442
4	303	0.1	989.3	4309.2	0.9365
5		0.01	981.5	4888.8	0.8832
6		0.001	967.8	5001.76	0.8204
7	308	0.1	988.8	3603.68	0.8993
8		0.01	980.7	4336	0.8032
9		0.001	967.2	4628	0.7463

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

Sr.No.	Temperature (^{0} K.)	Concentration (M)	Adiabatic Compressibility (β_S x 10^{-10})Pa^{-1}	Acoustic Impedance Z x 10^6($Kgm^{-2}S^{-1}$)	Free length L_f x 10^{-11} m
1	298	0.1	0.3846	5.0910	1.2195
2		0.01	0.3575	5.2399	1.1759
3		0.001	0.3388	5.3462	1.1441
4	303	0.1	0.5443	4.2630	1.4603
5		0.01	0.4262	4.7983	1.2926
6		0.001	0.4130	4.8407	1.2724
7	308	0.1	0.7787	3.5632	1.7660
8		0.01	0.5423	4.2523	1.4738
9		0.001	0.4827	4.4762	1.3904

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

Sr. No.	Temperature (^{0} K.)	Concentration (M)	Relative Association (R_A)	Apparent Molar Compressibility (Φ_k X 10^{-10})	Relaxation Time τ x 10^{-14}
1	298	0.1	1.0386	0.0575	5.1962
2		0.01	1.0077	0.1193	4.6657
3		0.001	0.9831	16.1166	4.2652
4	303	0.1	1.1111	2.2935	7.0058
5		0.01	1.0569	10.2914	5.0176
6		0.001	1.0342	97.1499	4.5166
7	308	0.1	1.2277	6.0480	9.3347
8		0.01	1.1448	35.8587	5.8067
9		0.001	1.1048	303.6851	4.8021

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

Sr. No.	Temperature (^{0} K.)	Concentration (M)	Rao's Constant (R)×10^{-3}	Wada's Constant (W)×10^{-3}	Free Volume (V_f) ×10^{-6}	Equivalent Conductance (λ) mhos
1	298	0.1	1.6849	3.0088	1.2307	77.8
2		0.01	1.7365	3.0876	1.3859	223
3		0.001	1.7799	3.1536	1.5380	2180
4	303	0.1	1.6005	2.8781	1.0700	83.7
5		0.01	1.6852	3.0088	1.4150	248
6		0.001	1.7225	3.0659	1.6362	2300
7	308	0.1	1.5056	2.7302	1.1438	94.2
8		0.01	1.6143	2.8984	1.3551	260
9		0.001	1.6712	2.9854	1.6660	2400

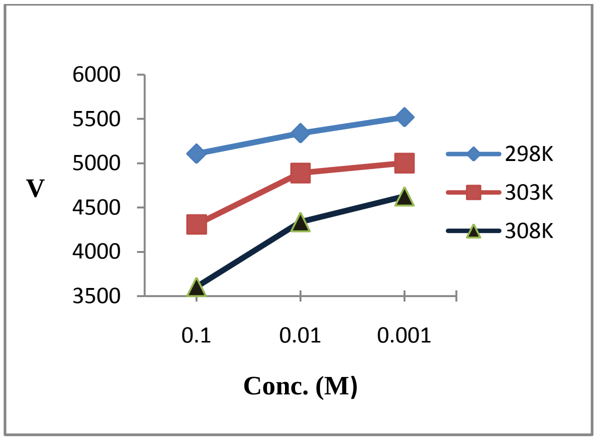

Fig-1.Ultrasonic velocity Vs Conc.

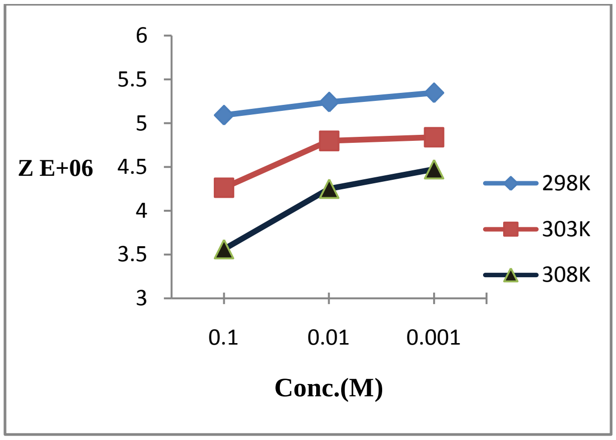

Fig-2.Acoustic impedance Vs Conc.

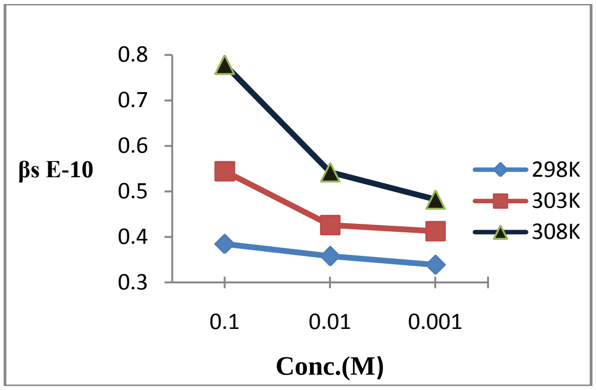

Fig-3. Adiabatic Compressibility Vs Conc.

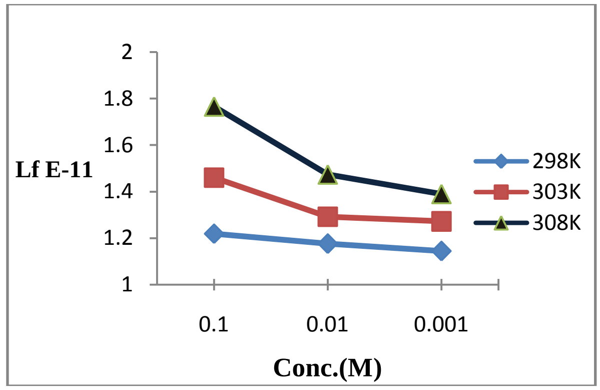

Fig-4. Free length Vs Conc.

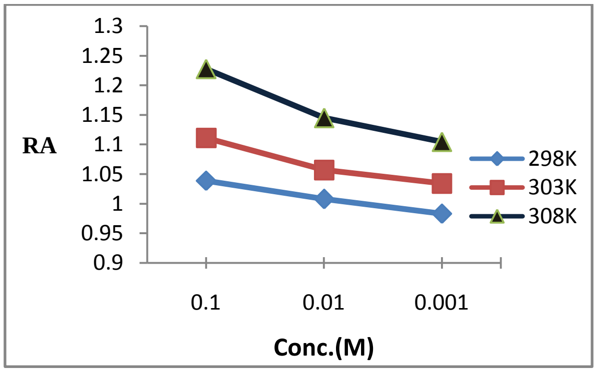

Fig-5. Relative Association Vs Conc.

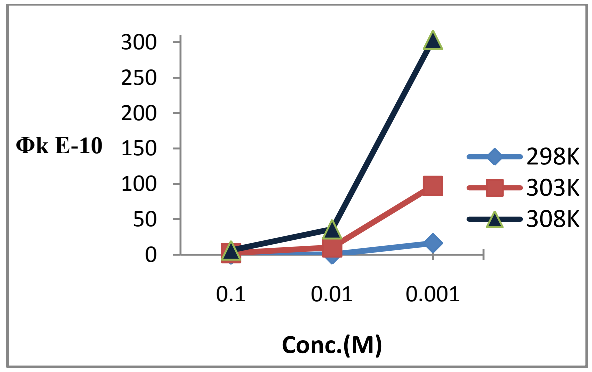

Fig-6. Apparent Molar Compressibility Vs Conc.

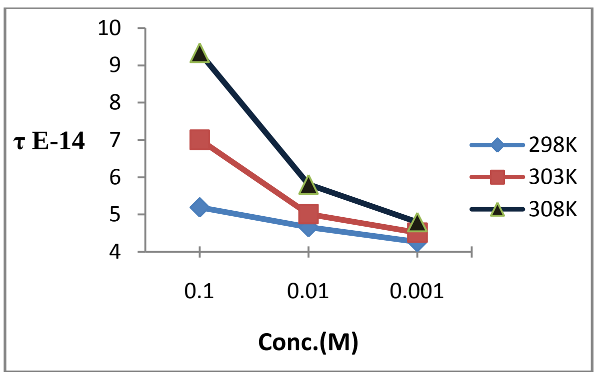

Fig-7. Relaxation Time Vs Conc.

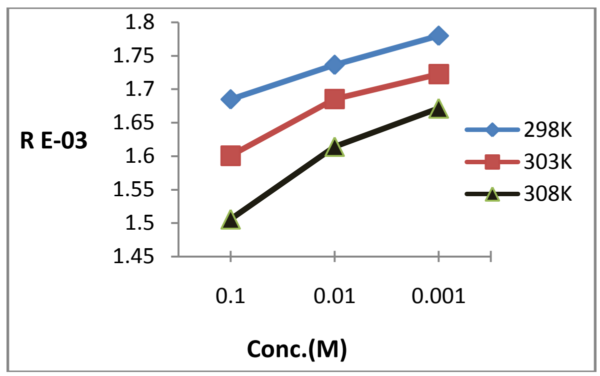

Fig-8. Rao's Constant Vs Conc.

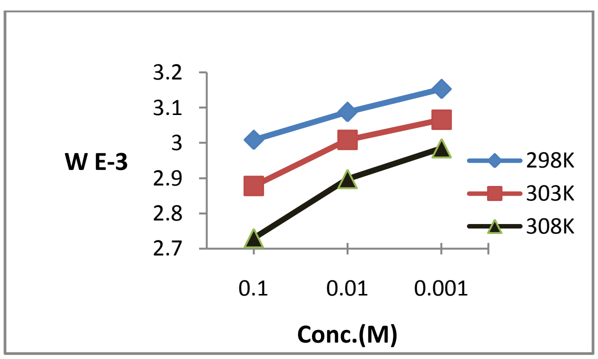

Fig-9. Wada's Constant Vs Conc.

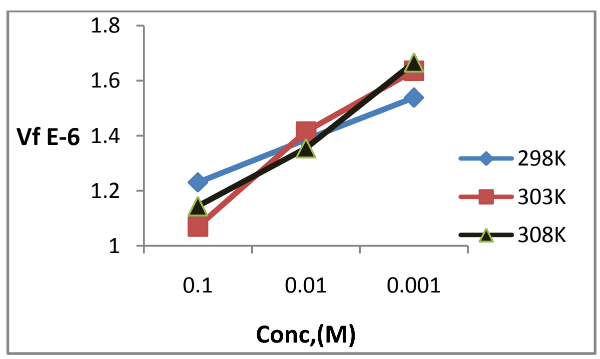

Fig-10. Free Volume Vs Conc.

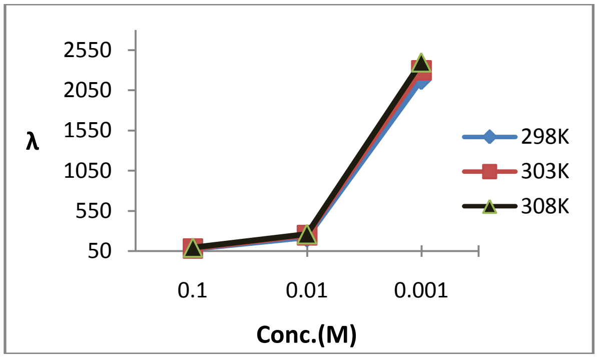

Fig-11. Equivalent Conductance Vs Conc.

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