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Investigation of Type of Interaction between Salicylic Acid and Ethanol at Different Temperatures

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ABSTRACT

The study of ultrasonic velocity leads to a better understanding of the nature of interactions between the solute and solvent. Density, viscosity and ultrasound velocity have been determined over the complete concentration range for binary liquid mixture of salicylic acid and ethanol. These data provide useful information about various types of interactions occurring in the solution. The derived acoustic parameters like adiabatic compressibility, intermolecular free length, specific acoustic impedance etc. Have been calculated from experimental data. The sign and magnitude of these properties have been used to interpret the experimental results in terms of molecular interactions.

Keywords- Ultrasound velocity, Density, Viscosity, Salicylic acid and Ethanol.

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INTRODUCTION

Knowledge of densities, viscosities and ultrasound velocity of liquid mixture is important to understand the molecular interactions between salicylic acid and ethanol to develop new theoretical models and also for engineering applications [1,2,10,12,16,17]. The behavior of these parameters suggests positive solute solvent interactions in the present system and solute acts as structure maker in the binary system. Salicylic acid is a mildly acidic organic molecule that can be derived from salicin, a compound found in the bark of the white willow tree and it is an effective drying and disinfecting agent [4,18]. The investigations regarding the molecular association in organic binary mixtures having ethanol group as one of the components is of particular interest, since ethanol group is highly polar and can associate with groups having some degree of polar attractions. The present work provides useful information in medical and pharmaceutical chemistry for the prediction of solute-solvent interaction. Ultrasound velocity. Density and viscosity of binary liquid mixture of salicylic acid with ethanol have been determined at 30°C, 35°C and 40°C. The data obtained during the study is used for determining the most significant acoustic parameters like adiabatic compressibility, specific acoustic impedance, intermolecular free length and shear's relaxation time. These parameters explore solute – solvent interactions in ethanol at different temperatures.

MATERIALS AND METHODS

The chemicals used in the present work were analytical reagent (AR) grade. Liquid mixtures of various compositions of salicylic acid in ethanol were prepared by mass in a 25cm^3 flask using a matter analytical balance. Density and viscosity measurements were carried out using a thermostatically controlled well-stirred water bath to maintain temperature, which was measured with a digital thermometer. The density of pure liquids and liquid mixture were determined using a double walled bicapillary pycknometer and viscosity was determined by Oswald's viscometer of 10 ml capacity. An ultrasonic interferometer (Model F-81) supplied by M/s Mittal enterprises, New Delhi, having the frequency 2 MHz with an overall accuracy of ± 0.05 has been used for velocity measurement. The purity of chemicals was checked by comparing with their densities with literature values.

Theory and Calculations

Using measured data, the following acoustical parameters such as adiabatic compressibility, intermolecular free length, specific acoustic impedance and shear's relaxation time have been calculated at 30°C, 35°C and 40°C with the help of following equations [7,9,13] -

| 1. Isentropic Compressibility | $(\beta_{s}) =$ | 1/ U ² ρ | (1) |
|--------------------------------|--------------------------------------|---------------------|-----|
| 2. Specific Acoustic Impedance | (Z) = | U.p | (2) |
| 3. Intermolecular Free Length | $(L_f) = K\sqrt{\beta_s}$ | | (3) |
| 4. Relative Association | $(R_A) = \rho / \rho_o [Uo \ 1/3/U]$ | | (4) |

| 5. Solvation Number | $(S_n) = (n_1 / n_2) (1 - \beta_s) / \beta_{so}$ | (5) |
|-----------------------------------|--|-----|
| 6. Apparent Molal Compressibility | $(\phi_{\rm K}) = 1000 (\rho_{\rm o}\beta_{\rm s} - \beta_{\rm so}\rho)/ \text{ C. } \rho_{\rm o} + \beta_{\rm so} \text{ M}/\rho_{\rm o}$ | (6) |

Where ρ_0 and Uo are the densities and ultrasonic velocities of solution and solvent respectively, K is Jacobson constant, M molecular weight of solute, β_{so} the isentropic compressibility of solvent, C is concentration in mole/litre n_1 and n_2 are the number of moles of solvent and solute respectively.

RESULTS AND DISCUSSION

In the present investigation, experimental values of density, viscosity and ultrasound velocity are shown in table (1). The observed data indicate that ultrasound velocity, density and viscosity of solutions increases with increase in the concentration of the salicylic acid in ethanol but values of these three parameters for same samples decreases on increasing temperature. These results are indicate that there is a significant interactions between the solute and solvent molecules because the presence of carboxylic group of salicylic acid and alcoholic group of ethanol create the possibility of interaction between the molecules [3,15].

| | Ultrasound Velocity (U) M/sec | | | Density (ρ) | | | Viscosity (η) | | |
|---------|-------------------------------|------|------|-------------------|--------|--------|---------------|--------|--------|
| С | | | | g/cm ³ | | | c.p. | | |
| Mol/lit | 30°C | 35°C | 40°C | 30°C | 35°C | 40°C | 30°C | 35°C | 40°C |
| 0.0276 | 1172 | 1167 | 1158 | 0.7778 | 0.7764 | 0.7756 | 1.1529 | 1.1425 | 1.1216 |
| 0.0552 | 1176 | 1171 | 1162 | 0.7830 | 0.7819 | 0.7811 | 1.1584 | 1.1480 | 1.1271 |
| 0.0828 | 1180 | 1175 | 1166 | 0.7894 | 0.7847 | 0.7839 | 1.1612 | 1.1508 | 1.1299 |
| 0.1104 | 1184 | 1179 | 1170 | 0.7910 | 0.7874 | 0.7866 | 1.1639 | 1.1535 | 1.1326 |
| 0.1380 | 1188 | 1183 | 1174 | 0.7924 | 0.7902 | 0.7894 | 1.1667 | 1.1563 | 1.1354 |
| 0.1656 | 1191 | 1186 | 1177 | 0.7937 | 0.7930 | 0.7922 | 1.1695 | 1.1591 | 1.1382 |
| 0.1932 | 1194 | 1190 | 1181 | 0.7944 | 0.7957 | 0.7949 | 1.1722 | 1.1618 | 1.1409 |
| 0.2208 | 1197 | 1193 | 1184 | 0.7980 | 0.7985 | 0.7977 | 1.1750 | 1.1646 | 1.1437 |
| 0.2484 | 1200 | 1196 | 1187 | 0.7985 | 0.8012 | 0.8004 | 1.1777 | 1.1673 | 1.1464 |
| 0.2760 | 1204 | 1199 | 1191 | 0.7993 | 0.8040 | 0.8032 | 1.1805 | 1.1701 | 1.1492 |

Table-1: Experimental values of ultrasound velocity, density and viscosity

The increase in velocity is due to the decrease in free length and increase in adiabatic compressibility of the liquid mixtures. Such decrease in free length may be attributed due to the strong packing of molecules inside the shield, and the adiabatic compressibility increases with increase of molar concentration it is shown that the presence of molecular interaction between the molecules of the liquid mixture. It is primarily the compressibility that increases due to structural changes of molecules in the mixture leading to a decrease in ultrasonic velocity [8,11,14]. In the present paper the elevation of temperature from 30° C - 40° C shows the same trend. (Table – 2)

| С | Intermolecu | lar free length (| L_f) | Adiabatic compressibility ($\phi_{\rm K} \times 10^9$) | | | | |
|---------|-------------|-------------------|---------|--|---------|---------|--|--|
| Mol/lit | A° | | | cm ² /dyne | | | | |
| | 30°C | 35°C | 40°C | 30°C | 35°C | 40°C | | |
| 0.0276 | 0.6105 | 0.6190 | 0.6295 | -0.6200 | -3.7785 | -0.3296 | | |
| 0.0552 | 0.6064 | 0.6147 | 0.6251 | -2.1552 | -3.8011 | -2.2198 | | |
| 0.0828 | 0.6019 | 0.6115 | 0.6219 | -2.9829 | -3.5381 | -2.0040 | | |
| 0.1104 | 0.5992 | 0.6084 | 0.6187 | -2.3495 | -2.8883 | -1.8840 | | |

Table-2: Experimental values of intermolecular free length, adiabatic compressibility



| _ | 0.1380 | 0.5968 | 0.6054 | 0.6157 | -1.8959 | -2.4426 | -1.7455 |
|---|--------|--------|--------|--------|---------|---------|---------|
| | 0.1656 | 0.5948 | 0.6025 | 0.6129 | -1.5207 | -2.0800 | -1.6373 |
| _ | 0.1932 | 0.5928 | 0.5998 | 0.6100 | -1.2005 | -1.8065 | -1.5704 |
| _ | 0.2208 | 0.5901 | 0.5971 | 0.6073 | -1.2290 | -1.7103 | -1.4810 |
| _ | 0.2484 | 0.5883 | 0.5946 | 0.6044 | -0.9830 | -1.5192 | -1.4439 |
| | 0.2760 | 0.5863 | 0.5920 | 0.6015 | -0.7991 | -1.3660 | -1.4102 |

The specific acoustic impedance is a product of the density of the solution and the velocity. Specific acoustic impedance increases with increase of molar concentration at all temperature [5] (Table-3). The shear's relaxation time decreases with increasing concentration the elevation of the ultrasonic velocity in the system should contain information about the characteristic time of the relaxation process that causes elevation. Thus the fact that increase of specific acoustic impedance with increase in molar concentration at all temperatures is an indicative of the increase in intermolecular forces with the addition of solute forming aggregates of solvent molecules around solute and supports the strong solute – solvent interactions, due to which structural arrangement is affected [6].

Table-3: Experimental values of specific acoustic impedance, shear's relaxation time

| С | Specific ac | oustic impedan | ce | Shear's relaxation time (τ) | | |
|---------|--------------------------|----------------|--------|----------------------------------|----------|----------|
| Mol/lit | $(Z \times 10^5)$ g/s.cm | | | | | |
| | 30°C | 35°C | 40°C | 30°C | 35°C | 40°C |
| 0.0276 | 0.9116 | 0.9061 | 0.8981 | 143.8822 | 144.0681 | 143.7877 |
| 0.0552 | 0.9208 | 0.9156 | 0.9077 | 142.6357 | 142.7618 | 142.4882 |
| 0.0828 | 0.9315 | 0.9220 | 0.9140 | 140.8566 | 141.6324 | 141.3593 |
| 0.1104 | 0.9365 | 0.9284 | 0.9204 | 139.9553 | 140.5162 | 140.2435 |
| 0.1380 | 0.9411 | 0.9346 | 0.9264 | 139.1682 | 139.4600 | 139.2593 |
| 0.1656 | 0.9451 | 0.9407 | 0.9323 | 138.5448 | 138.4855 | 138.3089 |
| 0.1932 | 0.9487 | 0.9466 | 0.9384 | 137.9604 | 137.5674 | 137.3215 |
| 0.2208 | 0.9553 | 0.9526 | 0.9441 | 136.9952 | 136.6354 | 136.4598 |
| 0.2484 | 0.9585 | 0.9582 | 0.9504 | 136.4776 | 135.8263 | 135.4691 |
| 0.2760 | 0.9620 | 0.9640 | 0.9566 | 135.9574 | 134.9793 | 134.4891 |

CONCLUSION

On the basis of the results obtained from this study, it is concluded that the solute solvent interaction in the mixture of salicylic acid with ethanol is significant and the computed acoustical parameters and their values indicate to the presence of molecular interaction in the mixture.

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