ISSN 0036-0244, Russian Journal of Physical Chemistry A, 2015, Vol. 89, No. 11, pp. 2150–2155. © Pleiades Publishing, Ltd., 2015.

BIOPHYSICAL CHEMISTRY

Acoustical Studies of Molecular Interaction in the Solution of Propranolol Hydrochloride Drug at Different Temperatures and Concentrations[1]

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Received September 16, 2014

Abstract—In the present study ultrasonic velocity (υ), density (ρ) and viscosity (η) have been measured at frequency 1 MHz in the binary mixtures of propranolol hydrochloride with water in the concentration range (0.1 to 0.0125%) at 303, 308, 313 K using Multifrequency ultrasonic interferometer. The measured value of density, ultrasonic velocity, and viscosity have been used the acoustical parameters namely adiabatic compressibility (β_a), relaxation time (τ), acoustic impedance (z), free length (L_f), free volume (V_f) and internal pressure (Π_i),Wada's constant (W), Rao's Constant (R), cohesive energy (CE) were calculated. These parameters explained formation of hydrogen bond and molecular interaction existing in the solution.

Keywords: propranolol hydrochloride, ultrasonic velocity, acoustical parameters.

DOI: 10.1134/S003602441511014X

INTRODUCTION

Ultrasound refers to sound waves of such a high frequency that it cannot be heard. High resolution ultrasound imaging has been used for determination of melanoma invasion depth in vivo for preoperative staging purposes [1, 2]. Now a day's Ultrasonic technology is employed in a wide range of applications in medicine, biology, industry, material science, agriculture, oceanography, sonochemistry research etc. due to its non-destructive nature [3–10].

These waves have also been used to extract and release intracellular enzymes such as invertase, to promote enzyme release, enhance productivity in biological processes [11] etc. In field of agriculture, ultrasound waves have been utilized extensively in chemical additives (fertilizers and plant protection preparations) for improving the production yield of food produced. In materials chemistry, ultrasound waves have been useful in the preparation of biomaterials, protein microspheres, in the modification of polymers and polymer surfaces etc. [12–17].

Much work has been done in solutions of polymers [18–23], amino acids [24, 25] and other electrolytes [26–33]. However, little work has been done for solutions of solid organic compounds [34–38].

Ultrasonic offers the most exciting and fascinating field of scientific research among the researchers since the ultrasonic and other related thermo acoustic parameters provide useful information regarding the structure of molecules, molecular order, molecular packing, inter and intra-molecular interactions [39, 40] etc. Ultrasonic study of liquid–liquid mixture has gained much importance during the last two decades in assessing the nature of molecular interaction and investigating the physiochemical behavior of this system [41, 42]. The review of literature reveals that lot of work has been done to investigate ultrasonic measurement of pure liquid and liquid mixture at different environment, but less effort has been made to investigate ultrasonic studies in binary mixture of propranolol hydrochloride (A syenthetic beta adrenergic receptor) i.e. with water. Thus in the present paper, acoustical studies of drug propranolol hydrochloride have been studied in water at different temperatures over a wide range of concentrations. From these experimental values a number of thermodynamic parameters namely adiabatic compressibility, acoustic impedance, relaxation time, free length, free volume, internal pressure, wada's constant, Rao's Constant have been calculated. The variation of these parameters with (%) concentration was found to be useful in understanding the nature of interactions between the components.

MATERIALS AND METHODS

Propranolol hydrochloride used in the present work was of analytical reagent (AR) grade with a minimum assay of 99.9%, It is used without purification.

[1] The article is published in the original.

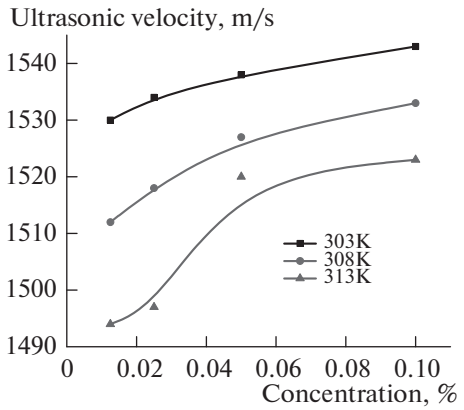

Fig. 1. Variation of Ultrasonic velocity.

Different concentrations of solution were prepared by adding sufficient amount of solvent water to propranolol hydrochloride. The ultrasonic velocity (υ) have been measured in ultrasonic interferometer Mittal Model-F-05 with an accuracy of 0.1%. The viscosities (η) of binary mixtures were determined using Ostwald's viscometer by calibrating with double distilled water with an accuracy of ±0.001 PaSec. The density (ρ) of these binary solution was measured accurately. using 25 mL specific gravity bottle in an electronic balance precisely and accurately The basic parameter U, η, ρ were measured at various concentration (0.0125 to 0.1%) and temperature of 303, 308 and 313 K. The various acoustical parameters were calculated from υ, η & ρ value using standard formulae.

On using ultrasonic velocity, density and viscosity the following acoustical parameters like adiabatic compressibility (β_{ad}), intermolecular free length (L_f), relaxation time (T), free volume (V_f), internal pressure (Π_i), acoustic impedence (Z), ultrasonic attenuation (α/f^2), Rao's constant (R), molar volume (V_m),cohesive energy (CE) were calculated by applying the following expressions [43–50].

1. Ultrasonic velocity (υ): The relation used to determine the ultrasonic velocity is given by,

$$\upsilon = f\lambda \ \ ms^{-1}$$

Where, f–Frequency of ultrasonic waves, λ–Wave length.

2. Adiabatic compressibility (κ): Adiabatic compressibility which is defined as,

$$\beta_{ad} = (1/\upsilon^2\rho) \ \ kg^{-1}\ ms^2,$$

where, υ–Ultrasonic velocity, ρ–Density of the solution.

3. Free volume (V_f): Free volume in terms of the ultrasonic velocity (υ) and the viscosity of the liquid (η) calculated by formula

$$V_f = (M\upsilon/_k\eta)^{3/2} \ \ m^3,$$

where, M is the molecular weight and 'k' is a temperature independent constant equal to 4.28×10^9 for all liquids.

4. Acoustic impedance (Z): The acoustic impedance is computed by the formula

$$Z = \upsilon\rho \ \ kg\ m^{-2}\ s^{-1}.$$

5. Free length (L_f): It is calculated on using formula,

$$L_f = (K\sqrt{\ }\kappa)$$

K–Jacobson temperature dependent constant defined as $K = (93.875 + 0.345T) \times 10^{-8}$, κ = Adiabatic compressibility.

6. Attenuation (α/f^2): It is calculated by,

$$\alpha/f^2 = 8\pi^2\eta/3\rho\upsilon^3.$$

7. Viscous relaxation time (T): It is calculated by using the relation,

$$T = 4\eta/3\rho\upsilon^2.$$

8. Rao's Constant (R): Rao's constant is calculated by using formula,

$$R = V\upsilon_2^1 \quad \text{or} \quad R = \left(\frac{M}{\rho}\right)\upsilon_2^1$$

M = Molecular Weight.

9. Wada constant (W): It was calculated by formula,

$$W = M\kappa^{-1/7}/\rho$$

10. Internal pressure (Π_i): On using below cited formula Internal pressure is calculated,

$$\Pi_i = bRT\left[\frac{kn}{v}\right]^2 \frac{\rho_3^2}{M_6^7}$$

11. Molar volume: It is the ratio of density and molecular weight.

$$V_m = \frac{\rho}{M}$$

12. Cohesive energy (CE): Cohesive energy is calculated by formula quoted below,

$$CE = \Pi_i V_m$$

RESULT AND DISCUSSION

The measured values of ultrasonic velocity, density and related thermo acoustical parameters of propranolol hydrochloride with water at 303, 308, 313 K temperatures in different concentrations are shown in supplimetry file. The variation of acoustical parameters with concentrations and temperature is shown graphically in Fig. 1 to 14. It is observed that ultrasonic velocity and acoustic impedance show nonlinear increasing variation with increase in molar concentration. This indicates that the complex formation and intermolecular weak association which may be due to

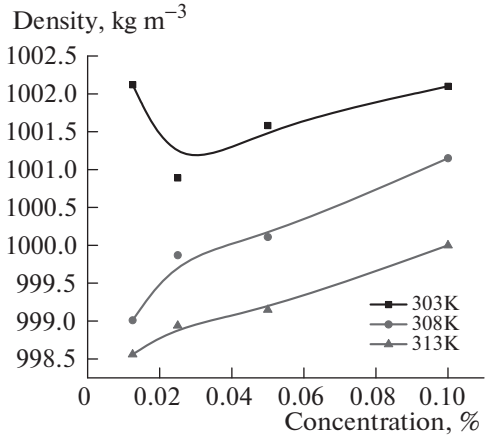

Fig. 2. Variation of Density with concentration and temperature with concentration and temperature.

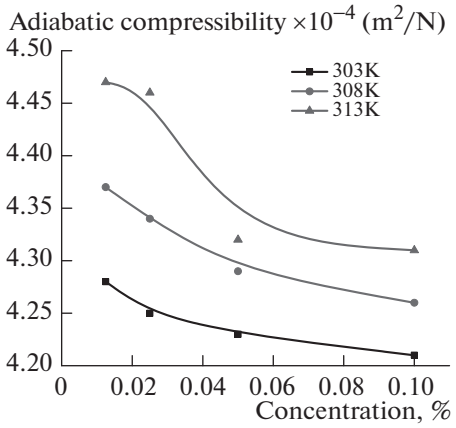

Fig. 3. Variation of Adiabatic compressibility.

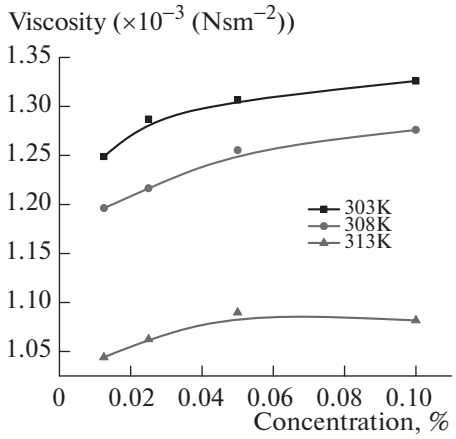

Fig. 4. Variation of Viscosity with concentration and temperature with concentration and temperature.

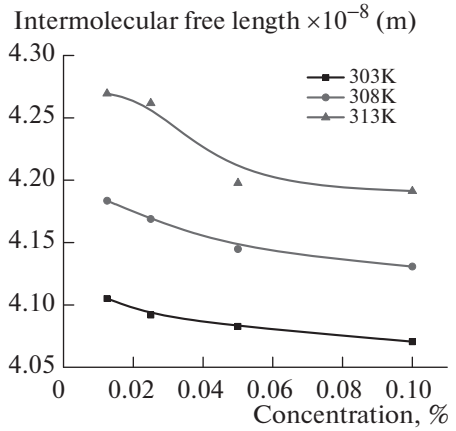

Fig. 5. Variation of Intermolecular free length.

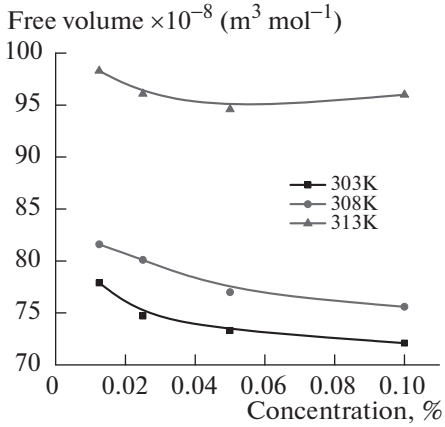

Fig. 6. Variation of free volume with concentration and temperature with concentration and temperature.

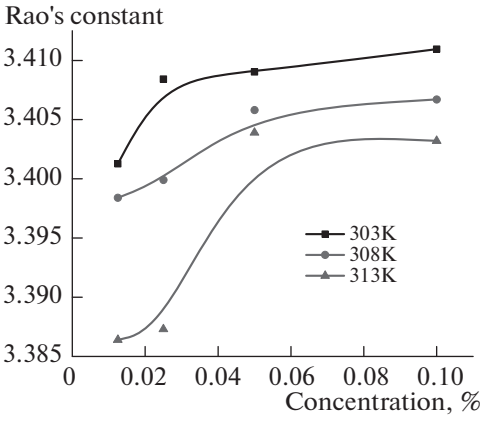

Fig. 7. Variation of Rao's constant.

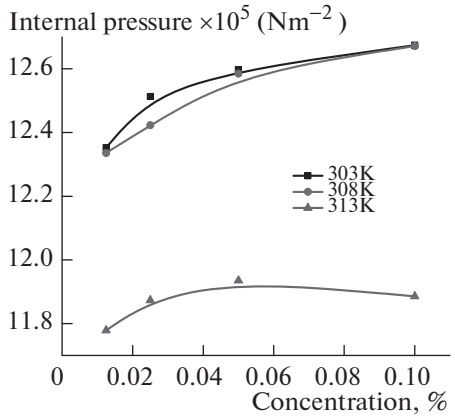

Fig. 8. Variation of Internal pressure with concentration and temperature with concentration and temperature.

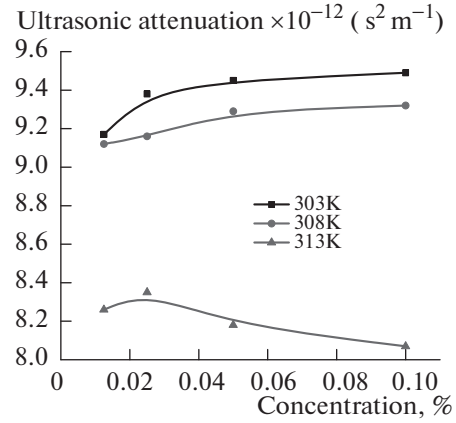

Fig. 9. Variation of Ultrasonic attenuation.

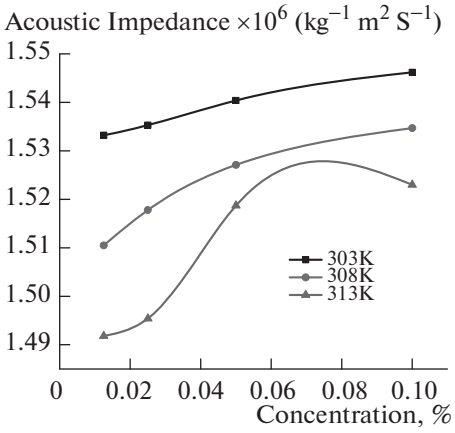

Fig. 10. Variation of Acoustic Impedance with concentration and temperature with concentration and temperature.

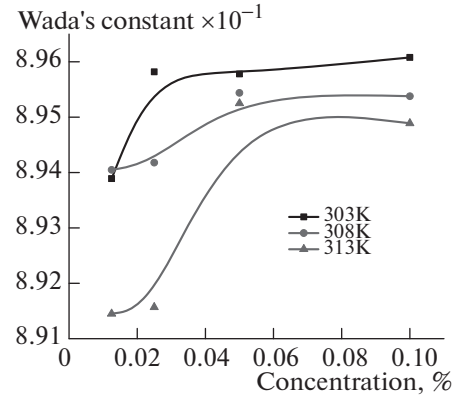

Fig. 11. Variation of Wada's constant.

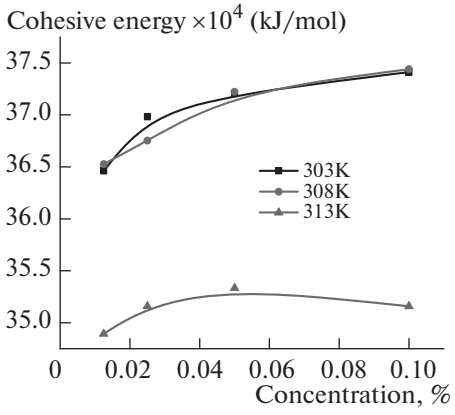

Fig. 12. Variation of cohesive energy with concentration and temperature with concentration and temperature.

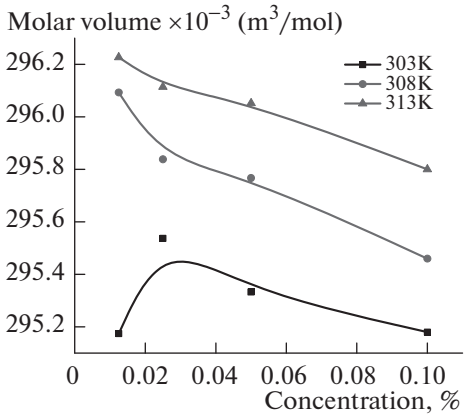

Fig. 13. Variation of Molar volume.

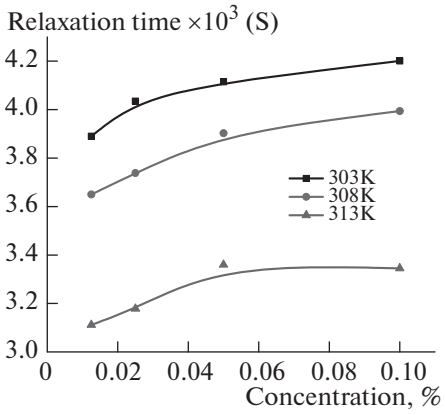

Fig. 14. Variation of Relaxation time with concentration and temperature with concentration and temperature.

hydrogen bonding. Thus complex formation can occur at these molar concentrations between the component molecules. Adiabatic compressibility (β_a) shows an inverse behavior compared to the ultrasonic velocity. Adiabatic compressibility decreases with increase in concentration of propranolol hydrochloride. The decrease in compressibility implies that there is an enhanced molecular association in the system with increase in solute concentration.

The opposite trend of ultrasonic velocity and adiabatic compressibility indicate that the association among interacting propranolol hydrochloride and water molecules. In the present system of aqueous 3 propranol hydrochloride, free length varies nonlinearly with increase in molar concentration which suggests the significant interaction between solute and solvent due to which structural arrangement is also affected.

Relaxation time decreases with increase in concentration. Nonlinear trend of density with concentration indicates the structure-making and breaking property of solvent due to the formation and weakening of H-bonds. The free volume increases and internal pressure decreases with increases in molar concentration indicate the association through hydrogen bonding. It shows the increasing magnitude of interaction between the propranolol hydrochloride and water.

CONCLUSION

The ultrasonic study of the liquid mixtures serves as a probe to detect the molecular association arising from the hydrogen bonding between the molecules of propranolol and water. The non-linear variation of thermo acoustical parameters with concentration reveals the complex formation between the component molecules. In the present paper the ultrasonic velocity (υ), density, viscosity and acoustical parameters viz. adiabatic compressibility, intermolecular free length, relaxation time, acoustic impedance, attenuation, Rao's constant, molar volume, cohesive energy, Wada's constant have been measured at different concentrations. The parameters indicate that there is a strong molecular interaction between molecules as the concentration of drugs solution increases and the interaction decreases as temperature increases.

ACKNOWLEDGMENTS

The Authors are thankful to Department of chemistry, Jankidevi Bajaj College of science, Wardha for their kind support in the present research work.

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SPELL: 1. adrenergic, 2. impedence, 3. propranol