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Solute-Solvent Interactions in Water Solutions of Methyl Cobalamine Drug at 303 and 313 K On Ultrasonic and Viscometric Data

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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 methyl cobalamine with water in the concentration range (0.1 to 0.0125%) at 303 K and 313 K using a multifrequency ultrasonic interferometer . The measured value of density, ultrasonic velocity, and viscosity have been used to estimate the acoustical parameters, namely adiabatic compressibility (κ), relaxation time (τ), acoustic impedance (z), free length (L_f), free volume (V_f), and internal pressure (Πi),Wada's constant(W), The obtained results support the complex formation, molecular association by intermolecular hydrogen bonding in the binary liquid mixtures.
Key Words: Methyl cobalamine, free volume, acoustical parameters, ultrasonic velocity.

Introduction:

Ultrasonic waves are used in many applications including plastic welding, medicine, jewelry cleaning, pipe inspection, and nondestructive test. Within nondestructive test, ultrasonic waves give us the ability to 'see through' solid / opaque material and detect surface or internal flaws without affecting the material in an adverse manner. It had been identified, about 200 years ago, that dogs could hear [1]. This canine ability is often used in police departmental work and by dog trainers. These sound waves are used by bats as a kind of navigational radar for night flying [2].Even blind people unconsciously develop a similar method by which obstacles are sensed by the reflected echoes of their footsteps or the tapping of a cane. In the field of technology, the waves are being used to measure depth of sea, directional signalling in submarine, and mechanical cleaning of surface soldering [3], and to detect shoals of fish. Acoustic sonograms have become an important medicinal diagnostic tool which is widely used nowadays [4-5]. Ultrasonic waves are used for both diagnosis and therapy. It includes the detection of wide variety of anomalies, such as tumor, bloodless surgery, proper extraction of broken teeth, cardiology, and stone fragmentation [6]. Ultrasound is more sensitive than X-rays in distinguishing various kinds of tissues. It is believed to be less hazardous than X-rays, although possible hazards of ultrasound have not yet been thoroughly explored [7]. The unique feature of sound wave property is that it gives direct and precise information of the adiabatic properties of solution. The data of velocity of sound in very few liquids were available up to 1930. The discovery of interferometer and optical diffraction method improved the investigation, both qualitatively and quantitatively. Most of the information extracted from ultrasonic study of fluids is confined to the determination of hydration number and compressibility [8-9]. The successful applications of acoustic methods to physicochemical investigations of solution become possible after the development of adequate theoretical approaches and methods for precise ultrasound velocity measurements in small volumes of liquids [10-12]. In the present paper, acoustical studies have been studied in water at different temperatures over a wide range of methyl cobalamine concentrations. From the experimental values a number of thermodynamic parameters namely ultrasonic velocity, adiabatic compressibility, acoustic impedance, relaxation time, free length, free volume, internal pressure, Rao's constant, ultrasonic attenuation, cohesive energy, and molar volume, Wada's constant has been calculated. The variation of these parameters with concentration was found to be useful in understanding the nature of interactions between the components [13-16].

Materials and Methods

Chemicals were purchased from local commercial suppliers and are of laboratory grade. Methyl cobalamine used in the present work was of analytical reagent (AR) grade with a minimum assay of 99.9%, Solution of different concentration of methyl cobalamine were prepared by water as solvent. The ultrasonic velocity (υ) has 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 doubly distilled water with an accuracy of ±0.001 PaSec. The density (ρ) of these binary solutions was measured accurately using 25 mL specific gravity bottle in an electronic balance, precisely and accurately. The basic parameter υ, η, and ρ were measured at various concentrations (0.1 to 0.0125%) and temperatures (303 K & 313 K).The various acoustical parameters were calculated from υ, η, and ρ values using standard formulas. On using ultrasonic velocity ,density and viscosity the following acoustical parameters like adiabatic compressibility (κ) [17] , intermolecular free length[18] (Lf) , relaxation time [19] (τ), free volume [20] (V_f) , internal pressure [21] (Πi) , acoustic impedance [22] (Z), Wada's constant [23] (W), ultrasonic attenuation [24] (α/f^2), Rao's constant [25] (R), molar volume (Vm), and cohesive energy (CE) were calculated by applying the following expressions.

1.Ultrasonic velocity (υ): The relation used to determine the ultrasonic velocity is given by, $\upsilon = f \times \lambda$ ms^{-1}; Where, f - Frequency of ultrasonic waves, λ - Wavelength

2. Adiabatic compressibility (κ): Adiabatic compressibility is defined as,
$\kappa = (1/\upsilon^2 \rho)$ 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) are 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
$Z = \upsilon \times \rho$ $kg\ m^{-2} s^{-1}$

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. Ultrasonic Attenuation (α/f^2): It is calculated by, $\alpha/f^2 = 8\pi2\eta/3\rho\upsilon^3$

7. Viscous relaxation time (τ): It is calculated by using the relation,
$\tau = 4\eta/3\rho\upsilon^2$

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

$R = V . u^{1/3}$ or $R = \left(\frac{M}{\rho}\right) u^{1/3}$; M= Molecular Weight.

9. Wada's constant (W): It was calculated by formula, W=M. $\kappa^{-1/7}/\rho$

10. Internal pressure (Πi): On using below-cited formula, Internal pressure is calculated, $\Pi i = b\ RT \left[\frac{k\eta}{v}\right]^{1/2} \frac{\rho^{2/3}}{M^{7/6}}$

11. Molar volume: It is the ratio of density & molecular weight. $Vm = \frac{\rho}{M}$

12. Cohesive energy (CE) : Cohesive energy is calculated by formula quoted below, $CE = \Pi i Vm$

RESULT AND DISCUSSION

The measured values of ultrasonic velocity, density and related thermo-acoustical parameters like adiabatic compressibility (κ), intermolecular free length (L_f) , relaxation time (□), free volume (V_f) , internal pressure (Πi) , acoustic impedance (Z), Wada's constant (W), ultrasonic attenuation (α/f^2), Rao's constant (R), molar volume (Vm),cohesive energy (CE) of methyl cobalamine with water at 303 K, 313 K in different concentrations are shown in figure 1 to 14 .

Figure: The following figures shows the variation of various acoustical parameters with concentration and temperature

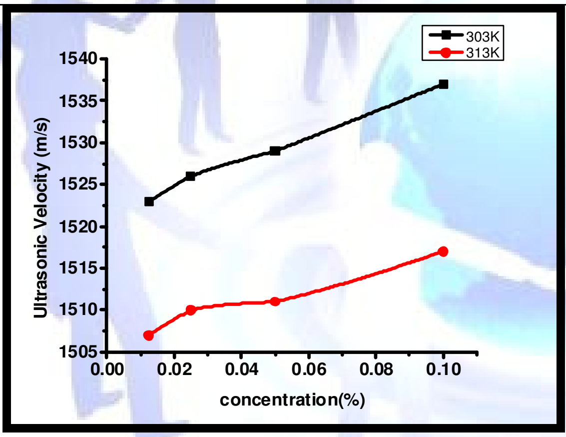

Fig.1:-Variation of Ultrasonic velocity with concentration and temperature

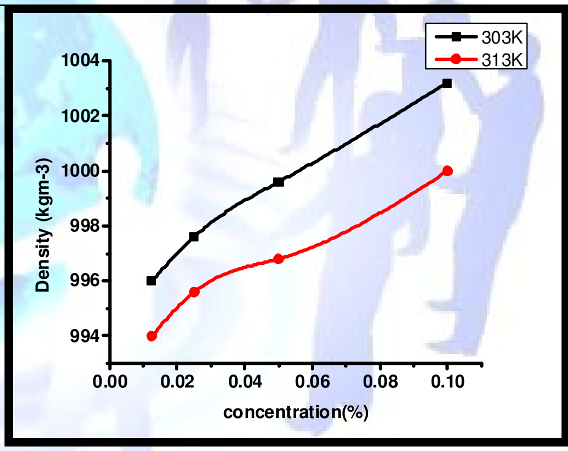

Fig.2:-Variation of Density with concentration and temperature.

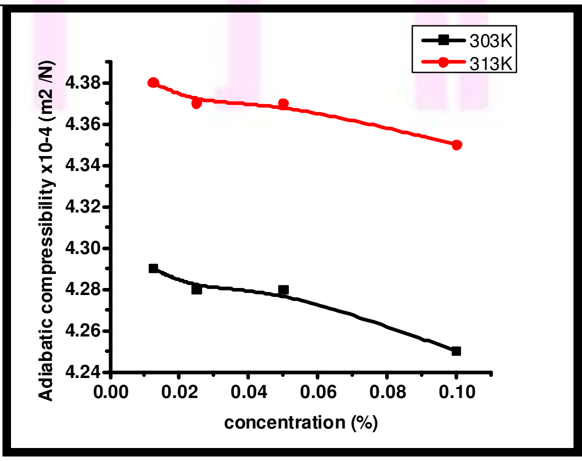

Fig.3:-Variation of Adiabatic compressibility with concentration and temperature

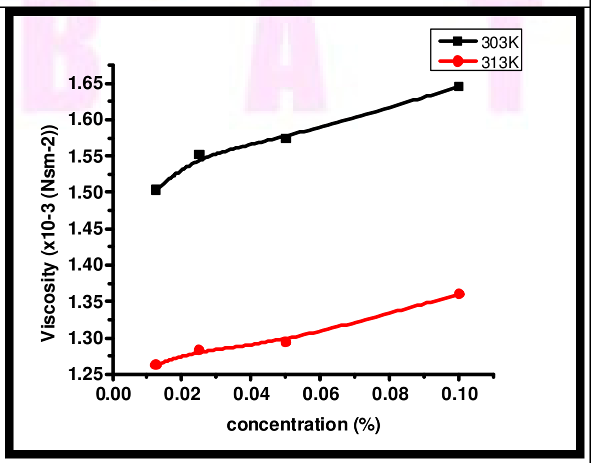

Fig.4:-Variation of Viscosity with concentration and temperature

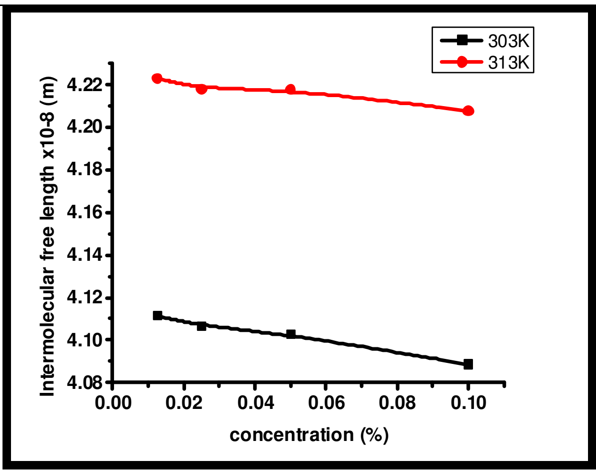

Fig.5:-Variation of Intermolecular free length with concentration and temperature

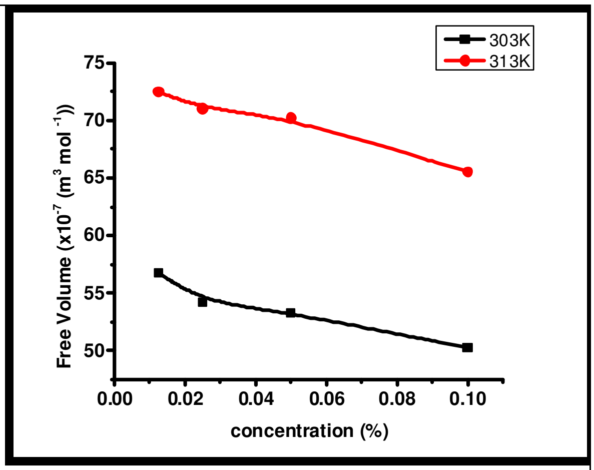

Fig.6:-Variation of free volume with concentration and temperature

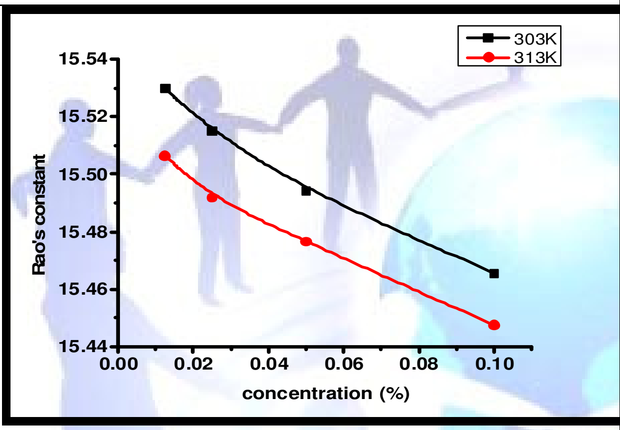

Fig.7:-Variation of Rao's constant with concentration and temperature

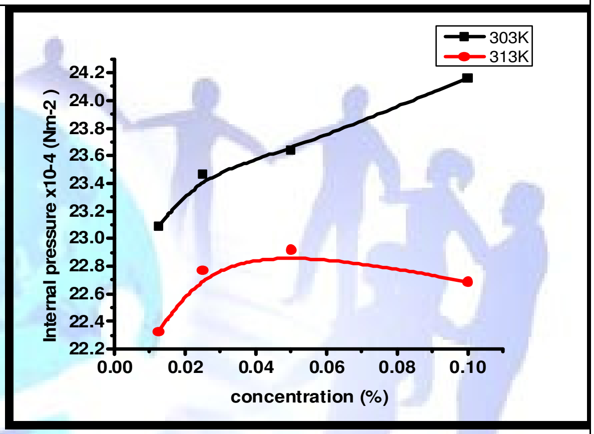

Fig.8:-Variation of Internal Pressure with concentration and temperature

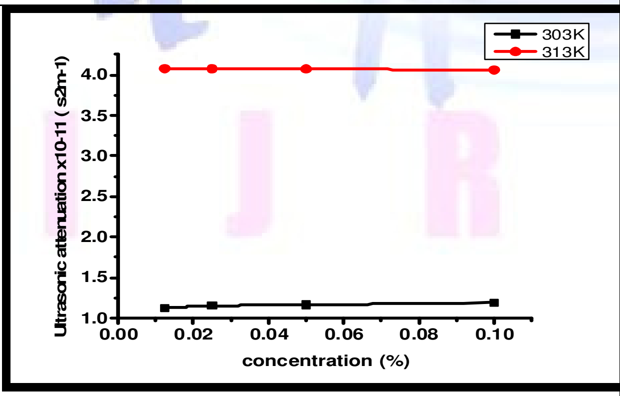

Fig.9:-Variation of Ultrasonic attenuation with concentration and temperature

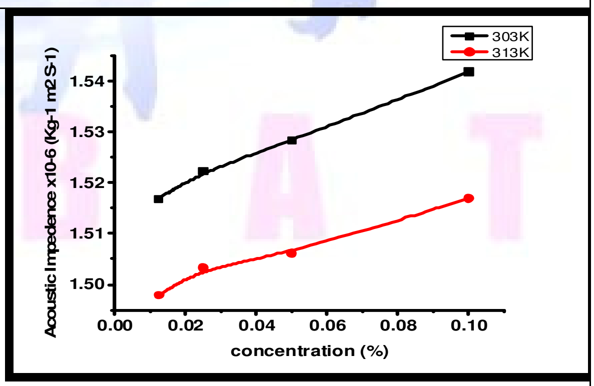

Fig.10:-Variation of Acoustic Impedance with concentration and temperature

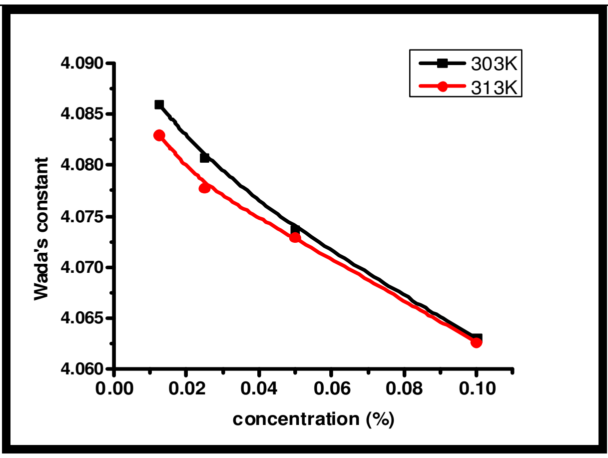

Fig.11:-Variation of Wada's constant with concentration and temperature

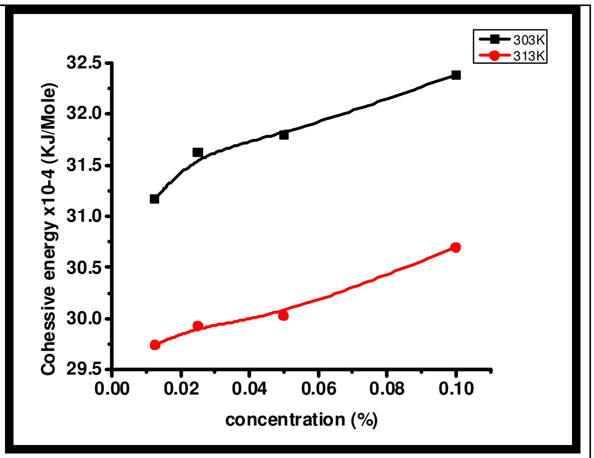

Fig.12:-Variation of Cohesive energy with concentration and temperature

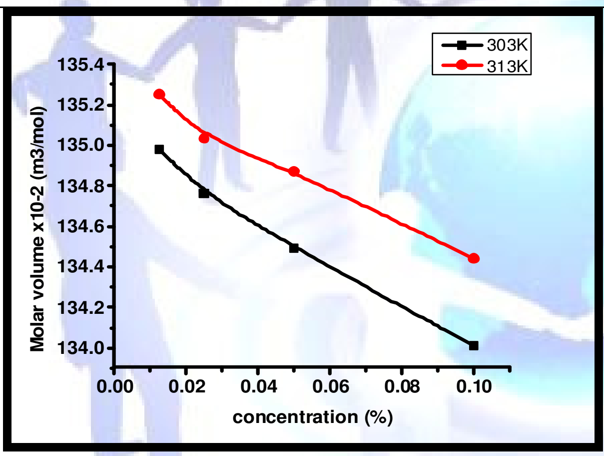

Fig.13:-Variation of Molar volume with concentration and temperature

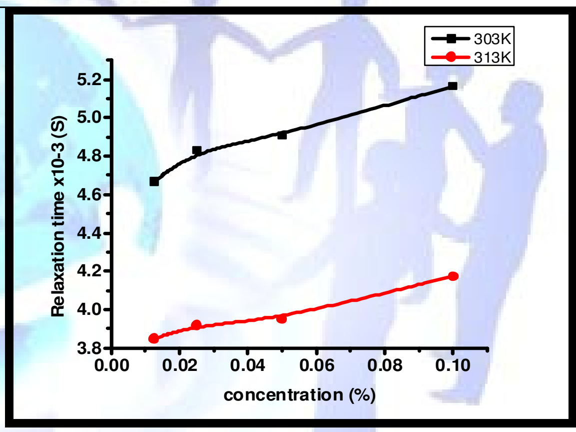

Fig.14:-Variation of Relaxation time with concentration and temperature

CONCLUSION

Ultrasonic velocity and density of the binary mixtures along with thermodynamic values such as adiabatic compressibility, free length, and impedance at different temperature were determined. It is observed that ultrasonic velocity increases with increase in concentration which may be due to solute-solvent interaction. The adiabatic compressibility decreasing with an increase in concentration shows that there is strong solute-solvent interaction. Acoustic impedance shows nonlinear increasing variation with an increase in molar concentration. This indicates the complex formation and intermolecular weak association which may be due to hydrogen bonding. Thus complex formation can occur at these molar concentrations between the component molecules. The opposite trend of ultrasonic velocity and adiabatic compressibility indicates the association among interacting methyl cobalamine and water molecules. In the present system of methyl cobalamine, 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 an 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 decreases and internal pressure increases with an increase in molar concentration, indicating that there is a weak interaction between solute and solvent molecules. Rao's constant and Wada's constant decrease with increasing concentration, which indicates that there is a weak interaction between solute and solvent 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 unlike molecules as the concentration of drug solution increases. The molecular interaction decreases with an increase in temperature.

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