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Study of molecular interactions in antihistamine drug cinnarizine and benzene at different temperatures

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ABSTRACT

In the present work, the ultrasonic studies have been conducted on the binary mixtures of Cinnarizine and Benzene at 2.9979 MHz and at different temperatures from 299K to 328 K using Ultrasonic interferometer. Further, the experimentally determined ultrasonic velocity and density are used to calculate the various thermo-acoustical parameters like adiabatic compressibility (β), intermolecular free length(L_f), specific acoustic impedance(Z), molar volume(V_m), available volume V_a(S), Rao's number(R_a) and Wada's number(W). The intermolecular interactions responsible for the changes in thermo-acoustical parameters with respect to temperature are discussed. It is noticed that weak molecular interactions are present between the components of the mixture and the molecular interactions are observed to be decreasing with increase in temperature.

Keywords: Ultrasonic velocity, adiabatic compressibility, intermolecular free length, Wada's number, molecular interactions.

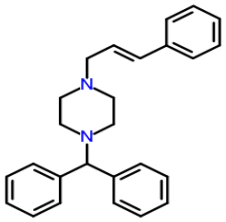
INTRODUCTION

The understanding of intermolecular interactions between polar and non-polar molecules can be best made by ultrasonic investigations and they find applications in several industrial and technological processes [1-3]. In many industrial applications, liquid mixtures rather than single component liquid system are used in processing and product formulations. The ultrasonic study of liquids and liquid mixtures are very important in understanding the nature and strength of molecular interactions. The biological activity of drug molecules and the activation energy of the metabolic process basically depend on the type and strength of intermolecular interactions [4-6]. Though the molecular interaction studies can be best carried out through spectroscopic methods, the other non spectroscopic techniques such as dielectric, magnetic, ultrasonic velocity measurements have been widely used in the field of interactions and structural aspect evaluation studies [7-11]. The unique property of sound wave is that it gives direct and precise information of adiabatic properties. The use of ultrasound is one of the well recognized approaches for the study of molecular interactions in fluids. Speed of sound itself is highly sensitive to the structure and interactions present in the liquid mixtures as it is fundamentally related to the binding forces between the constituents of the medium [12-13]. Properties of liquid and liquid mixtures are thermodynamically very important as part of studies of the thermodynamic, acoustic and transport aspects. The compositional dependence of thermodynamic properties have proved to be very useful tool in understanding the nature and extent of pattern of molecular aggregation resulting from intermolecular interactions between the components [14-16].

Cinnarizine is a drug derivative of Piperazine and it is characterized as an antihistamine and calcium channel broker. It is also known to promote cerebral blood flow and so is used to treat cerebral apoplexy, post trauma cerebral symptoms and cerebral arteriosclerosis. However it is more commonly prescribed for nausea and vomiting due to motion sickness or other sources such as chemotherapy. It helps to prevent travel sickness and dizziness. In view of all these various biological applications of the drug, we have studied the thermo-acoustical parameters of Cinnarizine and Benzene mixture in order to understand the molecular interactions.

MATERIALS AND METHODS

The molecular formula of Cinnarizine is $C_{26}H_{28}N_2$ and its molecular weight is 368.514 g/mol.
The molecular structure of Cinnarizine is as follows.



The compound Cinnarizine is procured from Sigma-Aldrich and AR grade Benzene from s d fine-chem. Ltd., India. Both the chemicals are used without any further purification. The ultrasonic velocity and density for a single weight fraction of 0.0147 using Cinnarizine as solute and Benzene as solvent are measured using Ultrasonic Interferometer (M/s Mittal Enterprises, Model F-84) working at 2.9979 MHz frequency with the accuracy of 0.5%. Further, the density of the liquid mixture is determined by using a bicapillary pycnometer. The accuracy in the density measurement is of the order of ± 0.0003 gm^{-3}. Both, ultrasonic velocity and density are measured at different temperatures ranging from 299K to 328K. The temperature of the mixture is maintained within ± 0.1K using an electronically operated constant temperature water bath. From these experimental data, various thermo-acoustic parameters like adiabatic compressibility(β), intermolecular free length(L_f), specific acoustic impedance(Z), molar volume(V_m), available volume V_a(S), Rao's number(R_a) and Wada's number(W) have been determined using the following relations [17]:

$$\beta = (1/u^2 \rho) \quad (1)$$

$$L_f = K \beta^{1/2} \quad (2)$$

Where $K = (93.875+0.375T) \times 10^{-8}$

$$Z = \rho u \quad (3)$$

$$V_m = (M_1f_1+M_2f_2) / \rho_{12} \quad (4)$$

$$V_a(S) = (1- u / u_\infty) V_m \quad (5)$$

Where u_∞ = 1,600 m/s

$$R_a = V_m u^{1/3} \quad (6)$$

$$W = V_m \beta^{-1/7} \quad (7)$$

Where K is the temperature dependent constant known as Jacobson constant [18], M is the molecular mass, f is the mole fraction, ρ is the density, u is ultrasonic velocity, T is the absolute temperature, while the suffixes 1, 2 and 12 indicate the relevant quantity for the solute, solvent and solution respectively.

RESULTS AND DISCUSSION

The experimentally determined values of ultrasonic velocity and density at different temperatures are given in table 1. The calculated thermo-acoustic parameters like adiabatic compressibility, intermolecular free length, and specific acoustic impedance values are presented in the table 2. The molar volume, available volume, Rao's number and Wada's number values are presented in table 3.

Table 1. Ultrasonic velocity and Density at different temperatures

T /K	u /m s^{-1}	ρ /kg m^{-3}
299	1289.70	875.14
303	1271.71	872.33
308	1252.52	867.47
313	1229.74	862.19
318	1207.55	857.41
323	1187.17	851.37
328	1164.38	846.31

Table 2. Adiabatic compressibility, Intermolecular free length, Specific acoustic impedance at different temperatures

T /K	β 10^{-10} / m^2 N^{-1}	L_f 10^{-10} /m	Z 10^6 /kg $m^{-2}s^{-1}$
299	6.8699	0.5399	1.1287
303	7.0883	0.5524	1.1093
308	7.3481	0.5676	1.0865
313	7.6696	0.5850	1.0603
318	7.9983	0.6027	1.0354
323	8.3341	0.6207	1.0107
328	8.7152	0.6402	0.9854

Table 3. Molar volume, Available volume, Rao's number, Wada's number at different temperatures

T /K	V_m 10^{-3} /m^3 mol^{-1}	V_a (s) 10^{-6} /m^3 mol^{-1}	R_a 10^{-4} /$m^{10/3}$ $s^{-1/3}$ mol^{-1}	W 10^{-3} /m^3 mol^{-1}
299	0.0903	17.5139	9.8298	1.8397
303	0.0906	18.5888	9.8154	1.8374
308	0.0911	19.7854	9.8205	1.8382
313	0.0917	21.2119	9.8204	1.8382
318	0.0922	22.6080	9.8153	1.8374
323	0.0928	23.9513	9.8291	1.8396
328	0.0934	25.4241	9.8241	1.8388

In order to understand the molecular interactions, the variation of ultrasonic velocity, density, adiabatic compressibility, intermolecular free length, specific acoustic impedance, molar volume, available volume, Rao's number and Wada's number with temperature are studied and the corresponding graphs are shown in the figures from I-IX respectively.

Fig.I. Variation of u /m s^{-1} with T/K

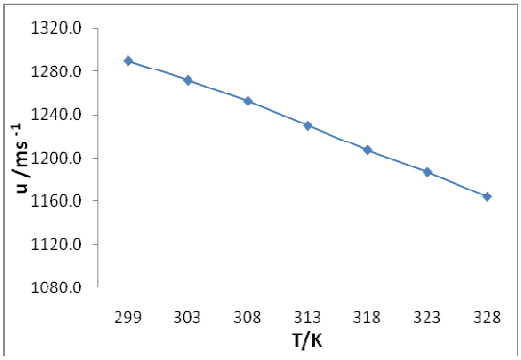


Fig.II. Variation of ρ /Kg m^{-3} with T/K

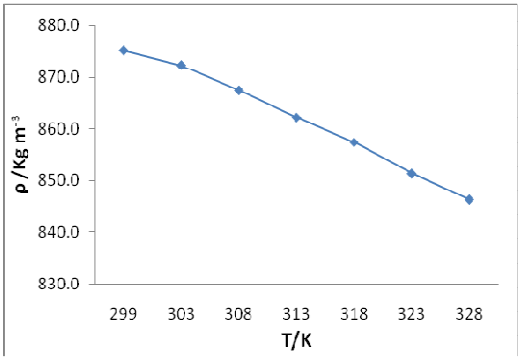


Fig.III. Variation of β 10^{-10} / m^2N^{-1} with T/K

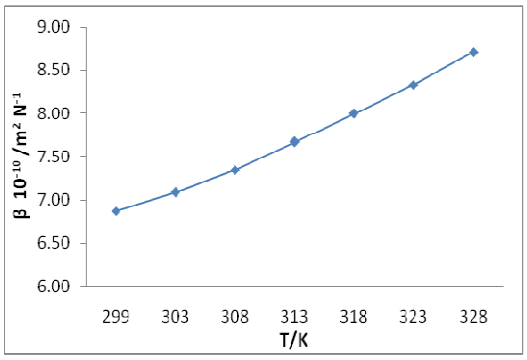


Fig.IV. Variation of L_f 10^{-10} /m with T/K

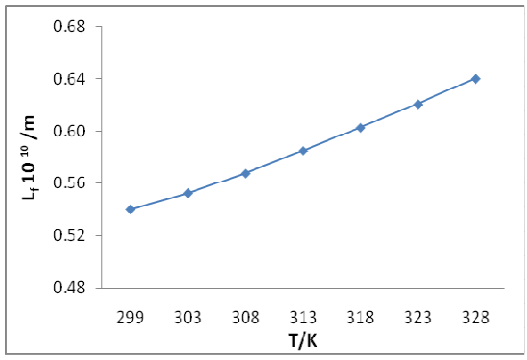


Fig.V.Variation of Z 10^6/Kg $m^{-2}s^{-1}$ with T/K

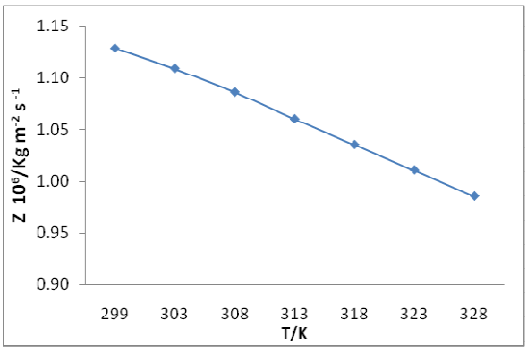


Fig.VI. Variation of V_m 10^{-3}/m^3 mol^{-1} with T/K

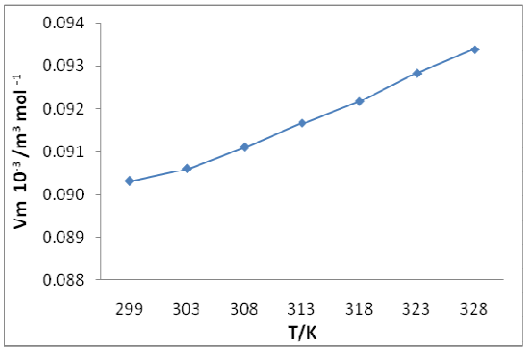


Fig.VII. Variation of V_a 10^{-6}/m^3 mol^{-1} with T/K

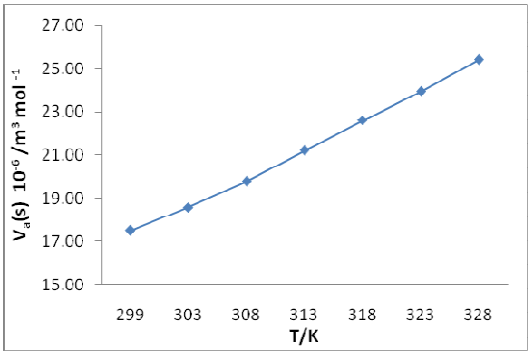


Fig.VIII .Variation of R_a 10^{-4}/m $^{10/3}$ $s^{-1/3}$ mol^{-1} with T/K

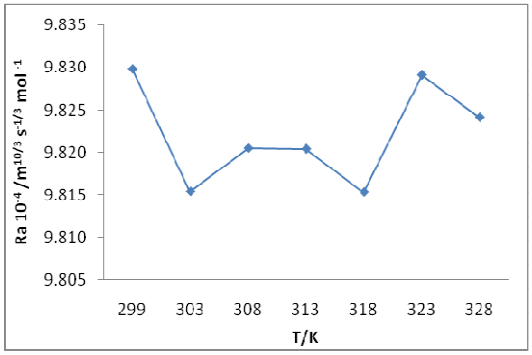
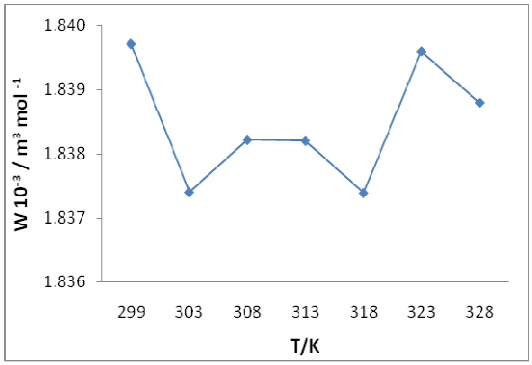


Fig.IX. Variation of W 10^{-3} /m^3 mol^{-1} with T/K



The variation of ultrasonic velocity in a mixture depends upon the increase or decrease of intermolecular free length [20]. Based on the model for sound propagation, Eyring and Kincaid have proposed that intermolecular free length is the dominant factor in determining the variation of ultrasonic velocity of the solution at different temperatures [19]. It is observed from table 2 that, the intermolecular free length increases with increase in temperature, which implies that the mean distance between the molecules increases thereby decreasing the potential energy of interaction between them thus leading to the decrease in the values of velocity and density [21]. The decrease in density with temperature is mainly due to decrease of intermolecular forces due to thermal agitation [22]. The decrease in ultrasonic velocity with increase in temperature indicates the presence of weak molecular interactions between the components of the mixture [23].

It is also observed from table 2 that, the adiabatic compressibility increases with increase in temperature. The adiabatic compressibility increases as the ultrasonic velocity and density decreases as it is evident from the equation 1. This trend is very much observed in our present investigation. Further it is observed that molar volume and available volume also increases with increase in temperature. The increase in adiabatic compressibility, molar volume and available volume with temperature is an indication of weak molecular interactions between the components of the mixture [25]. In the present study the variation of R_a and W with temperature is found to be non-linear and it may be due to the interaction between the solute molecules rather than the solvent benzene [24]. Further, it is also observed from table 2 that, the specific acoustic impedance also decreases with increase in temperature indicating the presence of weak molecular interactions between the components of the mixture.

CONCLUSION

In the present study the various thermo-acoustical parameters viz. adiabatic compressibility, intermolecular free length, specific acoustic impedance, molar volume, available volume, Rao's number and Wada's number have been evaluated from ultrasonic velocity and density at different temperatures. The ultrasonic velocity, density and acoustic specific impedance decreases with increase in temperature, whereas adiabatic compressibility, intermolecular free length, molar volume and available volume increase with increase in temperature. From the above studies, it is observed that weak molecular interactions are present between the components of the mixture and these interactions are found to be decreasing with increase in temperature.

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