Available online www.jocpr.com

Journal of Chemical and Pharmaceutical Research, 2016, 8(2):237-241

Research Article

ISSN : 0975-7384
CODEN(USA) : JCPRC5

Study of molecular interactions in antidepressant drug amitriptyline and benzene at different temperatures

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ABSTRACT

Acoustical studies have been conducted on the binary mixtures of Amitriptyline and Benzene at 2.9979 MHz and at different temperatures from 299K to 328 K using Ultrasonic interferometer. 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). From these various parameters the molecular interactions present in the binary mixture are studied with respect to change in temperature. It is observed that, there are weak molecular interactions present between the components of the mixture and these interactions are found to be decreasing with increase in temperature.

Keywords Ultrasonic velocity, Intermolecular free length, Available volume, Wada's number, molecular interactions

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INTRODUCTION

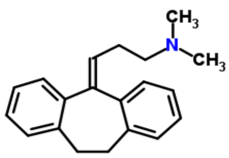
Ultrasonic's offers the most exciting and fascinating field of scientific research among the researchers, since the ultrasonic and other related thermo-acoustical parameters provide useful information regarding the structure of molecules, molecular order, molecular packing, inter and intra molecular interactions[1-3] etc. The ultrasonic study of liquid, liquid mixtures have gained much importance during the last two decades in assessing the nature of molecular interaction and investigating the physico-chemical behavior of the system [4-5]. The study of molecular interactions in the liquid mixtures is of considerable importance in understanding the structural properties of the molecules. The intermolecular interactions influence the structural arrangement along with the shape of molecule. Lagemann and Dunbar were the first to point out the sound velocity approach for qualitative determination of the degree of association in liquids. Recent developments have made it possible to use ultrasonic energy in medicine, agriculture, engineering and other industrial applications [6-12]. The ultrasonic velocity measurements are used in understanding the molecular interactions in pure liquids and binary or ternary mixtures, since the deviations from the linear dependence of velocity and compressibility on the mole fractions provide an insight into the physico-chemical properties of liquid mixtures such as molecular association and dissociation as well as the strength of interaction between the components [13].

Amitriptyline is a tricyclic antidepressant. It is used in pharmaceutical industry to treat symptoms of depression. It works by increasing the amounts of certain natural substances in the brain that are needed to maintain mental balance. It may help to improve mood and feelings of well being, relative anxiety and tension. It may also be used to treat nerve pain, eating disorder etc. It is used to prevent migraine headaches, relieve the long term pains of arthritis and related conditions. It is also used as a weight gainer. In view of these various biological applications of the drug, we have studied the thermo-acoustical parameters of Amitriptyline and Benzene mixture in order to understand the molecular interactions.

EXPERIMENTAL SECTION

The molecular formula of Amitriptyline is $C_{20}H_{23}N$ and its molecular wt is 277.4033 g/mol.

The molecular structure of Amitriptyline is as follows.



The compound Amitriptyline is obtained from Sigma-Aldrich and Benzene of AR grade from s d fine chem. Ltd, India and are used without any further purification. The ultrasonic velocity in the binary mixture is measured for a single weight fraction of 0.0138 using Amitriptyline as solute and Benzene as solvent using the 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 was determined by using a bicapillary pycnometer. Both, ultrasonic velocity and density are measured at different temperatures ranging from 299K to 328K. The accuracy in the density measurement is of the order of ± 0.0003 gm^{-3}. The temperature of the solution was maintained within ± 0.1K using an electronically operated constant temperature water bath. From the experimental data of ultrasonic velocity and density, the various thermo-acoustical parameters like adiabatic compressibility, intermolecular free length, specific acoustic impedance, molar volume, available volume, Rao's number and Wada's number have been determined using the following relations[14],

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

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

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

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

$$V_m = (M_1 f_1 + M_2 f_2) / \rho_{12} \quad (4)$$

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

Where u_∞ = 1,600 m/s

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

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

Where u is ultrasonic velocity, ρ is density, β is adiabatic compressibility, L_f is intermolecular free length, K is the temperature dependent constant known as Jacobson constant [18], Z is specific acoustic impedance, V_m is molar volume, $V_a(s)$ is available volume, R_a is Rao's number , W is Wada's number, M_1 is the molecular mass of solute, M_2 is the molecular mass of solvent, f_1 is the mole fraction of solute, f_2 is the mole fraction of solvent, ρ_{12} is the density of the solution, and T is the absolute temperature.

RESULTS AND DISCUSSION

The experimentally measured values of ultrasonic velocity and density at different temperatures are given in table 1. The calculated parameters like adiabatic compressibility (β), intermolecular free length (L_f), specific acoustic impedance (Z) are presented in the table 2. The molar volume (V_m), available volume V_a(s), Rao's number (R_a), Wada's number (W) 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	1285.50	876.10
303	1272.31	872.88
308	1249.52	868.37
313	1226.74	863.20
318	1203.96	857.76
323	1183.57	852.53
328	1163.78	847.73

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	6.9072	0.5414	1.1262
303	7.0772	0.5520	1.1106
308	7.3757	0.5686	1.0850
313	7.6981	0.5861	1.0589
318	8.0429	0.6044	1.0327
323	8.3734	0.6221	1.0090
328	8.7096	0.6400	0.9866

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	0.9005	17.7006	97.9137	1.8331
303	0.9038	18.5110	97.9370	1.8335
308	0.9085	19.9009	97.8545	1.8321
313	0.9140	21.3216	97.8388	1.8319
318	0.9198	22.7665	97.8457	1.8320
323	0.9254	24.0853	97.8873	1.8327
328	0.9306	25.3726	97.8903	1.8327

The variation of ultrasonic velocity, density, 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), Wada's number(W) with temperature are shown in the figures from I-IX respectively.

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

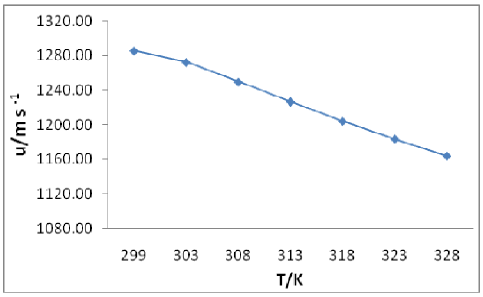


Fig. II. Variation of ρ /Kg m^{-3} with T/K

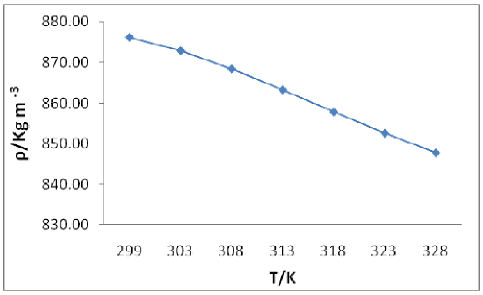


Fig.III. Variation of β 10^{-10} / m^2N^{-1} with T/K

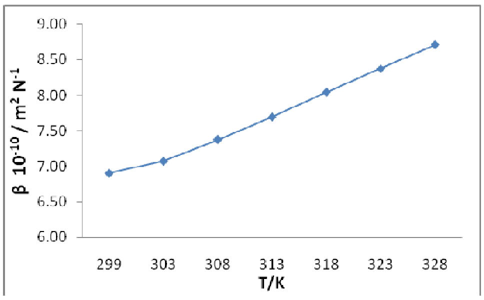


Fig.IV. Variation of L_f 10^{-10} /m with T/K

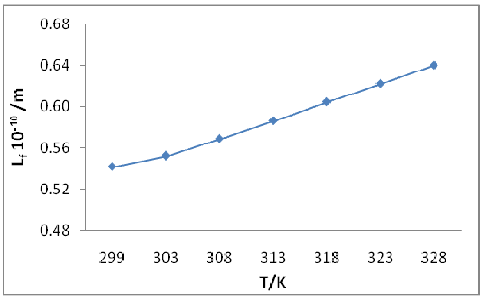


Fig.V. Variation of Z 10^6/Kg $m^{-2}s^{-1}$ with T/K

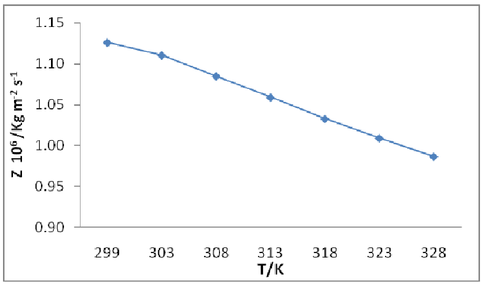


Fig.VI. Variation of V_m 10^{-3}/m^3 mol^{-1} with T/K

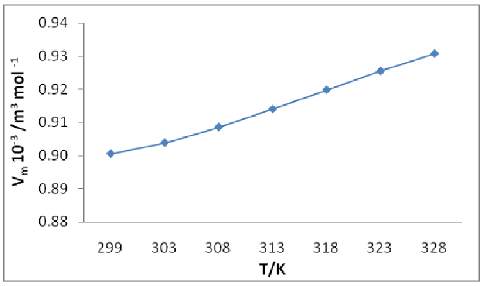


Fig.VII. Variation of V_a 10^{-6}/m^3 mol^{-1} with T/K

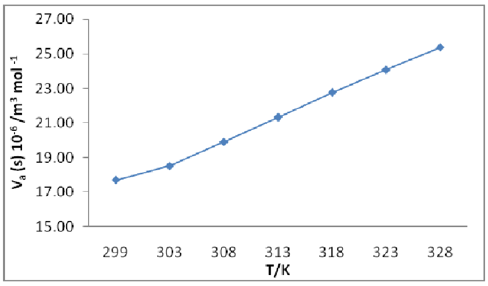


Fig.VIII .Variation of R_a 10^{-4}/m $^{10/3}$ $s^{-1/3}$ mol^{-1} with T/K

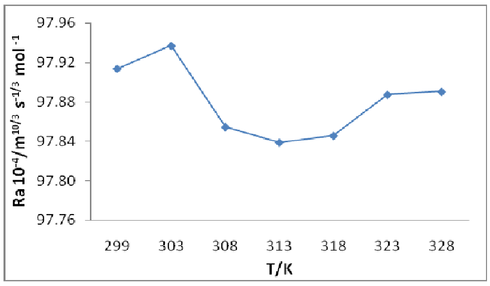
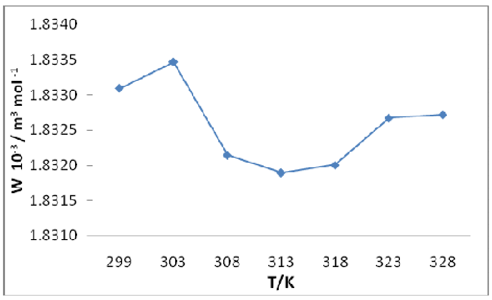


Fig.IX. Variation of W 10^{-3} /m^3 mol^{-1} with T/K



The intermolecular free length is the distance covered by a sound wave between the surfaces of the neighboring molecules and it depends upon the intermolecular attractive and repulsive forces. The variation of ultrasonic velocity in a mixture depends upon the increase or decrease of intermolecular free length [17]. Based upon the model for sound propagation, Eyring and Kincaid have proposed that free length is the dominant factor in determining the variation of ultrasonic velocity of the solution [16]. It is observed from table 2 that, the intermolecular free length increases with increase in temperature. The increase in the value of intermolecular free length with temperature 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 [18]. The decrease in density with temperature is mainly due to decrease of intermolecular forces due to thermal agitation [19]. The decrease in ultrasonic velocity with increase in temperature indicates the presence of weak interactions between the components of the mixture [20].

The compressibility is a measure of the ease with which a medium can be compressed. In the present study, it is found that, adiabatic compressibility increases with increase in temperature, which implies that the molecules tend to become loosely packed with increase in temperature. Further, the molar volume also increases with increase in temperature as it is evident from table 3. The increase in adiabatic compressibility and molar volume with temperature is an indication of weak molecular interactions between the components of the mixture [22].

The available volume is the direct measure of compactness and strength of binding between the molecules of the mixture. In the present study, it is observed that, available volume increases with increase in temperature indicating the decrease of compactness in the mixture. The variation of R_a and W with temperature is found to be non-linear and it may be due to the interactions between the solute molecules rather than the solvent benzene [21]. The acoustic impedance is the impedance offered to the sound wave by the components of the mixture. It is found that, in the present study, acoustic impedance decreases with increase in temperature, which also implies that, the molecular interactions decreases with increase in temperature.

CONCLUSION

The ultrasonic study of the binary mixtures serves as a probe to detect the presence of molecular interactions occurring between the components. In the present study the ultrasonic velocity and density have been measured experimentally and 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 are calculated for different temperatures ranging from 299K to 328 K. The decrease of ultrasonic velocity, density, acoustic impedance and increase of intermolecular free length, adiabatic compressibility, molar volume and available volume with temperature indicates the presence of weak molecular interaction between the components of the mixture and further it is observed that, these interactions are found to be decreasing with increase in temperature.

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