STUDY OF INTERMOLECULAR INTERACTIONS FOR BUTAMBEN AND BENZOCAINE BY USING ACETONE AND MIXTURE OF WATER-ACETONE AT 305.15K

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Abstract:
Ultrasonic velocity (U) and density (ρ) have been measured for Butamben and Benzocaine in acetone and water-Acetone (1:1) mixtures at 305.15K. Using that experimental values acoustical parameters like adiabatic compressibility (β), apparent molar compressibility (Kϕ) and relative association (RA) were calculated and the results of these parameters have been comparatively discussed in terms of solute –solvent and solute-co-solute interactions between the components.

Key words: Ultrasonic interferometer, adiabatic compressibility, apparent molar compressibility and Relative association.

Introduction:

The term "Ultrasonic" applied to sound refers to anything above the frequencies of audible sound and nominally includes anything over 20,000 Hz. These sound waves are used by bats as a kind of navigational radar for night flying[1]. Ultrasonic velocity studies have contributed significantly to chemical physics, industrial technology, biomedical sciences and food industries (A. Ali et al., 2000)[2]. Nowadays Acoustic sonograms have become important medicinal diagnostic tool [3-11].

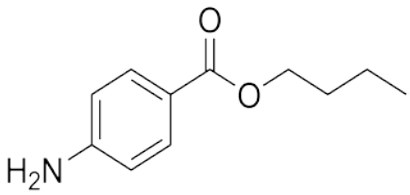
The principle behind interferometer is that the solvent molecules are attached to the ions strongly by the electrostatic forces which introduce a greater cohesion in the solution. The increased association observed in these solutions may also be due to solvent structure enhancement brought about by the increase in electrostriction effect which brings about the shrinkage in the volume of solvent. From the experimental values of acoustical parameters namely ultrasonic velocity, adiabatic compressibility, apparent molar compressibility and Relative association has been calculated. The variation of these parameters was found to be useful in understanding the nature of interactions between the components of solute and solvent. Many scientists used this technique as an effective analytical tool to study acoustical and thermodynamic properties. Variations of thermo dynamical parameters with molar concentration of ChCl urea in aqueous L-Alaline were studied by S.S.Nandre[12].

Butamben is a non-steroidal anti-inflammatory drug (NSAID). It works as local anesthesia. It blocks nerve conduction when applied locally to nerve tissue in appropriate concentrations. It acts on any part of the nervous system and on every type of nerve fiber. In contact with a nerve trunk these anesthetics can cause both sensory and motor paralysis in the innervated area. Their action is completely reversible.

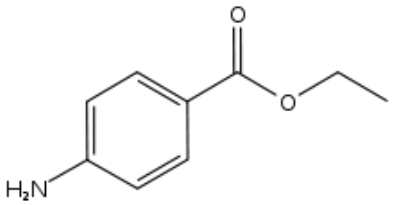
Benzocaine is used to reduce the pain which is caused by the stimulation of free nerve endings. When the nerve endings are stimulated then sodium enters the neuron because of this depolarization of the nerve happened and subsequent initiation of an action potential. The action potential is propagated down the nerve towards the central nervous system which interprets this as pain. Benzocaine acts to inhibit the voltage dependant sodium channels on the nerve membrane stopping the propagation of the action potential.

Selection of drugs

Butamben: Butyl 4-aminobenzoate



Benzocaine: Ethyl 4-aminobenzoate



Materials and Method:-

Butamben and Benzocaine API samples were provided by Ramdev Chemicals. Advanced electronic densitometer Anton Paar-35 having accuracy of ± 0.1 kg/m3 was used to measure the density which simultaneously shows the temperature and density of solutions.

Single crystal interferometer (Mittal Enterprises, Model F-81) with accuracy of ± 0.03% and frequency 2, 4, 6 MHz, were used in the present work.

AR grade Acetone and equal ratio mixture of double distilled water and acetone were used as diluents for preparation of sample solutions. Weighing of sample was done on digital balance Model CB/CA/CT-Series, Contech, having accuracy 0.0001g. Calibration of interferometer instrument was done by measuring the ultrasonic velocity of pure water at 303.15K. The measured value 1511 ms-1 is very close to theoretical[13] value 1515 ms-1 and thus confirms the accuracy of instrument. Constant digital temperature water bath was used to maintain the constant temperature with an accuracy of ±0.1K

Using standard relations some acoustical parameters have been calculated.

The adiabatic compressibility (β) is evaluated by using equation.

β = 1 / v2.□□ …… (1)

Where, v= ultrasonic velocity and □= density

Apparent molar compressibility (Kϕ) is an acoustic property which is determined by measuring density and ultrasonic velocity and depends upon the molality of solution and molecular weight of the solute by the relation,

Kϕ = [1000 (β s ρ 0 – β 0 ρs) / m ρs ρ0] + (β s M / ρs) …… (2)

Where, ρ0 = density of pure solvent, ρs = density of solution, m = molality of solution, M = molecular weight of solute, β 0 = adiabatic compressibility of pure solvent, and β s = adiabatic compressibility of solution.

The solute-solvent interactions may be interpreted in terms of acoustic impedance. Relative association is a function of ultrasonic velocity and is computed by the equation,

RA = ρs/ρ0 (v0/vs) 1/3 …. (3)

Where, v0 and vs. are ultrasonic velocities of solvent and solution

Results and discussion:

Table 1: 0.01M solution of Butamben at temperature 303.15 K

MHz	Solvents	Density of Solution (Kg/m3) (ρ)	Ultrasonic velocity of Solution m/s (v)	Adiabatic compressibility (β)	Apparent molar compressibility	Relative association
2	Acetone	777.73	3.2793	$1.1957E^{-10}$	$1.530E^{-08}$	0.9378
	Water: Acetone 1:1	929.16	1.7310	$3.5917E^{-10}$	$3.864E^{-08}$	0.9836
4	Acetone	777.73	6.7101	$2.8557E^{-11}$	$3.620E^{-09}$	0.9145
	Water: Acetone 1:1	929.16	4.2004	$6.1001E^{-11}$	$6.50\ E^{-09}$	0.8589
6	Acetone	777.73	12.0019	$8.9263E^{-12}$	$1.18\ E^{-09}$	0.9398
	Water: Acetone 1:1	929.16	9.5929	$1.1695E^{-11}$	$1.27\ E^{-09}$	0.8229

Table 2: 0.01M solution of Benzocaine at temperature 303.15 K

MHz	Solvents	Density of Solution (Kg/m3) (ρ)	Ultrasonic velocity of Solution m/s (v)	Adiabatic compressibility (β)	Apparent molar compressibility	Relative association
2	Acetone	777.20	1.7812	$4.0556E^{-10}$	$5.225\ E^{-08}$	1.1486
	Water: Acetone 1:1	929.79	1.7626	$5.8925E^{-11}$	$6.330\ E^{09}$	0.8547
4	Acetone	777.20	4.4031	$6.6368E^{-11}$	$8.547\ E^{-09}$	1.0517
	Water: Acetone 1:1	929.79	4.2723	$5.8925E^{-11}$	$6.330\ E^{-09}$	0.8547
6	Acetone	777.20	9.5832	$1.4010E^{-11}$	$1.804\ E^{-09}$	1.0123
	Water: Acetone 1:1	929.79	6.8056	$2.3221E^{-11}$	$2.497\ E^{-09}$	0.9233

These acoustic parameters are directly reflecting the structural interaction of solvents with solute and explore valuable and important information regarding internal structure and molecular association.

According to Pagare et.al[14] the increase in ultrasonic velocity in any solution shows the greater association among the components of the mixture. The greater association is due to hydrogen bonding between solute and solvent molecules. Looking towards the graph it was observed that from 2 to 4 MHz benzocaine gives somewhat same result in both the solvents i.e. in acetone and water: acetone (1:1). But in case of butamben shows greater velocity in acetone as compare to acetone: water (1:1). This increase in ultrasonic velocity is due to molecular association and cohesion brought about by the ionic hydration.

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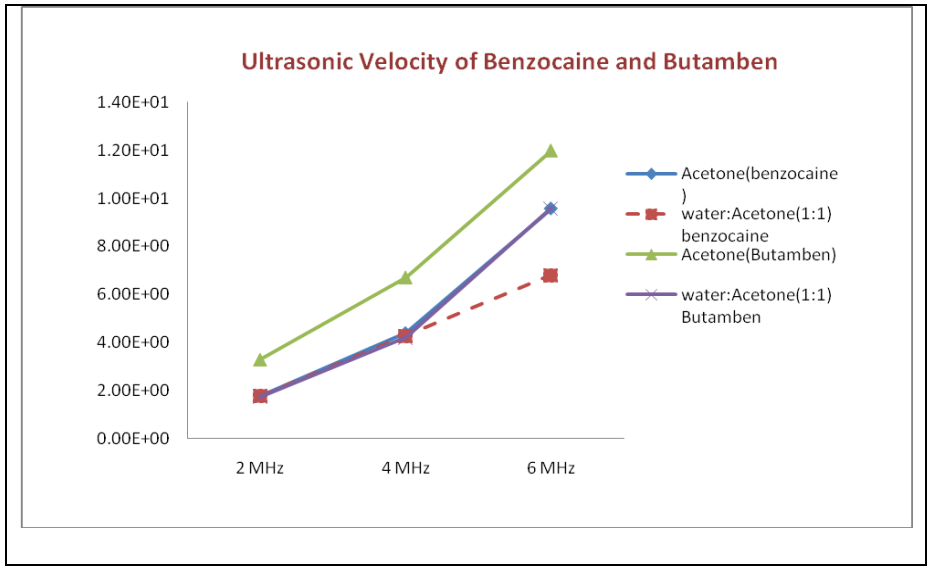

Figure 1: Ultrasonic Velocity of Benzocaine and Butamben at 0.01M and 303.15K

According to S. R. Kanhekar, decrease in compressibility indicates that there is enhanced molecular association in the system upon increment of solute[15]. The influence of the electrostatic field of solute molecules on the surrounding solvent molecules results the decrease in adiabatic compressibility. Butamben and Benzocain both shows decreasing trend of adiabatic compressibility in both the solvents. But butamben has less compressibility value in acetone as compared to the benzocain which has high compressibility value at all three frequencies. This may be due to additional methylene group present in butamben compare to benzocaine which contributes in formation of bulky structure of butamben with the acetone. Apart from that Butamben and Benzocain shows same behavior in water: acetone (1:1) solution at all 3 frequencies.

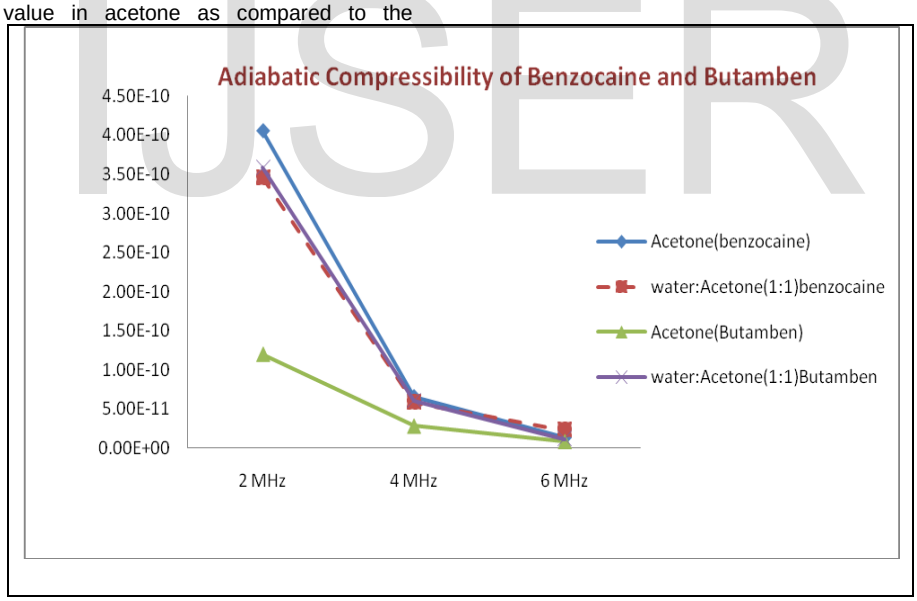

Figure 2: Adiabatic Compressibility of Benzocaine and Butamben at 0.01M and 303.15K

Both drugs show similar descending trend of apparent molar compressibility in both the solvents. But from fig 3, it was observed that, (Kϕ) values show greater decrease in acetone: water mixture for benzocaine as compare to acetone, this may be due to the weaker interaction between ions and solute molecules, which suggest the structure promoting behavior of solute. This may also imply that the increase in free ions, showing the occurrence of ionic dissociation due to weak ion-ion interaction.

Butamben shows somewhat reverse trend from that of benzocaine i.e. in acetone: water mixture apparent molar compressibility is greater decrease and in acetone it found lesser. The decreasing values of apparent molar compressibility in all the two system reveals that, more strengthening the solute–solvent interactions exist in these mixtures. Different results found may be because of additional methylene group in butamben.

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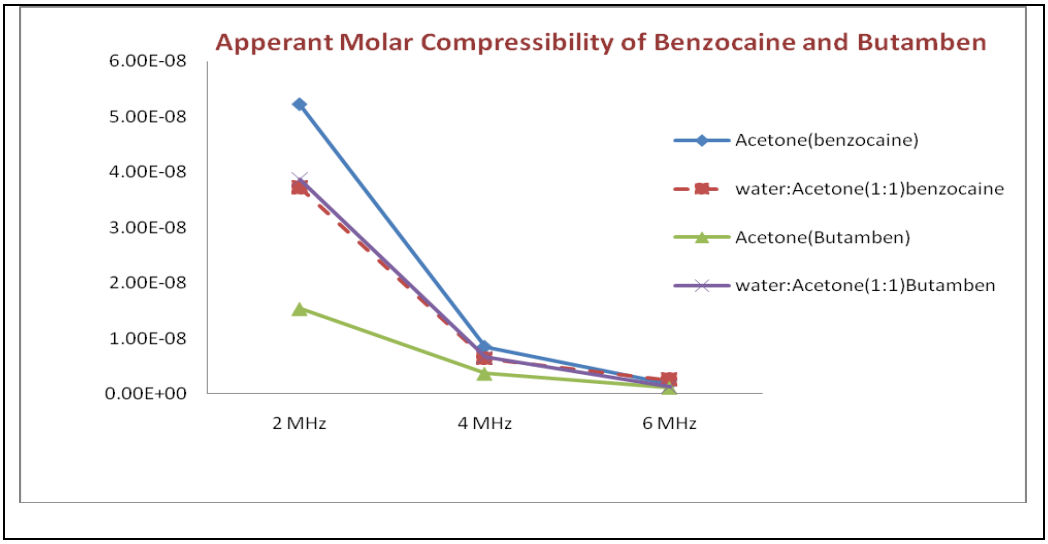

Figure 3: Apparent molar compressibility of Benzocaine and Butamben at 0.01M at 303.15K

Relative association is the measure of extent for association of components in the solution. The relative association depends on either of breaking up of the solvent molecules on addition of solute to it or the salvation of ions that are present. From fig 4 it was observed that Butamben and Benzocaine gives different results of Relative association in both the solvent (From fig 4). In acetone benzocaine shows decreasing trend from 2 to 6 MHz which may be due to breaking up of solvent molecules on addition of acetone in it.

Where as in acetone: water (1:1) system it decreases from 2 to 4 MHz and then slightly increases at 6 MHz this may be because of salvation of solute[16]. Butamben shows decreasing trend in acetone: water (1:1) and in pure acetone relative association shows decreasing trend from 2 to 4 MHz and then increases up to 6MHz. This change is may be because of nature of component in butamben there is presence of linkage of methylene group which is supported by higher density value which makes solution medium become denser.

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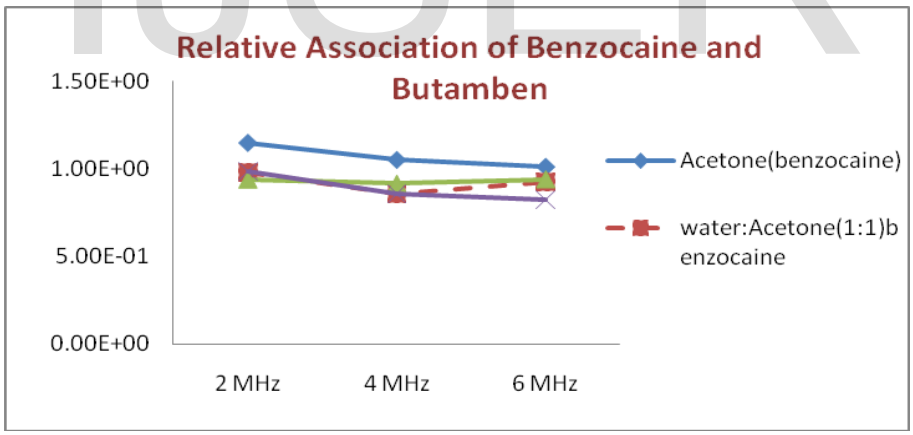

Figure 4: Relative association of Benzocaine and Butamben at 0.01M and 303.15K

Conclusion:

It can be concluded that there is an appreciable existence of solute-solute interactions in the benzocaine and butamben with acetone and Acetone-water mixture with varying degrees, hence it is evaluate that the ultrasonic velocity measurement in the given medium serves as a powerful probe in characterizing the physio-chemical properties of the media.

It is found that benzocaine has stronger interaction with acetone and weak interactions with solvent acetone: water (1:1). The strong interaction of benzocaine with acetone is due to dipole-induced dipole moment. Butamben shows strong interaction with solvent (acetone: water). The weak interactions are due to predominance of dispersive force over dipole-dipole interaction.

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