



MOLECULAR INVESTIGATION IN AQUEOUS SOLUTION OF DOXYCYCLINE AT DIFFERENT CONCENTRATIONS AND TEMPERATURES BY ULTRASONICALLY

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ABSTRACT:

Ultrasonic velocity plays a vital role to understand molecular interaction existing in the solution. Drugs are the compound which is used to cure diseases. Doxycycline is antimalarial drug. Densities, viscosities of aqueous solution of doxycycline were measured at different concentrations and at different temperatures. From the experimental values thermodynamic parameters were calculated. From it molecular interaction was predicted.

Keywords: - Antimalarial, Doxycycline, Ultrasonic, Molecular Interaction.

INTRODUCTION :

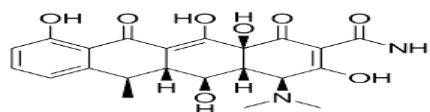
In the recent years Ultrasonic measurements play a vital role in chemical and food processing, pharmaceuticals, testing of material and mechanical machinery of materials¹⁻⁵. There is some considerable interest to aware the intermolecular interaction in liquid mixtures. The main usage of organic mixtures have used for processing and further formulations of product. Physicochemical properties of pure and mixtures of organic liquids are having great importance in the field of science and industrial engineering. The thermodynamic properties like adiabatic compressibility, acoustic impedance is used to classify the various intermolecular interactions between the different species exist in solution.

A drug is any chemical substance that causes a change in an organism's physiology or psychology when consumed ⁶⁻⁷ Drugs are typically distinguished from food and substances that provide nutritional support. Consumption of drugs can be via inhalation, injection, and smoking, and ingestion, absorption via a patch on the skin, suppository, or dissolution under the tongue. Antimalarial drugs are used for the

treatment and prevention of malaria infection. Most antimalarial drugs target the erythrocyte stage of malaria infection. Doxycycline is an antibiotic that also can be used to prevent malaria. Doxycycline, a synthetically derived tetracycline, is a partially efficacious causal prophylactic (liver stage of Plasmodium) drug and a slow acting blood schizontocidal agent highly effective for the prevention of malaria.⁸

In the present study ultrasonic velocity, density and viscosities of aqueous solution of doxycycline at different concentration s and at different temperature was measured. This data is useful to calculate thermodynamic parameters such as adiabatic compressibility, acoustic impedance. From these reactivity and molecular interaction of the drug is predicted.

The structure of doxycycline is



Experimental:

The ultrasonic velocity (U) in liquid mixtures which prepared by taking purified AR grade samples, have been measured using an ultrasonic interferometer (Mittal type, Model F-

81) working at 2MHz frequency and at temperature 298K,303K and 308K . The accuracy of sound velocity was $\pm 0.1 \text{ ms}^{-1}$. An electronically digital operated constant temperature water bath has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desire temperature. The density of pure liquids and liquid mixtures was determined using density bottle by relative measurement method with an accuracy of $\pm 0.1 \text{ Kg m}^{-3}$.

RESULT & DISCUSSION :

The strength of the repulsive forces acting among solvent and solute molecules effects the molecular interaction. And hence intermolecular motion is affected accordingly. molecular association is due to attractive forces. Molecular association changes in mass and hence density changes.

From the table 1,2 and 3 and fig. 1 it shows that the density, and ultrasonic velocity of the solution increases with increase in concentration and temperatures . This linear increase in velocity, density and viscosity with concentration and temperature confirms an increase of cohesive forces because of strong molecular interactions ⁹.The variation of ultrasonic velocity in a solution depends on the intermolecular free length on mixing. On the basis of a model for sound propagation proposed by Kincaid and Eyring ¹⁰ ultrasonic velocity increases with decrease of free path length and vice versa.

From fig.2and fig.3 Decrease of adiabatic compressibility and free length with concentration and temperatures supports solvent-solute interactions. This indicates a strong intermolecular interaction between solute and solvent molecules due to formation of hydrogen bonding between doxycycline and water molecule. As a result of weakening of molecules interaction forces between donor and

acceptor free length decreases and hence strong solute solvent interaction exist in the solution ¹¹. Acoustic impedance increases with increase in concentration and temperatures suggest strong molecular in

CONCLUSION:

Teraction between solute and solvent.

From the values of ultrasonic velocity, density, adiabatic compressibility free length and acoustic impedance it shows that strong solute solvent interaction present in the the solution of doxycycline at 308K.

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Table 1: Ultrasonic velocity, densities, viscosities adiabatic compressibility's, intermolecular free length acoustic impedance of aqueous solution of Doxycycline at different concentrations and at 298K

Sr. No	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg)	Viscosity	Adiabatic Compressibility $\gamma \times 10^{-10}$	Intermolecular Free length (A°)	Specific impedance $\times 10^4$
1	0.01	1511.13	1260.90	1.143	3.47	0.0372	19.0617
2	0.02	1511.68	1273.65	1.150	3.43	0.0370	19.2535
3	0.03	1511.71	1277.36	1.165	3.42	0.0369	19.3076

Table 2: Ultrasonic velocity, densities, viscosities adiabatic compressibility's, intermolecular free length acoustic impedance of aqueous solution of Doxycycline at different concentrations and at 303K

Sr. No	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg)	Viscosity	Adiabatic Compressibility $\gamma \times 10^{-10}$	Intermolecular Free length (A°)	Specific impedance $\times 10^4$
1	0.01	1511.39	1265.46	1.015	3.45	0.0371	19.6828
2	0.02	1512.00	1274.35	1.033	3.43	0.0370	19.2681
3	0.03	1555.62	1279.20	1.039	3.23	0.0359	19.3366

Table 3: Ultrasonic velocity, densities, viscosities adiabatic compressibility's, intermolecular free length acoustic impedance of aqueous solution of Doxycycline at different concentrations and at 308K

Sr. No	Concentration (M)	Ultrasonic Velocity (m/s)	Density (Kg)	Viscosity	Adiabatic Compressibility $\gamma \times 10^{-10}$	Intermolecular Free length (A°)	Specific impedance $\times 10^4$
1	0.01	1554.19	1271.46	0.923	3.24	0.0360	19.7990
2	0.02	1554.96	1277.30	0.980	3.23	0.0359	19.8615
3	0.03	1557.48	1290.91	1.001	3.19	0.0357	20.0669

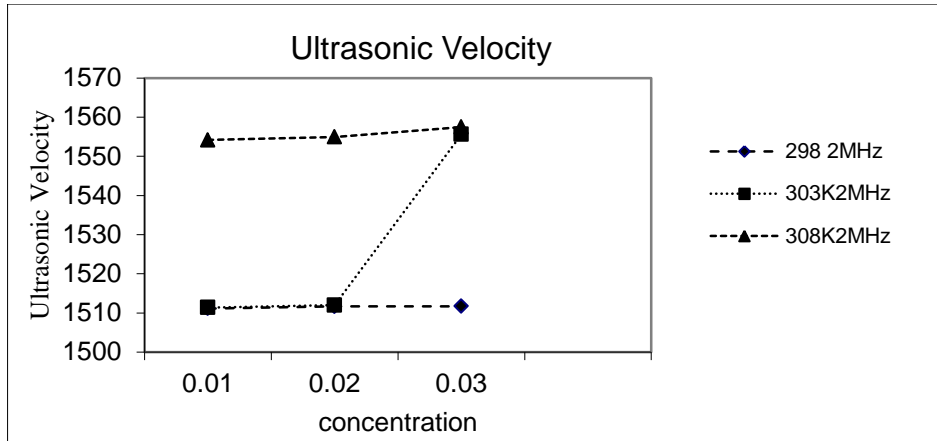


Fig. 1: Ultrasonic Velocity of aqueous solution of Doxycycline at different concentrations and temperatures

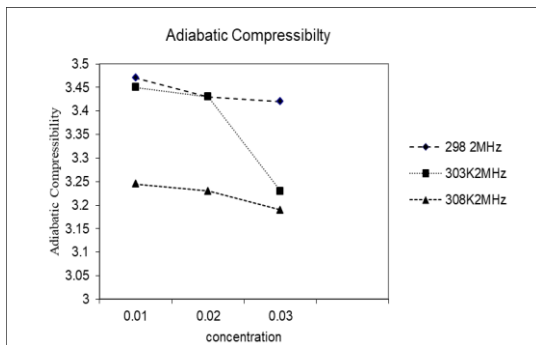


Fig. 2: Adiabatic Compressibility of aqueous solution of Doxycycline at different concentrations and temperature

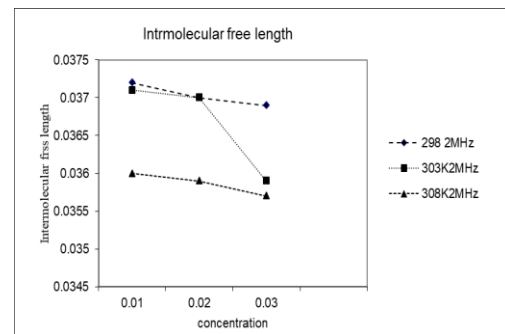


Fig. 3 : Intermolecular Free Length of aqueous of Doxycycline at different concentrations and temperature