

# An Ultrasonic Study of Molecular Interactions in the Leaf Extract Solution of *Thuja Occidentalis*

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## ABSTRACT

Ultrasonic Velocity, density, viscosity have been measured experimentally for the solution of leaf extract of *Thuja Occidentalis* in 50% ethyl alcohol with various concentrations at 298.15 K, 303.15 K, 308.15 K keeping constant frequency of 2 MHz. As the acoustical parameters like adiabatic compressibility, intermolecular free length, relative association, relaxation time, specific acoustic impedance would prove to be more useful to predict and confirm the molecular interactions, these have been determined by measuring the Ultrasonic Velocity, density, viscosity of the prepared solution. A variation in these parameters will provide a strong information regarding the molecular interactions taking place in the solution.

**Keywords :** Ultrasonic Velocity, Adiabatic Compressibility, Relative Association, Intermolecular Free Length.

## I. INTRODUCTION

In recent years ultrasonic technique has become a powerful tool in providing information regarding the molecular behavior of the liquids, polymer solutions and mixtures etc. owing to its ability of characterizing physico-chemical behavior of the medium. Ultrasonic velocity measurements and other acoustic parameters of liquid mixtures are the powerful technique in understanding of chemical nature and the molecular interactions. Our country is very well known for Ayurveda, in the Ayurveda medicines are largely made up from plants, herbs. One of such plants is which is also known as *Thuja Occidentalis*. *Thuja* is known for its antifungal nature. The solution of leaf extract of *Thuja Occidentalis* in 50% ethyl alcohol is studied at 2 MHz for the concentration of 1%, 0.5%,

0.25%, 0.125% at 298.15K, 303.15K, 308.15K. Here the effect of concentration at different temperature on molecular interaction will be predicted which may be helpful for predicting the reactivity of the extract.

## II. METHODS AND MATERIAL

The leaf extract used in this study was of analytical range. 50% ethyl alcohol was used for the preparation of solution. A special thermostatic water bath arrangement was made to maintain constant temperature. 1%, 0.5%, 0.25%, 0.125% solutions of leaf extracts of *Thuja Occidentalis* was Prepared by taking accurate weights on electronic digital balance (Model CB/CA/CT-Series, Contech having

accuracy ± 0.0001 g.) The ultrasonic velocity of the 1%, 0.5%, 0.25%, 0.125% solutions of leaf extracts of *Thuja Occidentalis* was measured with the Multifrequency ultrasonic interferometer (Model M-83, Mittal Enterprises) at 2 MHz frequency with an accuracy of ± 2 m/s. All the readings were taken at 298.15 K, 303.15K, 308.15K. The viscosity was measured by using Ostwald's viscometer and the density of the solution was measured by using Digital densitometer (DMA-35, Anton Paar)

**Computation :**

By using ultrasonic velocity following ultrasonic parameters are calculated.

**Adiabatic compressibility** -  $\beta = 1/v_s^2 d$

**Table 1 : Density, Viscosity and Velocity (at frequency 2 MHz) of Thuja occidentalis leaf extract solution.**

Sr. No.	Conc. (%)	Temp. (K)	Density (d <sub>s</sub> ) (Kg m <sup>-3</sup> )	Velocity (v <sub>s</sub> ) (m/s)	Viscosity (η) (Kg m <sup>-1</sup> s <sup>-2</sup> )
1	1%	298.15	931.6	1603	23.50 E <sup>-4</sup>
		303.15	922.5	1342	21.80 E <sup>-4</sup>
		308.15	920.4	1350	17.42 E <sup>-4</sup>
2	0.5%	298.15	936.7	1384	18.30 E <sup>-4</sup>
		303.15	930.4	1512	20.50 E <sup>-4</sup>
		308.15	968.9	1439	12.44 E <sup>-4</sup>
3	0.25%	298.15	924.5	1471	21.27 E <sup>-4</sup>
		303.15	927.0	1503	21.51 E <sup>-4</sup>
		308.15	927.4	1330	16.85 E <sup>-4</sup>
4	0.125%	298.15	925.0	1451	18.12 E <sup>-4</sup>
		303.15	921.8	1514	16.05 E <sup>-4</sup>
		308.15	918.4	1385	12.85 E <sup>-4</sup>

Where, v - velocity of solution,

d - density of liquid

**Intermolecular free length** -  $L_f = K\sqrt{\beta_s}$

Where, K - temperature dependent known as Jacobson's constant

**Specific acoustic impedance** -  $Z = v \times d_s$

**Relative association** -  $R_A = d_s / d_0 [v_0 / v_s]^{1/3}$

Where, v<sub>0</sub> - ultrasonic velocity of solvent

v<sub>s</sub> - ultrasonic velocity of solution

**Relaxation time** -  $\tau = 4/3 \beta_s \times \eta$

**III. RESULTS AND DISCUSSION**

The experimentally determined values are listed in the following table.

**Table 2 :- Acoustic parameters of Thuja leaf extract solution in 50% Ethyl Alcohol at 2 MHz.**

Sr. No.	Conc. (%)	Temp. (K)	Adiabatic Compressibility	Specific Acoustic Impedence Kg M <sup>-2</sup> S <sup>-1</sup>	Intermolecular free length	Relative Association	Relaxation time
1.	1%	298.15	4.177 E <sup>-10</sup>	1493354	4.20 E <sup>-11</sup>	3.169 E <sup>-1</sup>	13.05 E <sup>-13</sup>
		303.15	6.019 E <sup>-10</sup>	1237995	5.09 E <sup>-11</sup>	3.519 E <sup>-1</sup>	17.45 E <sup>-13</sup>

2.	0.5%	308.15	5.961 E <sup>-10</sup>	1242540	5.11 E <sup>-11</sup>	3.410 E <sup>-1</sup>	13.81 E <sup>-13</sup>
		298.15	5.573 E <sup>-10</sup>	1296392	4.85 E <sup>-11</sup>	3.689 E <sup>-1</sup>	13.56 E <sup>-13</sup>
3.	0.25 %	303.15	4.701 E <sup>-10</sup>	1406764	4.49 E <sup>-11</sup>	3.150 E <sup>-1</sup>	12.80 E <sup>-13</sup>
		308.15	4.984 E <sup>-10</sup>	1336687	4.67 E <sup>-11</sup>	3.367 E <sup>-1</sup>	8.24 E <sup>-13</sup>
		298.15	4.998 E <sup>-10</sup>	1359939	4.59 E <sup>-11</sup>	3.427 E <sup>-1</sup>	14.13 E <sup>-13</sup>
		303.15	4.775 E <sup>-10</sup>	1393281	4.53 E <sup>-11</sup>	3.156 E <sup>-1</sup>	13.66 E <sup>-13</sup>
		308.15	6.098 E <sup>-10</sup>	1233442	5.17 E <sup>-11</sup>	3.487 E <sup>-1</sup>	13.67 E <sup>-13</sup>
4.	0.12 5%	298.15	5.129 E <sup>-10</sup>	1342804	4.65 E <sup>-11</sup>	3.473 E <sup>-1</sup>	12.36 E <sup>-13</sup>
		303.15	4.730 E <sup>-10</sup>	1395973	5.99 E <sup>-11</sup>	3.117 E <sup>-1</sup>	10.09 E <sup>-13</sup>
		308.15	5.673 E <sup>-10</sup>	1272351	4.99 E <sup>-11</sup>	3.552 E <sup>-1</sup>	9.69 E <sup>-13</sup>

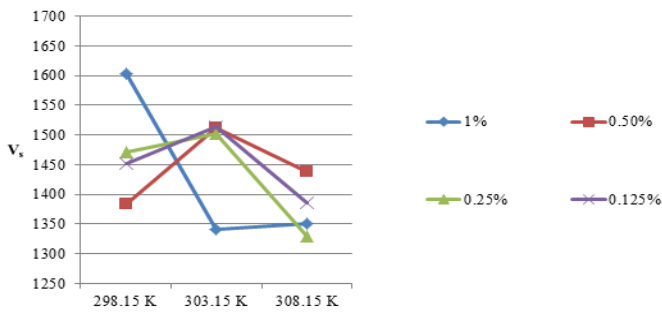


Fig.1 Variation of ultrasonic Velocity with temperature at different conc.

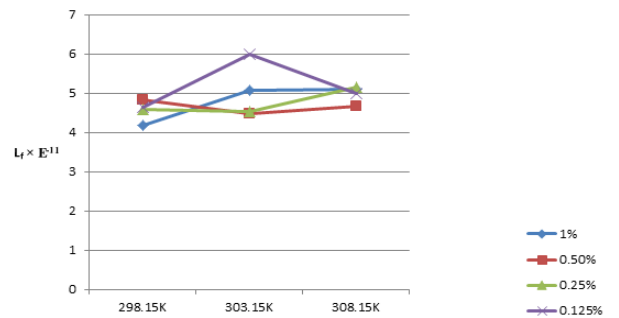


Fig. 4 Variation of Intermolecular free length with temperature at various concentrations

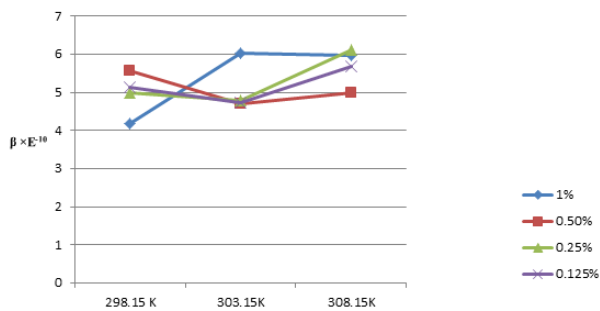


Fig.2-Variation of Adiabatic compressibility with temp. at different conc.

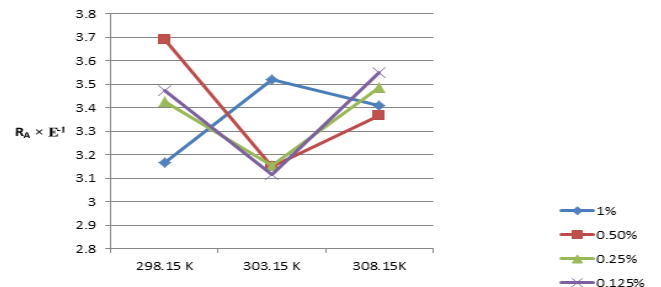


Fig. 5-Variation of Relative Association with temp.at various concentrations

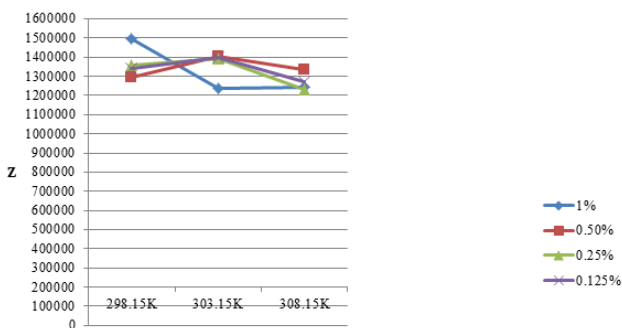


Fig.3 Variation of Specific acoustic impedance with temperature at different concentration

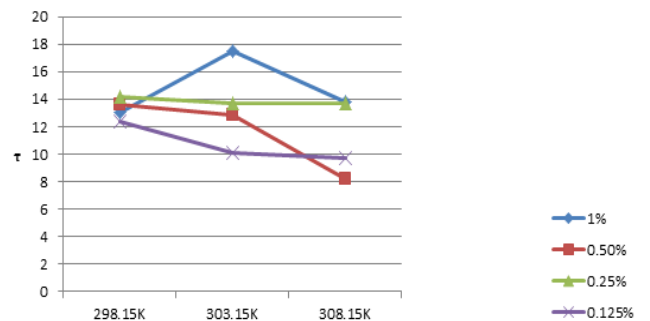


Fig.6. Variation of Relaxation time with temperature at different concentrations

The ultrasonic velocity of 1%, 0.5%, 0.25%, 0.125% *Thuja occidentalis* leaf extract solution in 50% ethyl alcohol was measured at 298.15 K, 303.15K, 308.15K at 2 mhz frequency. From table no.1, it is observed that the ultrasonic velocity increases with decrease in concentration particularly for 0.5% and 0.125% concentration, but this increase is not regular as we can see from the table no.1 and figure no.1. This may be due to the fact that solute molecules form a strong hydrogen bonds with solvent molecules H<sub>2</sub>O and C<sub>2</sub>H<sub>5</sub>OH. It affects the propagation of ultrasonic waves through the solution. Further it is observed for selected temperatures. From table no.2 and fig.2 it is observed that Adiabatic compressibility increase with increase in concentration. The increase in adiabatic compressibility shows significant molecular interactions. A strong evidence for solute - solvent interaction is that the value of specific acoustic impedance increases with increase in concentration in figure 3. The intermolecular free length is the distance between the surfaces of the neighbouring molecules. Here the intermolecular free length decreases with increase in concentration which clearly indicates strong solute- solvent interaction figure 4. Relative association is a measure of extent of association of components in the medium. It is a property of understanding the molecular interaction in liquid mixtures and solutions. As discussed relative association depends on either of breaking of solvent molecules on addition of solute to it or the salvation of ions that are present. The result shows that relaxation time and relative association increase with increase in concentration at a given temperature (fig.5 & fig.6).

#### IV.CONCLUSION

From the above discussion a non linear variation in adiabatic compressibility, specific acoustic impedance, free length, relative association, relaxation time is observed in the system. The ultrasonic velocity values significantly increases for lower concentrations

particularly for 0.5% and 0.125% due to strong hydrogen bonding with solvent molecules. It is observed that molecular association between *Thuja occidentalis* leaf extract molecules and 50% ethanol solvent may arise from intermolecular hydrogen bonding which supports the molecular association occurring in the solution.

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