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Research Article

MOLECULAR INTERACTION WITH RESPECT TO THERMO-DYNAMICAL AND ACOUSTICAL STUDIES OF AQUEOUS MESITOL AND PYROGALLOL

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ABSTRACT

The thermodynamic and acoustical study elucidates the nature of interactions between molecules in liquids and solutions. Also ultrasonic parameters are directly related to a number of thermodynamic parameters. As the different liquid state theories are based on thermodynamic considerations, the study of propagation of ultrasonic waves in liquid systems is established as a simple and effective tool in determining the nature of interactions between molecules in liquids and solutions. Using ultrasonic velocity measurements, Adiabatic Compressibility, Rao's Constant, Wada's Constant, Specific Acoustic Impedance and Intermolecular Free Length are evaluated and the variations are analyzed. Structure making and Structure breaking nature of solution is studied using Internal Pressure variations.

Keywords: *Compressibility, Rao's Constant, Wada's Constant, Acoustic Impedence*

INTRODUCTION

The structure of liquids is well established than that of gases or solids. Despite a great deal of research in this area, we still do not have a clear picture of the way in which molecules are arranged in even the most common liquid, water. Ultrasonic studies of electrolytic solutions yield valuable information about the nature and strength of molecular interactions. The estimation of ultrasonic velocity, help us to evaluate the Internal Pressure, Free Volume, Compressibility, Rao's Constant and Wada's Constant, which provides a wealth of information about the state of liquid. It explains many of the properties of liquids and solutions. Even microscopic changes occurring in the medium like in molecular orientations or temperature will change the value of Internal Pressure. From the acoustic parameters the ultrasonic behaviour of Mesitol and Pyrogallol was assessed.

MATERIALS AND METHODS

The aqueous solution of Mesitol and Pyrogallol (AR Grade) is dissolved separately in double distilled water for making up different concentrations under study. A Mittal type fixed frequency Interferometer (2 MHz) is used for the determination of Ultrasonic Velocity. A circulating thermostat is used to maintain the temperature of the system for constant temperature variation studies.

Mathematical Formula:

Ultrasonic Velocity (U) =λ x f

λ = wavelength f=frequency Where λ=2d/n

Adiabatic Compressibility: $\beta = (1/u^2\rho)$

Intermolecular free length (L_f): $L_f = \left(\frac{K}{U_P^{1/2}}\right) = K\left(\beta_{ad}\right)^{1/2}$

Relaxation time (ι) = $4\eta/(3\rho U^2)$

Specific Acoustic Impedance(z) = ρ*U

Rao's Constant(R) = $R = \frac{M}{\rho} \bullet u^{1/3}$

Wada's Constant(W) = $\left[\frac{M}{\rho}\right](\beta_{ad})^{-1/7}$

Table 1: Mesitol

Concentration	Velocity (U) (m/Sec)	Compressibility (β)	Free Length (L_f) (mt)	Impedance (Z) (Rayl)	Rao's constant(R)	Wada's constant (W)
1.00	1512	40.65	0.4053	16.268	993.55	568.77
2.00	1498	38.15	0.3926	17.503	1001.69	580.70
3.00	1491	36.15	0.3822	18.546	1021.65	597.67
4.00	1486	35.68	0.3797	18.860	1060.87	631.92

Table 2: Pyrogallol

Concentration	Velocity (U) (m/Sec)	Compressibility (β)	Free Length (L_f) (mt)	Impedance (Z) (Rayl)	Rao's constant(R)	Wada's constant (W)
0.15	1531	41.17	0.4104	15.659	974.34	553.60
0.30	1539	40.23	0.4031	16.144	982.99	560.37
0.45	1547	38.88	0.3935	16.623	991.03	566.79
0.60	1553	37.76	0.3906	17.053	1000.34	573.79
0.75	1560	36.63	0.3847	17.503	1008.80	580.32
0.90	1568	35.53	0.3790	17.950	1018.21	587.30
1.05	1575	34.47	0.3731	18.421	1025.79	593.32
1.20	1583	33.56	0.3682	18.829	1036.16	600.64

Table 3: Mesitol - Internal Pressure

Concentration	308K	313K	318K	323K	328K
1.00	23833	23071	22521	21701	21063
2.00	23632	23009	22399	21450	20824
3.00	23042	22527	22002	21099	20633
4.00	22770	22359	21704	20846	20341

Table 4: Mesitol - Free Volume

Concentration	308K	313K	318K	323K	328K
1.00	0.02741	0.03169	0.03569	0.04166	0.04754
2.00	0.02749	0.03118	0.03540	0.04206	0.04794
3.00	0.02843	0.03192	0.03583	0.04247	0.04733
4.00	0.02869	0.03218	0.03596	0.04226	0.04833

Table 5: Pyrogallol - Internal Pressure

Concentration	308K	313K	318K	323K	328K
0.15	24363	23438	22668	21921	21296
0.30	24162	23365	22599	21824	21224
0.45	24029	23251	22466	21666	21197
0.60	23847	23178	22297	21626	21116
0.75	23656	22886	22189	21276	20835
0.90	23547	22719	21994	21181	20642
1.05	23375	22515	21899	21117	20664
1.20	23076	22519	21728	21153	20566

Table 6: Pyrogallol - Free Volume

Concentration	308K	313K	318K	323K	328K
0.15	24363	23438	22668	21921	21296
0.30	24162	23365	22599	21824	21224
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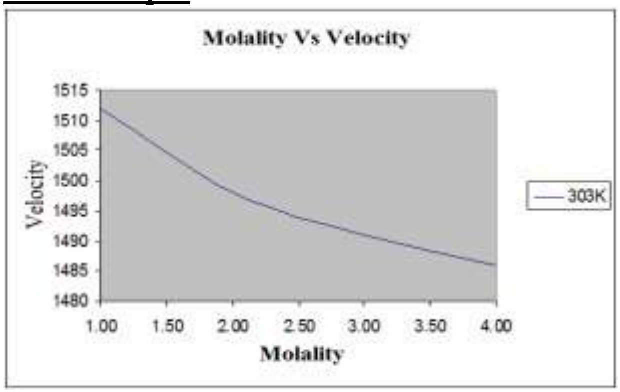
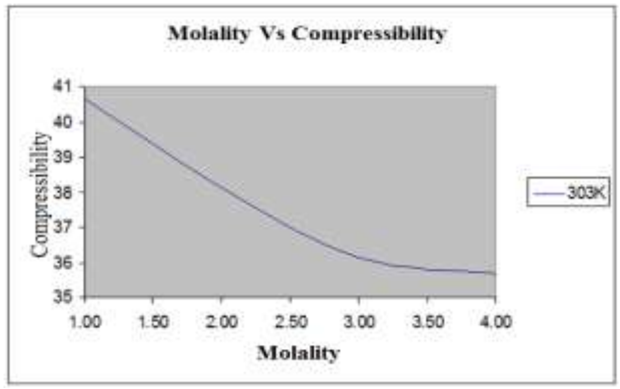
0.60	23847	23178	22297	21626	21116
0.75	23656	22886	22189	21276	20835
0.90	23547	22719	21994	21181	20642
1.05	23375	22515	21899	21117	20664
1.20	23076	22519	21728	21153	20566

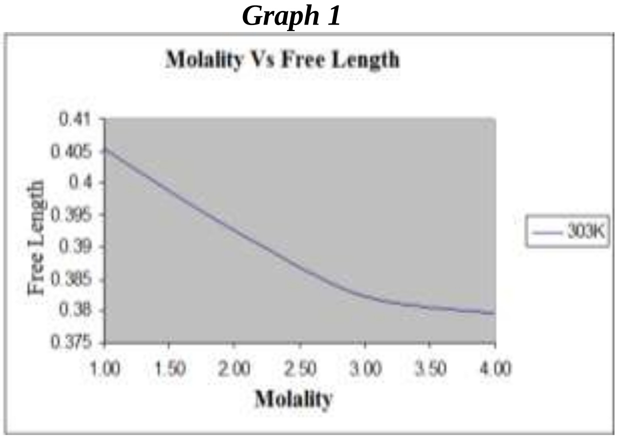
<u>Mesitol Graphs</u>



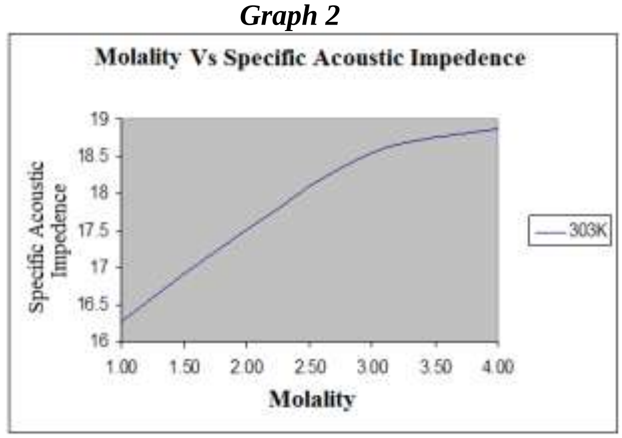
Graph 1



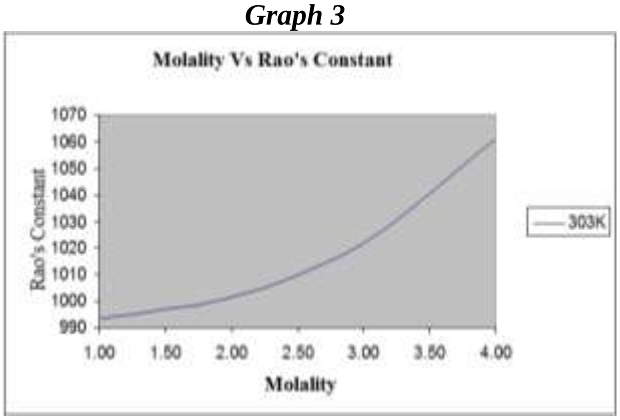
Graph 2



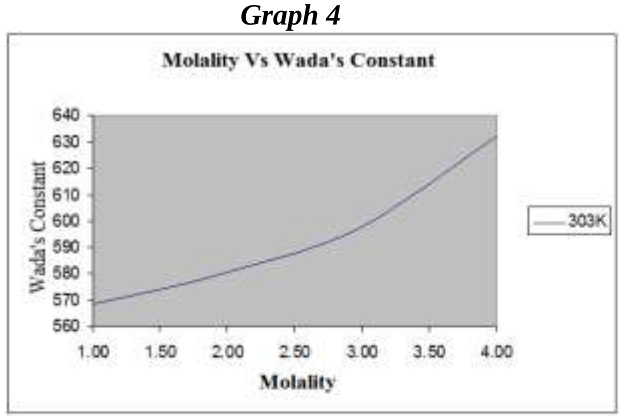
Graph 3



Graph 4



Graph 5



Graph 6

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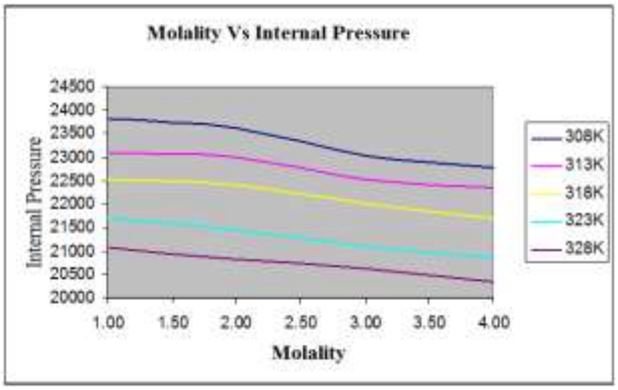
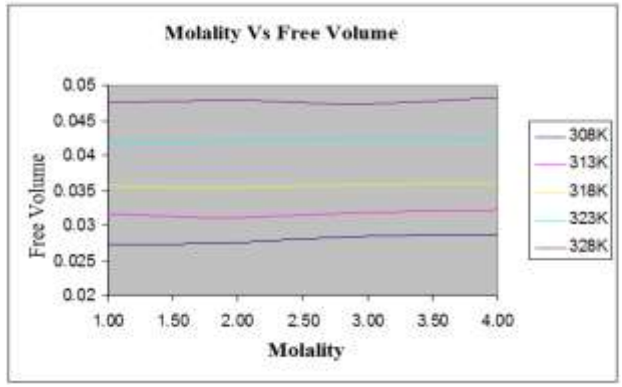
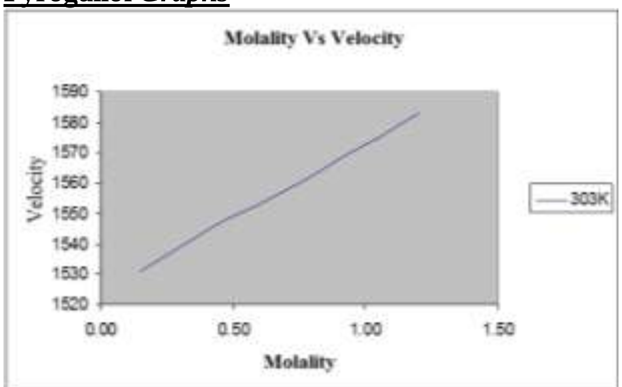


Graph 7

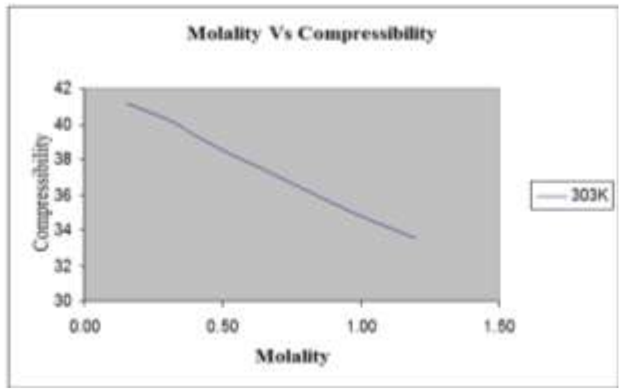


Graph 8

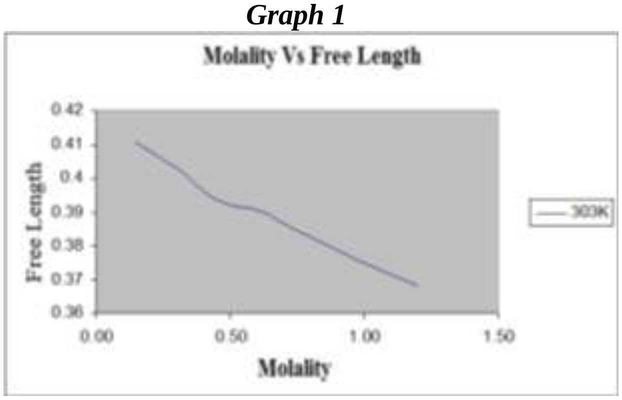
<u>Pyrogallol *Graphs*</u>



Graph 1



Graph 2



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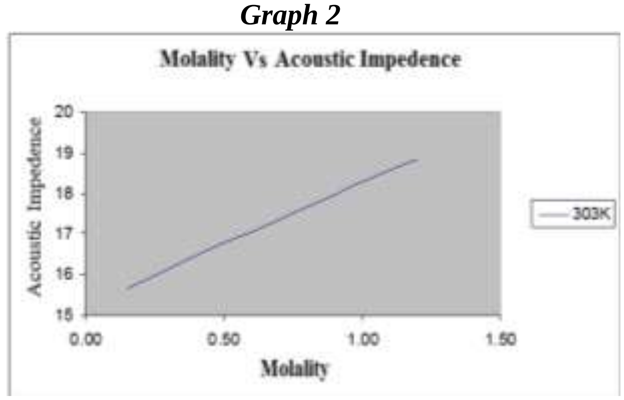
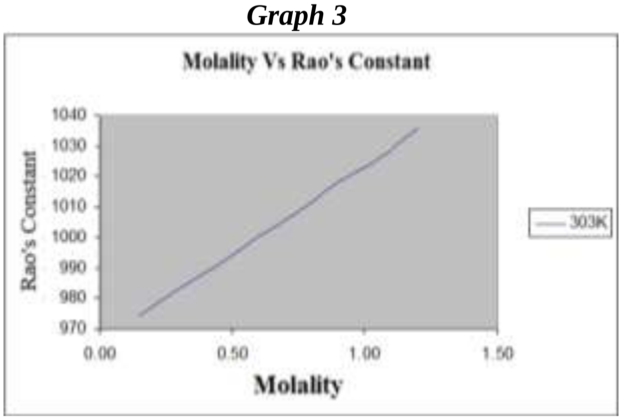
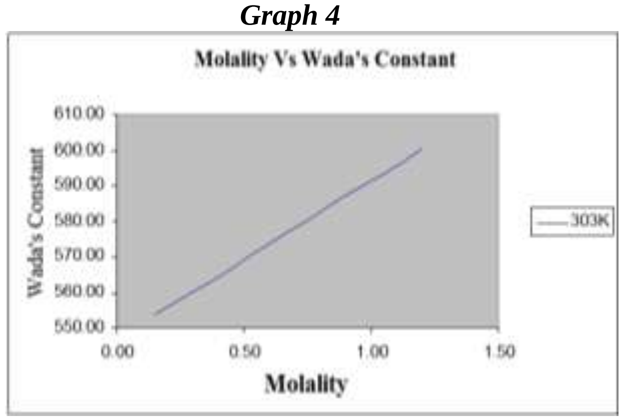


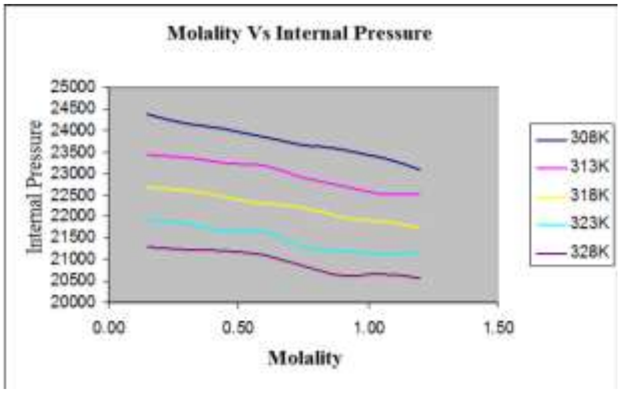
Graph 4



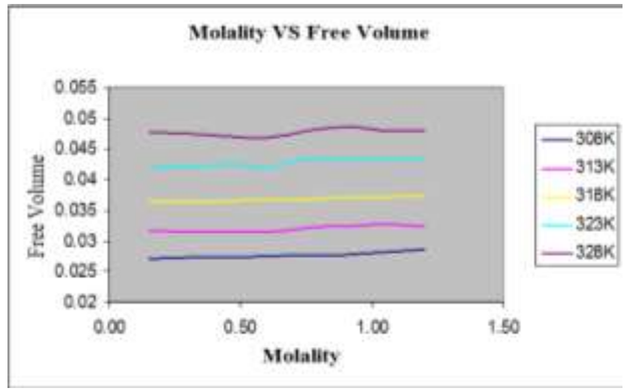
Graph 5



Graph 6



Graph 7



Graph 8

RESULTS AND DISCUSSION

The experimentally determined values of Ultrasonic Velocity for Mesitol and Pyrogallol at different concentrations are summarized in the table 1 and table 2.

The measurement of ultrasonic velocity is an important tool to study and understand the physical and chemical properties of the liquids. Ultrasonic velocity and allied parameters of Mesitol and Pyrogallol for various concentrations are presented in table 1 and table 2 respectively and graphically represented in figures.

The parameters derived from ultrasonic measurements such as Adiabatic Compressibility, Intermolecular Free Length, Specific Acoustic Impedance, molar sound velocity and molar compressibility provide a better insight into molecular environment in liquid mixtures and solutions.

In the system under study ultrasonic velocity decreases with increase in concentration in the case of Mesitol, but for Pyrogallol the ultrasonic velocity increases with concentration.

In the case of Mesitol the plot between the ultrasonic velocity and concentration shows that the ultrasonic velocity is found to linearly decrease with increase in concentration. This linear decrease suggests that there are weak solute-solvent interactions in the liquid solution. These interactions are both concentration and temperature dependent. The effects of temperature on the interactions are more than that of concentration. At low concentrations, the number of hydrogen bonds formed may be less and at higher concentrations, it may be more due to solute-solute interactions [Graph1]. In the case of Pyrogallol the ultrasonic velocity is found to increase with concentration

The compressibility is a macroscopic observable, which is sensitive to solute-solvent interactions. Any modifications induced by the solute on the local structure of the solvent generate changes in the Adiabatic Compressibility of the solutions and therefore compressibility can be used to characterize solvated properties of solute in dilute solutions. The decrease of Adiabatic Compressibility with Concentrations of both the solutions studied here indicates the formation of a more number of tightly bound systems. This implies, the β is decreasing with Concentration [1]. This is seen from the fact that the Velocity is equal to the square root of the reciprocal of β with density [Graph 2].

The intermolecular free length of the liquid systems decreases with increase in concentration. The free length is the distance between the surfaces of the neighboring molecules. It indicates significant interactions between the solute and solvent molecules, due to which the structural arrangement in the neighborhood of constituent solute particles is considerably affected. At lower concentrations, the molecules are not closer and then the Intermolecular Free Length will be high [2]. As the concentration increases, the molecules come closer, there by decreasing the intermolecular free length [Graph 3].

The usual behavior of the linear increase of Specific Acoustic Impedance with Concentration at a given temperature is observed in the systems studied here. The Specific Acoustic Impedance in liquids can also be used to assess the strength of Inter-Molecular Attraction [3]. As the strength of the intermolecular attraction increases, the ultrasonic velocity also increases consequently, the acoustic impedance value also increases. Acoustic impedance is a characteristic property of the medium [Graph 4].

The variations of Molar Sound Velocity (Rao's constant) and Molar Compressibility (Wada's constant) show increasing trend with the variation of concentration at 303k as expected [Graph 5 and 6].

As tabulated in Table-3 and Table-5 the variation of Internal Pressure with increase in concentration show a decreasing trend in both system studied here and this is exhibited in the graphs 7a & 7b. Thermodynamic importance of internal pressure is shown by bringing out its quantitative relationship with entropy and the partition function of the system. Internal pressure is shown to be related to the transport properties in liquids and solutions.

In the case of Free Volume, Mesitol system show an increasing trend and Pyrogallol system show a decreasing trend. This is represented in graphs 8a & 8b. The free volume plays an important role in ultrasonic wave propagation in liquids.

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