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Intermolecular Interaction through Ultrasonic Studies

KEYWORDS

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ABSTRACT *Molecular Interaction studies in liquids provide vivid information about the structural details of the molecules in solution phenomena. The Cohesive Energy of the Inter& Intra molecular interaction is the best revealed through ultrasonic studies. In the current paper by passing ultrasonic waves through aqueous solution of Digitaline the Acoustical and related Thermodynamical parameters are estimated. The study is carried out at different temperatures in order to understand the effect of temperature with the association of molecular phenomena of structure breaking or breaking.*

Introduction:

There are many approaches to determine the structure function relationship of molecules. Ultrasonic methods along with spectroscopic techniques are found to be powerful tools in the investigation of molecular interactions occurring in solutions. The Digitaline samples are more prominently used in Bio-medical & Pharmaceutical fields. The relative associations of the molecules from their pure to dilated forms are investigated through the variation of Ultrasonicvelocity, density, viscosity, compressibility studies. The formation of Hydrogen bonding as expressed in spectroscopic studies can be easily ascertained by the Thermodynamical studies through Ultrasonic & acoustical measurements. The Interactions confirm the structure making and breaking properties of solution phenomena.

Experimental studies:

The aqueous solution of Digitaline (AR Grade) is dissolved 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 10 ml specific gravity bottle& cannon Fenske Viscometer was used for determining both density & viscosity of the solutions respectively. A circulating thermostat to maintain the temperature of the system constant for temperature variation studies.

Mathematical formulas:

Ultrasonic Velocity (U) =λ x f

λ = wavelength f=frequency

Where λ=2d/n

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

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

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

Specific Acoustic Impedance(z)= ρ*U

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

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

Tabular columns

Ultrasonic Velocity(U)(m/sec) **Ultrasonic Density(ρ)(Kgm^{-3})**

Mol/Temp	303	308	313	318	323	303	308	313	318	323
0.6	1543	1559	1579	1599	1616	1.043	0.9927	1.038	1.036	1.034
1.2	1546	1562	1581	1602	1623	1.056	1.054	1.052	1.046	1.043
1.8	1547	1564	1587	1608	16273	1.073	1.051	1.068	1.064	1.062
2.4	1554	1569	1589	1612	1631	1.09	1.084	1.084	1.082	1.076
3	1558	1572	1594	1616	1634	1.105	1.099	1.099	1.09	1.087

UltrasonicViscosity(η)(Nsm^{-2}) **Adiabatic Compressibility(βx10^{-11})**

Mol/Temp	303	308	313	318	323	303	308	313	318	323
0.6	0.01064	0.0073	0.0082	0.0079	0.0073	4.0291	4.1471	3.8611	3.7762	3.7047
1.2	0.01153	0.0098	0.0091	0.0087	0.0082	3.962	3.887	3.8013	3.7237	3.64
1.8	0.01262	0.0106	0.0097	0.0092	0.0088	3.8929	3.8919	3.7179	3.637	3.5557
2.4	0.0136	0.011	0.0104	0.0099	0.0095	3.7979	3.7312	3.6558	3.5553	3.4917
3	0.01456	0.0119	0.0119	0.0106	0.0101	3.7282	3.6703	3.579	3.511	3.4451

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Intermolecular Free Length($L_f x10^{-11}$) **Specific Acoustical Impedance(Z)(Rayl)**

Mol/Temp	303	308	313	318	323	303	308	313	318	323
0.6	1.2695	1.2944	1.2614	1.2586	1.2538	160893	154719	163962	165636	167065
1.2	1.2589	1.2532	1.2516	1.2448	1.2429	163258	164669	166357	167603	169274
1.8	1.2479	1.2539	1.2378	1.2303	1.2284	166020	164331	169485	171040	172824
2.4	1.2326	1.2278	1.2274	1.2164	1.2173	169409	170841	172196	174453	175544
3	1.2212	1.2177	1.2145	1.2088	1.2092	172159	173277	175233	176196	177629

Molar Sound Velocity **Molar Compressibility**

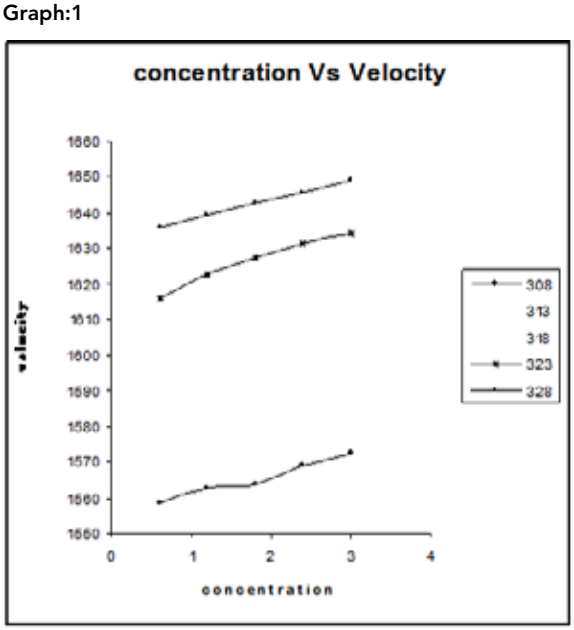
Mol/Temp	303	308	313	318	323	303	308	313	318	323
0.6	998.17	1048.87	948.13	953.8	959	568.53	592.92	539.06	541.81	544.35
1.2	1055.98	940	945.6	955.21	962.05	602.46	535.88	538.62	543.31	546.64
1.8	1106.32	952.62	942.1	949.71	955.4	632.6	542.83	537.69	541.41	544.19
2.4	1155.11	929.71	937.9	944.3	953.31	661.84	532.39	536.41	539.54	543.95
3	1202.57	928.63	935.5	947.55	953.6	690.31	532.61	535.99	541.9	544.87

Vanderwaal's Constant **Relaxation Time(sec)**

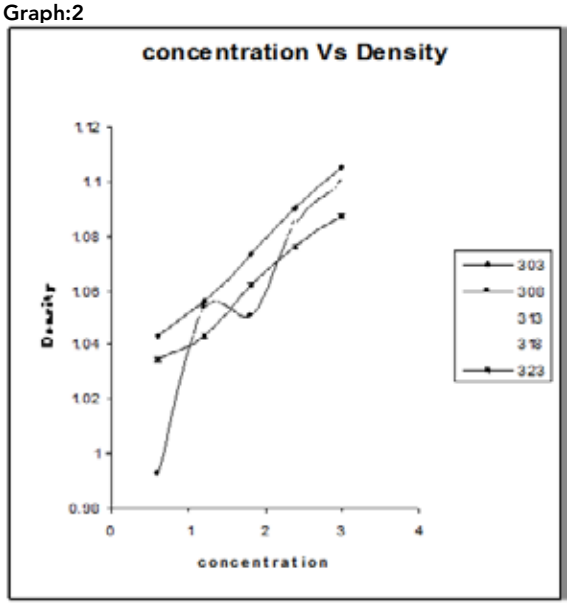
Mol/Temp	303	308	313	318	323	303	308	313	318	323
0.6	28.32	29.85	28.8	29.05	29.23	5.716	4.0139	4.2163	3.9826	3.6059
1.2	31.72	31.89	32.16	32.61	32.96	6.091	5.0843	4.5971	4.3244	3.9555
1.8	34.92	35.78	35.58	35.99	36.3	6.5055	5.5058	4.8036	4.4566	4.1672
2.4	38.31	38.41	38.85	39.14	39.79	6.887	5.4873	5.0694	4.674	4.4042
3	41.64	41.81	42.3	43.02	43.33	7.2377	5.799	5.2969	4.9622	4.6394

Graphs

Graph:1



Graph:2



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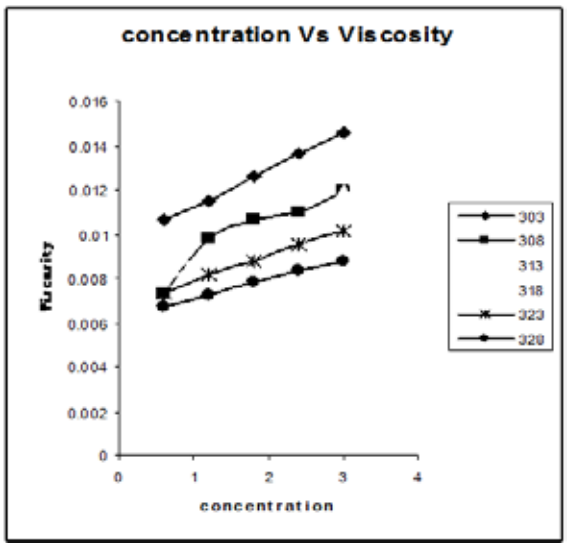
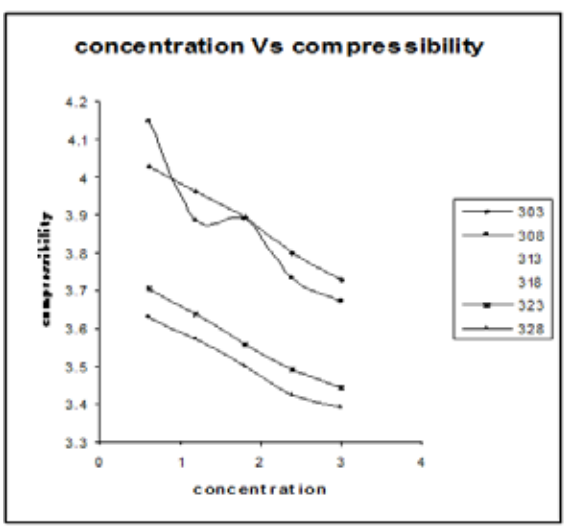
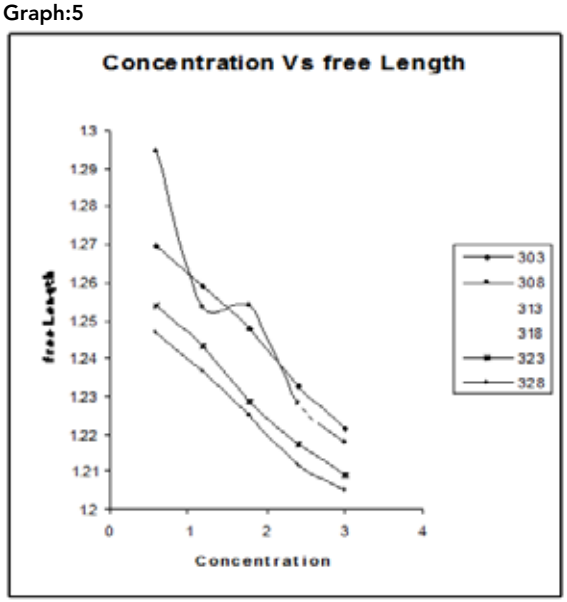
Graph:3



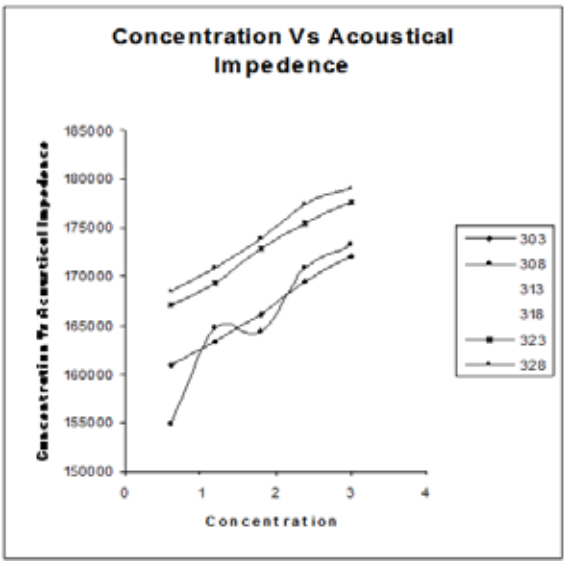
Graph:4



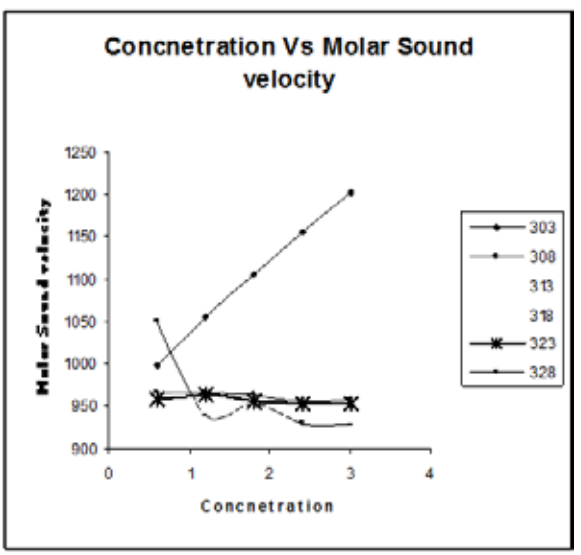
Graph:5



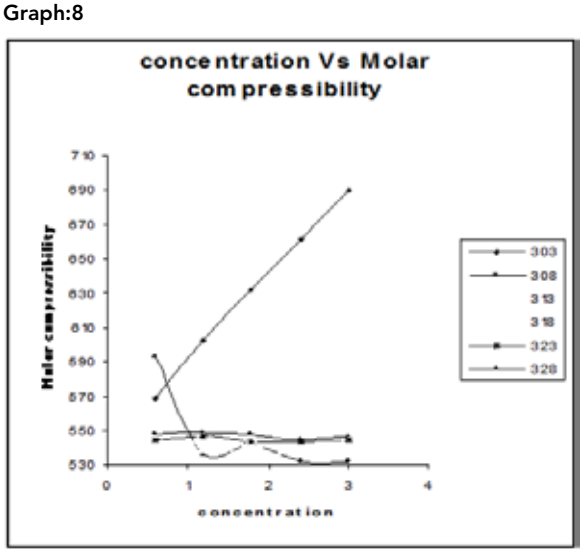
Graph:6



Graph:7



Graph:8



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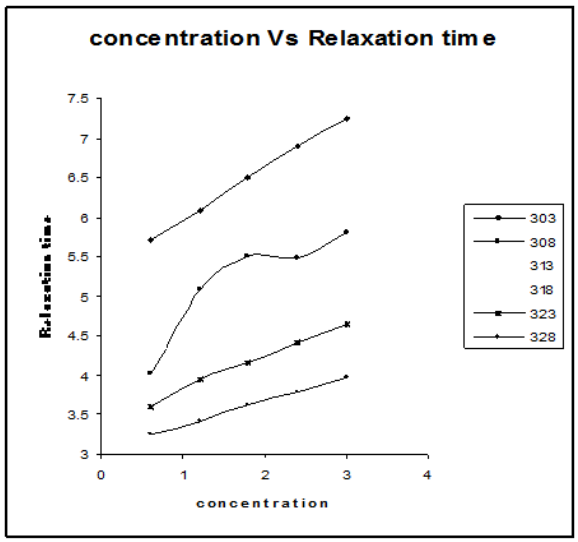
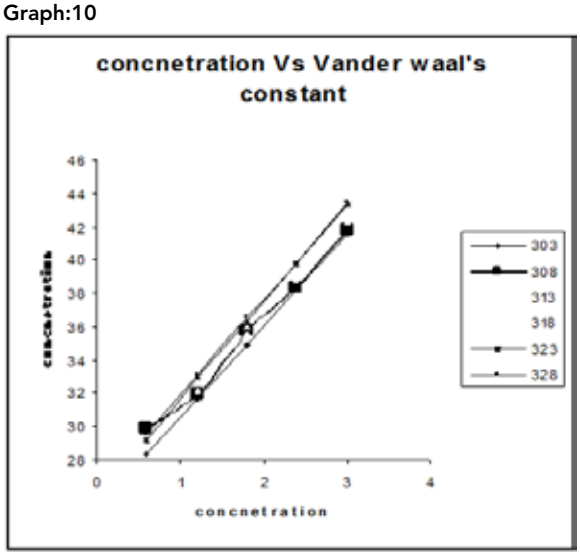
Graph:9



Graph:10



Results and Discussion

The experimentally determined values of ultrasonic velocity for Digitaline at temperatures at 303K,308K, 313K, 318K and 323K are summarized in the table.

The measurement of ultrasonic velocity is an important tool to study the physical & chemical properties of the liquid. Ultrasonic velocity and allied parameters of Digitaline for various concentrations, at different temperatures are presented in tables and represented graphically in figures.

The parameters derived from ultrasonic measurements such as adiabatic compressibility, acoustical relaxation time, intermolecular free length, specific acoustic impedance, molar sound velocity and molar compressibility prove a better insight into molecular environment in liquid mixtures and solutions.

In this the ultrasonic velocity increases with increase in both temperature and concentration.

The plots between the ultrasonic velocity and concentration potential shows that the ultrasonic velocity is found to linearly increase with concentrations and temperatures. This linear increase suggests that there are strong 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].

Ultrasonic density, Viscosity increases with increase in concentration and decreases with increase in temperature [Graphs 2, 3].

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 all the solutions studied here indicates the formation of a more number of tightly bound systems. This implies, since the density should increase with concentration, the is also decreasing with concentration[1]. This is seen from the fact that the velocity is equal to the square root of the reciprocal of the with density[Graph 4].

The intermolecular free length of the liquid systems decreases with increase in velocity. 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 5].

The usual behavior of the linear increase of specific acoustic impedance with concentration at a given temperature is observed in all 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 6].

The variations of molar sound velocity (Rao's constant) and molar compressibility (Wada's constant) show increasing trend with the variation of concentrations and temperatures as expected[Graphs 7,8].

Acoustical relaxation time of all the systems studied here, is found to decrease with increase in temperatures. It is directly proportional to adiabatic compressibility and viscosity. Acoustical relaxation time increases with rise in concentration at a give temperature and decreases with rise in temperature at a given concentration. These changes with respect to concentrations are not similar to those found in adiabatic compressibility. These changes in acoustical relaxation time with respect to concentrations and temperatures are similar to those found in viscosity[4]. This supports the view that viscous forces play a dominant role in the relaxation processes[Graph 9].

Vanderwaal's Constant increases with increase in temperature[Graph 10].

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