Original Article

Molecular Interaction of Polymer Dextran in Sodium Hydroxide through Evaluation of Thermo Acoustic Parameters

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ABSTRACT

Aim: To find out the molecular interaction of solute dextran of different concentration with sodium hydroxide as a solvent. **Materials:** Dextran of molecular weight 70000 dalton and aqueous 1(N) Sodium hydroxide. **Methods:** To Measure the density by specific gravity bottle, Viscosity by Ostwald's viscometer and ultrasonic velocity through ultrasonic interferometer of the solution and to calculate the thermo acoustical parameters using the measured parameters. **Results:** Ultrasonic wave propagation affects the physical properties of the medium and hence furnishes information on the physics of liquid and solution. I have used the measured parameters, like ultrasonic velocity, density, viscosity and evaluated parameters to understand the solute-solute and solute-solvent interactions in the solution containing dextran with sodium hydroxide. **Conclusion:** The effect of frequency on thermo acoustical parameters had been studied. From the above studies, the nature of forces between molecules such as hydrogen bonds, charge transfer complexes, breaking of hydrogen bonds and complexes had been interpreted. Intermolecular forces (electrostatic forces between charged particles of a permanent dipole and an induced dipole molecules) are weak. Structural characteristics of the components arising from geometrical fitting of one molecules in to another due to the difference in shape and size of the molecules. In the present study ultrasonic velocity (U), viscosity (η) and density (ρ) have been measured at temperature 308 K in the solution of sodium hydroxide with polymer dextran in the concentration range 0.1% to 1 % at four different frequencies i.e. 1 MHz, 5 MHz, 9 MHz and 12 MHz using ultrasonic interferometer. The measured values of ultrasonic velocity (U), viscosity (η) and density (ρ) have been used to calculate the thermoacoustic parameters namely free volume (V_f), internal pressure (ϖi), attenuation coefficient /absorption coefficient (α), Rao's constant (R) and Wada's constant (W) etc, These acoustical parameters are highly essential in studying various types of molecular interactions in liquid solution and provide qualitative information regarding the physical nature and quality of the molecular interaction in binary mixture dextran 1(N) sodium hydroxide. The molecular interactions like electrostriction, acceptor-donor association, dipole-dipole association and hydrogen bonding have been analyzed based on these parameters. Molecular interactions provide an understanding of the fundamental problems concerned with the mechanism of chemical and biochemical catalysis and the paths of the chemical reaction.

Key words: IJPER, Citation profile, Scientometrics, Pharmaceutics, Journal evaluation.

Submission Date: 04-09-2019;
Revision Date: 18-02-2020;
Accepted Date: 19-05-2020

DOI: 10.5530/ijper.54.3.112

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INTRODUCTION

The study of the molecular interaction of polymer has been the focus of intense research activities for the past few years.[1] Test and hypothetical investigations have offered ascend to renewed interest in the field due to its commercial application in the field of medical science, chemical and agricultural industries.

In continuation of earlier work on different solute and solvent,[2-7] we have made further attempt to study the molecular interaction of dextran in NaOH by calculating different thermo-acoustic parameters like, free volume (V_f), internal pressure (πi), attenuation coefficient/absorption coefficient (α), Rao's constant (*R*) and Wada's constant (*W*). From these values, we have assessed the nature and force of the molecular interaction of dextran in sodium hydroxide. Measurement of some bulk properties like ultrasonic velocity (U), viscosity (η) and density (ρ) provide insight into the intermolecular arrangements of the solute and solvent in solutions and helps to understand the thermo-acoustic properties of the solutions.

In this paper, solute-solvent interactions was investigated by estimations of U, ϱ, η and related acoustic parameters for the aqueous solution of polymer dextran in the concentration range 0.1%, 0.25%, 0.5%, 0.75% and 1 % (0.1) have been studied at four various frequencies i.e. 1, 5, 9 and 12 MHz using ultrasonic interferometer at constant temperature 308 K.

Ultrasonic wave propagation through solids and liquids provides valuable information regarding the structure of solids and liquids. By ultrasonic speed estimations, the molecular interaction in pure liquids, and liquid solutions have also been studied. The ultrasonic speed in a fluid gives a ground-breaking, viable and dependable device to examine properties of arrangements of polymers, amino acid, carbohydrates, amino acid, and vitamins, etc. It is generally related to the binding powers among the particles or molecules and has been effectively utilized in understanding the idea of molecular interaction in the liquid solution. The measurement of ultrasonic velocity enables the accurate evaluation of some useful acoustical parameters which are highly sensitive to molecular interactions.

Dextran, a water-soluble polymer, is an α-D-1, 6-glucose connected glucan with side chains l-3 connected to the backbone units of polymer. It has involved a different region of examinations by analysts due to its flexible pharmaceutical, biomedical and modern application.

Sodium hydroxide is one of the most well-known inorganic bases or alkali. It is soluble in polar solvents, for example, water, ethanol and methanol and insoluble in organic solvents. Dissolving solid sodium hydroxide in water is a highly exothermic reaction and the resulting aqueous sodium hydroxide solution is a colorless, odorless and important base used in the laboratory. Its fundamental uses are in the paper industry, petroleum industry, textile industry, in the manufacture of soaps and detergents, in the Bayer process of aluminum generation, industrial cleaning and pH guideline. It is additionally utilized in the food industry for some applications.

Experimental Section

Materials

The solution prepared in aqueous sodium hydroxide as a solvent for preparing the dextran solution of different concentrations. Dextran of MW 70,000 (Da) utilized as a solute, is of analytical reagent grade.

Measurements

(a) Velocity Measurement

Using an ultrasonic interferometer, the speed of the ultrasonic wave in solution was measured, operating at 11 different frequencies. The interferometer measuring cell is a specially designed double walled vessel with temperature constant arrangement. An electronically operated advanced steady temperature shower installed operating in the temperature range -10°C to 85°C with an accuracy of ± 0.1 K was used to circulate water through the outer jacket of the double walled estimating cell containing the test solution.

The expression used for assessing ultrasonic speed is

$$U = 2d/T \text{ (m/s)}$$

$$\text{Or.} \quad U = 2d \times v$$

$$\text{Or, } U = \lambda \times v \text{ -------------------------- (1)}$$

(Here-2d=λ)

Where, *v* is the frequency of the generator which is used to excite the crystal; (In the present investigation, different frequency frequencies (1MHz, 5MHz, 9MHz and 12MHz interferometer was employed) d- Separation between the reflector and crystal; T. Travel time of the ultrasonic wave.

(b) Density Measurement

A 10ml Pycnometer bottle was used to measure the solution densities. The Pycnometer bottle was submerged in temperature-controlled shower of water with the investigational solution.

The density was estimated using the equation

$$\rho_2 = \frac{w_2}{w_1}\rho_1 \text{ -------------------------------- (2)}$$

Where, w_1 = weight of distilled water, w_2 = Weight of investigational solution, ρ_1 = Density of water, ρ_2 = Density of investigational solution.

(c) Viscosity measurement

The solutions viscosities were measured using the standardized Ostwald viscometer. The Ostwald's viscometer was immersed in a temperature –controlled water bath with the investigational solution. The flow time was measured using an advanced, 0.01 s precision stopwatch

The viscosity was calculated using the equation,

$$\eta_2 = \eta_1 \left(\frac{t_2}{t_1}\right)\left(\frac{\rho_2}{\rho_1}\right) \quad \text{-------------------(3)}$$

Where, η_1 = Viscosity of distilled water, η_2 = Viscosity of solution, ρ_1 = Density of distilled water, ρ_2 = Density of investigational solution. t_1 = Flow time of water, t_2 = Flow time of investigational solution.

Theoretical Aspect

The data of ultrasonic velocity, density and viscosity lead to the determination of various thermo-acoustical parameters, using standard formula.

(i)Free volume

It can be calculated using the relation[8] as given below

$$V_f = \left(\frac{M_{eff}U}{K\eta}\right)^{\frac{3}{2}} \quad \text{---------------------- (4)}$$

(ii)Internal pressure

It can be calculated using the relation[9]

$$\pi_i = bRT\left(\frac{k\eta}{U}\right)^{3/2}\left(\frac{\rho^{2/3}}{M_{eff}^{7/6}}\right) \quad \text{------ (5)}$$

(iii)Absorption coefficient / attenuation coefficient

It is given by the formula[10]

$$\propto = \frac{8\pi^2\eta f^2}{3\rho U^3} \quad \text{---------------------- (6)}$$

(iv)Rao's constant

The derived empirical relation[11] as

$$R = \frac{M_{eff}}{\rho}U^{1/3} \quad \text{---------------------- (7)}$$

(v)Wada's constant

The derived the empirical relation.[12]

$$W = \frac{M_{eff}}{\rho}\beta^{-1/7} \quad \text{---------------------- (8)}$$

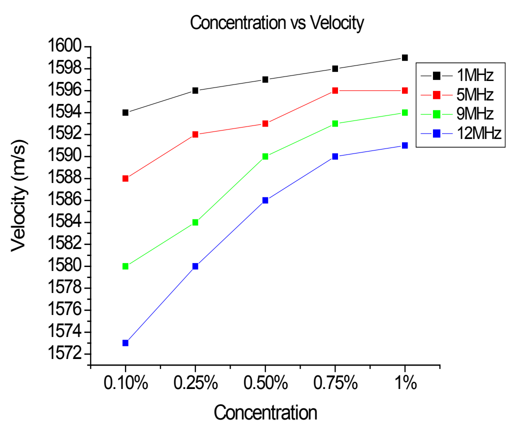

Figure 1: Plot of ultrasonic speed with concentration.

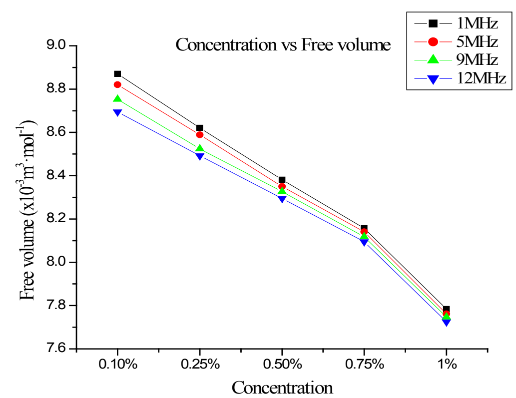

Figure 3: Plot of free volume with concentration.

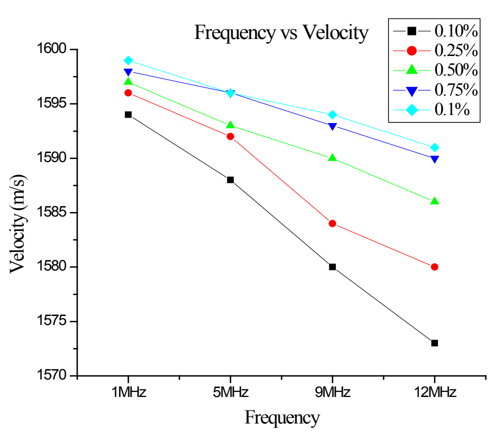

Figure 2: Plot of ultrasonic speed with frequency.

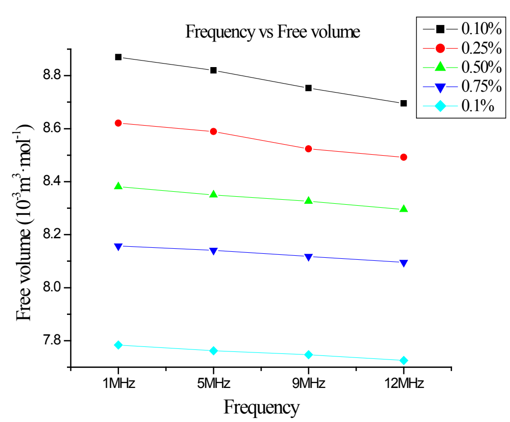

Figure 4: Plot of free volume with frequency.

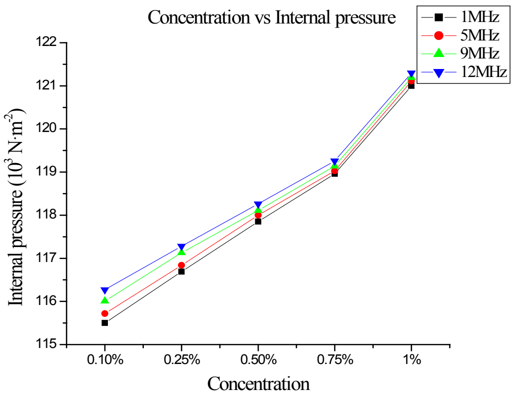

Figure 5: Plot of internal pressure with concentration.

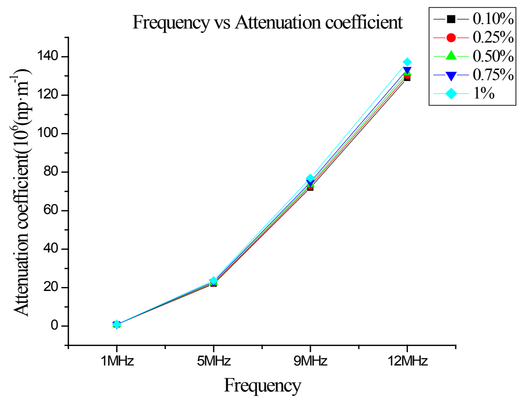

Figure 8: Plot of attenuation coefficient with frequency.

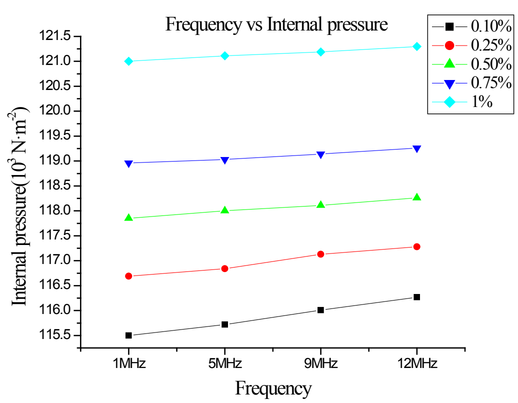

Figure 6: Plot of internal pressure with frequency.

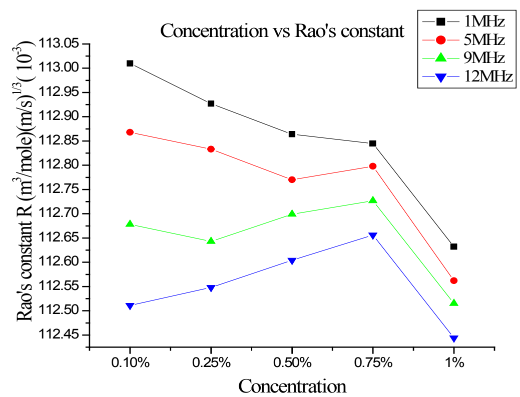

Figure 9: Variation of Rao's constant with concentration.

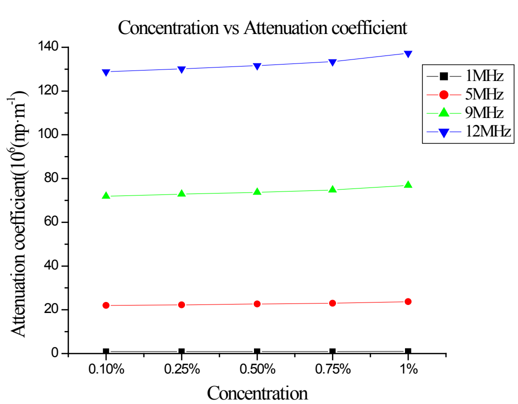

Figure 7: Plot of attenuation coefficient with concentration.

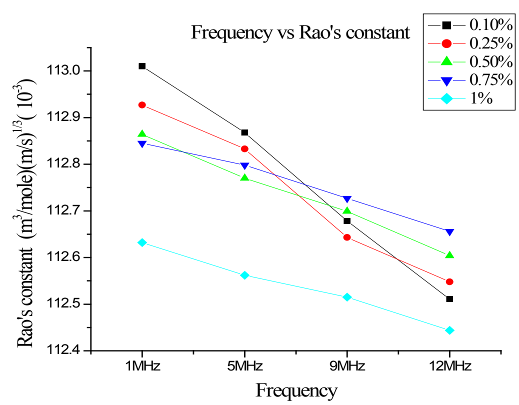

Figure 10: Variation of Rao's constant with frequency.

RESULTS AND DISCUSSION

The measured datas of ρ, η and U of sodium hydroxide with aqueous dextran and calculated acoustic parameters at frequencies likes 1, 5, 9 and 12 MHz for 308K temperature in different concentration of dextran have been presented in Tables 1 to 4 and Figures 1-12.

The plot of the velocity of dextran with NaOH at 308 K and frequencies 1, 5, 9 and 12 MHz are shown in Figures 1 and 2. It is observed that U rises gradually with a rise in the concentration of dextran up to 0.75% of dextran, then saturate. This indicates the existence of the molecular association, which may involve

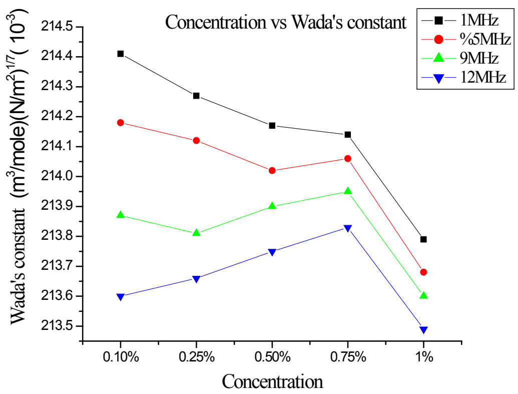

Figure 11: Variation of Wada's constant with concentration.

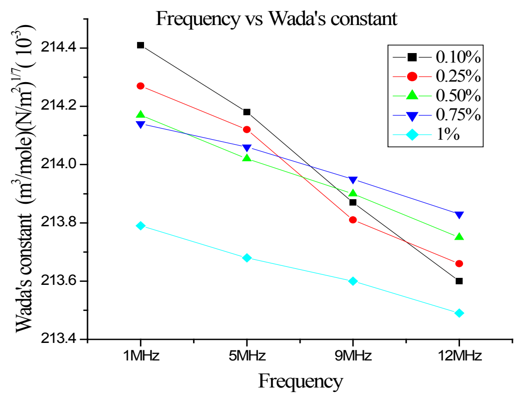

Figure 12: Variation of Wada's constant with frequency.

Table 1: Values of and of dextran with sodium hydroxide at various concentrations at 308 K.

T (kelvin)	Concentration									
	0.10%		0.25%		0.50%		0.75%		1%	
	ρ $Kg.m^{-3}$	η*10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η*10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η*10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η*10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η*10^{-3} $N.s.m^{-2}$
308 K	1033.667	0.869	1034.855	0.887	1035.647	0.904	1036.043	0.921	1038.212	0.951

Table 2: Values of U and Vf of dextran with sodium hydroxide in various concentrations and frequencies at 308 K.

Conc, (%)	(U) m/s				(V_f) ($x10^{-3}m^3 \cdot mol^{-1}$)			
	1MHz	5MHz	9MHz	12MHz	1MHz	5MHz	9MHz	12MHz
0.10	1594	1588	1580	1573	8.870	8.820	8.753	8.695
0.25	1596	1592	1584	1580	8.621	8.589	8.524	8.492
0.50	1597	1593	1590	1586	8.381	8.350	8.326	8.295
0.75	1598	1596	1593	1590	8.157	8.141	8.118	8.095
1	1599	1596	1594	1591	7.784	7.762	7.747	7.725

Table 3: Values of and of dextran with sodium hydroxide in various concentrations and frequency at 308 K temperature.

Conc. (%)	(π_i)($\times10^3$ $N \cdot m^{-2}$)				(α) ($x10^6$($np \cdot m^{-1}$))			
	1MHz	5MHz	9MHz	12MHz	1MHz	5MHz	9MHz	12MHz
0.10	115.50	115.72	116.01	116.27	0.87	21.95	71.85	128.87
0.25	116.69	116.84	117.13	117.28	0.89	22.26	72.86	130.19
0.50	117.85	118.00	118.11	118.26	0.90	22.65	73.68	131.64
0.75	118.96	119.03	119.14	119.26	0.92	22.99	74.76	133.40
1	121.00	121.11	121.19	121.30	0.94	23.68	76.92	137.26

due to dipole-dipole or hydrogen bonding between NaOH and water. The association due to ion-dipole interaction among Na^+ of sodium hydroxide and water molecules than the ion-dipole interaction between Na^+ of sodium hydroxide and dextran molecule.

Variation in the velocity perhaps because of the self-relationship of the solvent particles and dipole-induced dipole cooperation between the segment atoms, which is concentration-dependent. At saturation region of the mixture, there is a constancy in velocity indicating dipole-

Table 4: Values of R and W of dextran with sodium hydroxide at various concentrations and frequency at 308 K temperature.

Conc. (%)	R (m^3/mole)(m/s)$^{1/3}$(10^{-3})				W (m^3/mole)(N/m^2)$^{1/7}$(10^{-3})			
	1MHz	5MHz	9MHz	12MHz	1MHz	5MHz	9MHz	12MHz
0.10	113.010	112.868	112.678	112.511	214.408	214.177	213.869	213.597
0.25	112.927	112.833	112.643	112.548	214.274	214.121	213.813	213.658
0.50	112.864	112.770	112.699	112.604	214.172	214.019	213.903	213.749
0.75	112.845	112.798	112.727	112.656	214.140	214.063	213.948	213.833
1	112.632	112.562	112.515	112.444	213.795	213.680	213.604	213.489

induced dipole force dominated by dispersive force and the molecular association stops. This is because the size of dextran is more than the size of the water molecule. Hence higher the size more will be polarizability and the process may lead to strong interaction forces.

An increase in frequencies weakens the interaction which may be due to an increase in agitation between molecules resulting in a decrease in ultrasonic velocity at higher frequencies and hence dissociation. This is because the number of dextran molecules decreases and hence more polarized molecules are not available for strong ion-dipole interaction between Na^+ of NaOH and aqueous dextran. This process leads to weak interaction force. Further, in higher frequency range intermolecular gap decreases which leads to a decrease in velocity.

The strength of the interaction is well reflected in the deviations of free volume and internal pressure. The structural changes due to strong repulsive forces in the fluid solution with the moderately feeble attractive forces give the internal pressure which held the fluid solution together. The V_f signifies repulsive forces whereas the π_i is more delicate to attractive forces. These two acoustic parameters together extraordinarily decide the entropy of the system.

The V_f and at four different frequencies for the entire range of concentration of dextran are presented in Figure 3, 4 and Figure 5, 6. It is observed that the V_f diminution with a rise in concentration and π_i rises with a rise in concentration, at all concentrations range. This decrease of V_f and rise in π_i may be because of the mutual loss of the dipolar association of NaOH and the breaking up of molecular clusters. Changes in a way inverse to that of V_f at all concentrations and frequencies. With a rise in frequencies, agitation energy of the molecules increases, subsequently accessible free volume rises or π_i decreases. It is likewise the development of hard and/or tight solvation layer around the ion due to more solute-solvent interaction. The ultrasonic attenuation/absorption is a characteristic of the medium and it relies on the outer condition such as temperature, pressure and frequency. Ultrasonic attenuation increases slowly with the rise in dextran content in NaOH may be due to the compact packing of the medium. As concentration raises, the absorption coefficient increases progressively, the absorption coefficient at low frequency (1MHz) is negligible and more effective if we increase the frequency. The increase in the absorption coefficient with a rise in concentration suggests that the atoms arrange themselves in such a way that the void space is less usable showing a reduction in free volume. As frequency increases, the absorption coefficient increases rapidly because of its proportionality to the square of the frequency.

Also equally important are *R* and *W* constant to study the role of molecular cooperation. It is observed that *R* and *W* constant differ none linearly with the concentration increase. It may be due to the interaction between the solute molecules rather than the solvent sodium hydroxide. Further *R* and *W* constant diminishing with an increment in frequency as appeared in Figures 10 and 12. This shows close pressing of solute and solvent molecules.

CONCLUSION

Ultrasonic experiments are conducted to include a thorough analysis of molecular interaction in the liquid solution. Summarizing the trends and variation of thermodynamic parameters with the frequency of the ultrasonic wave has been studied in detail which will give us an idea about the nature of molecular interactions in the aqueous dextran solution.

ACKNOWLEDGEMENT

The author sincerely thanks the staff members and HOD of the Physics department, Centurion University of Technology and Management, Odisha, India and ABIT management, Cuttack for their strategic help and support.

CONFLICT OF INTEREST

This is my original research work and it has no conflict of interest with any other research work or person. This manuscript is not submitted elsewhere for same purpose.

ABBREVIATIONS

U: Ultrasonic velocity; **ϱ:** Density; **η:** Viscosity; **Vf:** Free volume; **πi:** Internal pressure; **α:** Attenuation coefficient /Absorption coefficient; **R:** Rao's constant; **W:** Wada's constant; **β:** Adiabatic compressibility; **KT:** Jacobson constant; **k:** Boltzmann's constant; **T/K:** Temperature; **NaOH:** Sodium hydroxide; **HOD:** Head of the department; **ABIT:** Ajay Binay Institute of Technology.

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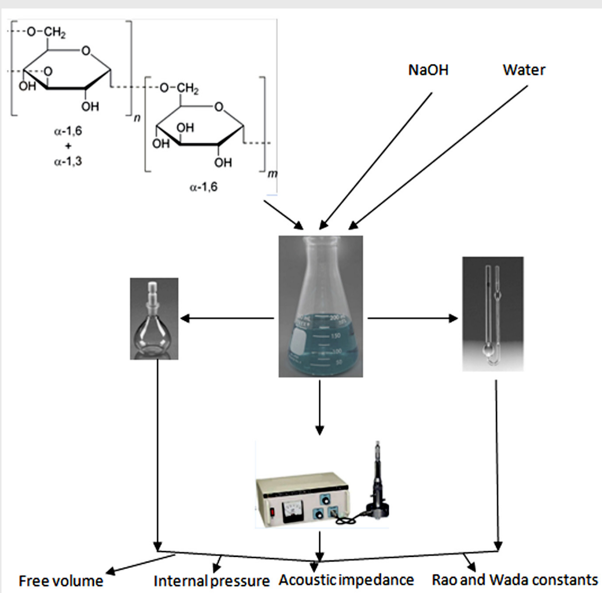
PICTORIAL ABSTRACT



SUMMARY

- In this appealing research work the main problem was to find out the molecular interaction of dextran with sodium hydroxide in simpler method. In past work in this area has not been carried out, so it become difficult to find background on this topic. So out of interest through this paper, the relationship between solute and solvent was find out with proper analysis of the results.
- As dextran it is used as drugs, especially as blood plasma volume expander, since plasma is required to circulate red blood cells supplying oxygen throughout the body. It is used to reduce the amount of circulating blood plasma which can result from surgery, trauma or injury, serious burns, or other bleeding causes. Because of the importance of dextran, a systematic study of it with sodium hydroxide has been undertaken in the present investigation.

About Authors

Dr. Subhraraj Panda is working as an Associate Professor of Physics in Centurion University of Technology and Management, Bhubaneswar, Odisha since 2008 and has 19 years of experience in teaching. He had his Ph.D. from Ravenshaw University, Cuttack in 2019 and got eight years of research experience. His research interests are fluid and molecular acoustic He has published 24 research articles in his area of research in different national and international journals.

Cite this article: Panda S. Molecular Interaction of Polymer Dextran in Sodium Hydroxide through Evaluation of Thermo Acoustic Parameters. Indian J of Pharmaceutical Education and Research. 2020;54(3):630-6.