Gurukul International Multidisciplinary Research Journal (GIMRJ)*with* International Impact Factor 8.357
Peer Reviewed Journal
https://doi.org/10.69758/GIMRJ/2504I5VXIIIP0050

e-ISSN No. 2394-8426
Monthly Issue
APR-2025
Issue–IV, Volume–XIII

Acoustical Studies on molecular interactions of Agarose and DMSO at 303K

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Abstract:
This study investigates the molecular interactions of Agarose dissolved in Dimethyl Sulfoxide (DMSO) at different concentrations at 303K using ultrasonic techniques. Ultrasonic velocity, density, and viscosity were measured for various Agarose concentrations to examine the intermolecular forces, solute-solvent interactions, and structural behavior of the solution. Acoustical parameters such as adiabatic compressibility (βad), intermolecular free length (L_f), acoustic impedance (Z), Rao's constant (RA), and Wada's constant (W) were derived and analyzed. These parameters provide insights into the influence of hydrogen bonding, dipole-dipole interactions, and the solvation dynamics between Agarose and DMSO. The results highlight the nature and strength of molecular interactions, enhancing our understanding of Agarose's behavior in solution. These findings have potential applicable in various field like pharmaceuticals, biotechnology, and material sciences.

Keywords: Ultrasonic velocity (u), density (ρ), viscosity (η), free length (L_f), adiabatic compressibility (βad), solvation dynamics, solute-solvent interactions.

INTRODUCTION:

In recent years ultrasonic is an area of intense scientific research in material science. Materials are classified in different ways e.g. ionic crystals, covalent crystals, amorphous materials, metals, alloys, semiconduzctors, electronic and magnetic materials nano-materials, polar and non-polar liquids, bio-fluids, polymer, biopolymers[1-3]etc. Research and development studies in material science deals with the different methods used to process the material and study various properties possess by the materials. These properties include the structural, mechanical, chemical, thermal, optical and many other properties. The measurement of ultrasonic speed enables us to the accurate measurement of some useful acoustic and thermodynamic parameters and their excess values [4-6]. In order to have clear understanding of intermolecular interaction between component molecules an attempt has been made to study the ultrasonic behaviors of Agarosein DMSO at 303K.

Agarose, a polysaccharide widely used in biophysics and material science. Agarose is chosen due to its excellent gel-forming ability,biocompatibility, and relevance in biological and pharmaceutical applications. Its interaction with solvents like DMSO helps in understanding solute-
solvent interactions, which are crucial in drug delivery and biomaterial studies.

MATERIAL & METHODS:

In the reported study, Agarose with 99.5% purity of analytical grade was obtained from Vedayukt India Private Ltd. Initially, a standard solution of 1–6 % concentration of Agarose in DMSO in steps of 1% was prepared. The ultrasonic velocities (U) in the liquid mixtures have been measured by a digital ultrasonic velocity meter supplied by Vi Microsystem Pvt. Ltd., Chennai, at a central frequency of 2 MHz with an accuracy of ± 0.01 m/s. The viscosity (η) of the solution is measured by an Ostwald's viscometer with accuracy ± 0.001Nm^{-2}s. The density (ρ) is measured using a Pycnometer Specific Density Gravity Bottle with an accuracy of ±0.1 kg/m^3.The temperature of the solution is maintained constant at 303K using a temperature-controlled water bath with an accuracy of ± 0.01K.

The data measured are used to calculate derived acoustical parameters such as adiabatic compressibility (β_{ad}), intermolecular free length (L_f), free volume (V_f), acoustical impedance (Z) and relaxation time (τ) etc.

THEORY:

- The Density of experimental liquid was measured using the formula

  $$\rho_2 = \left(\frac{W_2}{W_1}\right)\rho_1 \quad \text{---------- (1)}$$

  Where, w_1& ρ_1 = weight & density of distilled water.

  w_2& ρ_2 = weight & density of experimental liquid.
- Viscosityof the experimental liquid was determined using relation.

  $$\eta_2 = \left(\frac{t_2}{t_1}\right)\left(\frac{\rho_2}{\rho_1}\right)\eta_1 \quad \text{---------(2)}$$

  Where, η_1, ρ_1& t_1 is viscosity, density & time flow of water.

  η_2, ρ_2 &t_2 is viscosity, density & time flow of mixture.
- Adiabatic Compressibility (β_{ad}) has been calculated using the relation

  $$\beta ad = \frac{1}{\rho\, U^2} \quad \text{-------------(3)}$$
- Intermolecular free length(L_f) has been determined by the equation:

  $$L_f = K_T\sqrt{\beta_{ad}} \quad \text{-----------(4)}$$

  Where K_T is a Jacobsen's constant

  (93.875 + 0.375 T) X 10^{-8} and T being the absolute temperature.
- Free Volume (V_f) is determined using the equation:

  $$V_f = \left(\frac{M_{eff}U}{K\eta}\right)^{3/2} \text{----------(5)}$$

Where, $M_{eff} = \Sigma\, m_i x_i$ & K = 4.28 × 10^9 for all liquids in MKS system.

- Specific Acoustic Impedance is calculated using relation:

  $$Z = U.\rho \text{----------------- (6)}$$
- Relaxation Time is calculated from the relation.

  $$\tau = 4/3.\ (\beta_{ad}.\eta) \text{ -------------(7)}$$

RESULTS & DISCUSSION:

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The ultrasonic velocity, density, viscosity, and other relevant thermodynamic parametersi.e adiabatic compressibility (β_{ad}), intermolecular free length (L_f), acoustic Impedance (Z), free volume (V_f) and relaxation time (τ) of Agarose in DMSO were tabulated in Table-1.These parameters were evaluated and analyzed at various concentration percentages, at a fixed temperature of 303K.

Table-1

Measured parameters of ultrasonic Velocity(U), density(ρ), viscosity(η), adiabatic compressibility (βad), intermolecular free length (Lf), acoustic Impedance (Z), free volume (Vf) and relaxation time (τ) of Agarose in DMSO at 303 K

% Concentration	(U) (*m/s*)	(ρ) (Kg/m^3)	$\eta x\ 10^{-3}$ ($Nm^{-2}\ s$)	$\beta_{ad} \times 10^{-10}$ ($m^2\ N^{-1}$)	L_f X 10^{-11} (m)	$Zx10^6$ ($Kg\ m^{-2}s^{-1}$)	$V_f x10^{-8}$ (m^3)	τ x 10^{-13} (s)
0.1	1485.201	1087.52	3.8904	4.16862	4.2366	1.6152	1.8424	21.6238
0.2	1512.078	1090.12	5.4683	4.01215	4.1563	1.6483	1.1374	29.2533
0.3	1528.228	1091.44	5.9985	3.92305	4.1099	1.6680	1.0074	31.3766
0.4	1543.326	1092.52	6.5066	3.84287	4.0677	1.6861	0.9064	33.3389
0.5	1564.084	1093.56	8.3267	3.73798	4.0118	1.7104	0.6397	41.5005
0.6	1581.208	1093.72	9.8581	3.65692	3.9680	1.7294	0.5055	48.0670

Ultrasonic velocity (U) (fig.1) and density (ρ) (fig.2) increased with increasing agarose concentration, indicating stronger intermolecular interactions.

fig.1

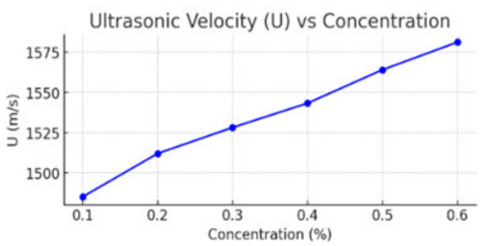
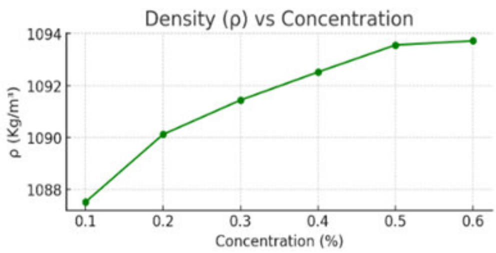
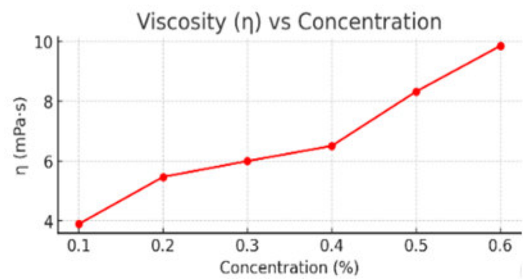


fig.2



Viscosity (η) (fig.3) increased significantly, particularly at higher concentrations, implying increased resistance to molecular motion due to stronger hydrogen bonding.

fig.3



Adiabatic compressibility (βad) (fig.4) and intermolecular free length (Lf) (fig.5) decreased, suggesting tighter molecular packing and reduced intermolecular spaces.

fig.4

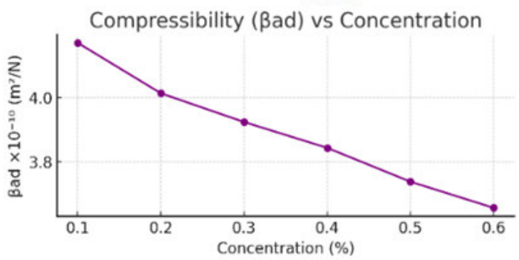


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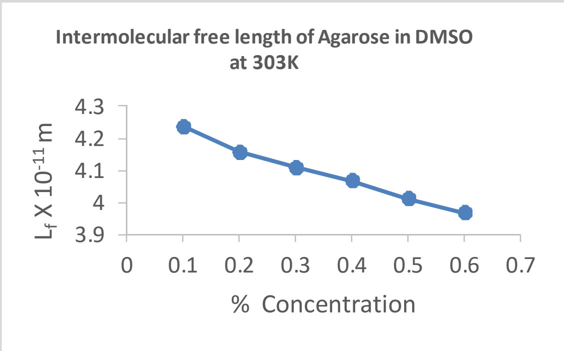
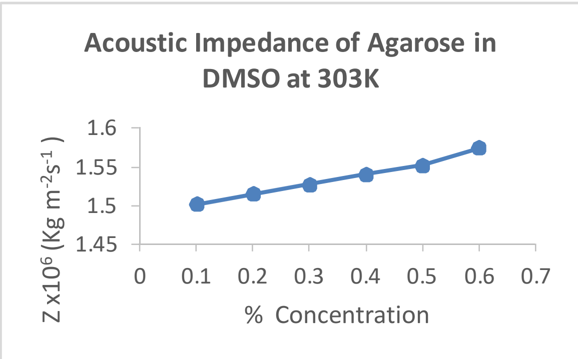
fig.5



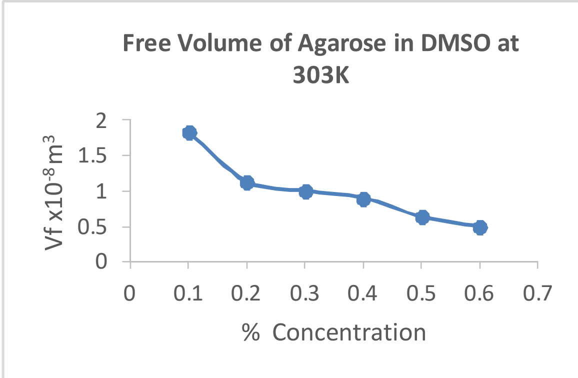
Acoustic impedance (Z) (fig.6) increased, confirming enhanced molecular interactions as the solution became denser and less compressible.

fig.6



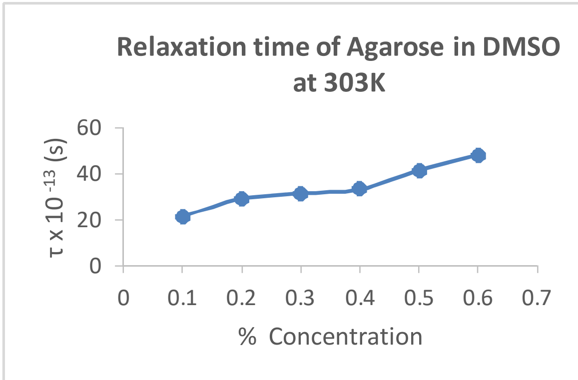
Free volume (Vf) (fig.7) decreased, indicating a reduction in the available space for molecular movement, which aligns with the increase in viscosity.

fig.7



Relaxation time (τ) (fig.8) increased, reflecting longer time scales for molecular rearrangements due to enhanced interactions in the system.

fig.8



Conclusion:

This study highlights the significant role of molecular interactions, particularly hydrogen bonding and dipole-dipole interactions, in influencing the physical properties of agarose solutions in DMSO. As the concentration of agarose increases, these interactions become more pronounced, leading to systematic variations in ultrasonic velocity, density, viscosity, compressibility, intermolecular free length, acoustic impedance, free volume, and relaxation time. Understanding these concentration-dependent changes is essential for optimizing the use of agarose in various scientific and industrial applications, including gel formation, biopolymer research, and drug delivery systems, where its structural and dynamic properties can be strategically utilized for desired outcomes

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