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# Investigation of Molecular Interactions of Polyvinyl Pyrrolidone (PVP-40) with Water and DMSO using Acoustic Spectroscopic Technique

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**ABSTRACT: This paper deals with investigating molecular interaction of Polyvinyle pyrolidone polymer having molecular weight 40,000 (PVP-40) with water and Dimethyl Sulfoxide (DMSO). Ultrasonic velocity (u), density (ρ) and coefficient of viscosity (η) were measured for solutions of PVP-water and PVP-DMSO system for different concentrations with range 0-50 Wt%. Ultrasonic velocity measurements were done by pulse-echo technique at frequency 5 MHz. The measurements were made at atmospheric pressure and room temperature. The experimental results have been used to calculate various acoustical parameters such as adiabatic compressibility (*β*), acoustical impedance (Z) free length ($L_f$) and relaxation time (τ), absorption coefficient ($\alpha/f^2$). The variations of these parameters under different conditions of concentration have been used to discuss the nature and extent of intermolecular interactions between the component molecules. The effect of polymer on solvent has also been studied.**

**Keywords:** Acoustical parameters; Dimethyl Sulfoxide; Molecular interaction; Polyvinyle pyrolidone; Ultrasonic velocity.

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**INTRODUCTION:** Acoustic spectroscopy is one of the most widely used techniques to study the molecular interaction in polymer solutions. The information about different interactions involved among the various polymer-solvent systems and of the complex formation, association or dissociation, structural and destructural nature of the solvents can be directly given using Adiabatic compressibility, computed from ultrasonic velocity and density of the solution. The relationship between material properties and acoustic parameters has been studied for a long time. This technique has been employed as excellent tools for non-destructive testing and imaging[1]. We can characterize the viscoelastic properties of polymer melts, as well as those of semicrystalline polymers. When propagated in polymeric materials, acoustic waves are influenced by the polymer structure and molecular relaxation process. Ultrasonic method has been successfully used to monitor polymer processing[2], chemical reactions such as polymerization or curing of thermo sets[3,4], film formation from aqueous polymer dispersions[5], glue processes or crystallization in polymers[6]. Literature studies on polymer solutions revealed that ultrasonic velocity measurements are used to understand the nature of polymer-solvent, polymer-polymer interactions in these systems.

Polyvinyl pyrrolidone (PVP) has many important applications in all the fields like medicine, industry, agriculture and so on. It is used as a binder in many pharmaceutical tablets. Polyvinyl pyrrolidone (PVP) having molecular formula $(C_6H_9NO)_n$ and used as binders for the formulation of pharmaceutical tablets, for moistening various personal care products, as food additives and adhesives, etc. It is readily soluble in water, physiologically compatible, non-toxic, essentially chemically inert, temperature-resistant, pH-stable, non-ionic, and colorless[7].

Dimethyl Sulfoxide (DMSO) with molecular formula $(CH_3)_2SO$ is an important polar solvent that dissolves both polar and nonpolar compounds and miscible in water as well as different organic solvents. It is widely used in different fields as drug, solvent, extractant etc.

**MATERIALS AND METHODS:** The chemicals used for the present investigation were of analytical grade. The purity of these compounds was >99.8%. Polyvinyle pyrolidone (PVP-40) and DMSO was obtained from Sigma Aldrich. The mixtures were prepared by mixing known amount of polymer in HPLC grade water and DMSO in airtight bottles and adequate precautions were taken to minimize evaporation loses during the actual measurements.

The ultrasonic velocities in pure liquids and liquid mixtures were measured by pulse echo technique at 5MHz frequency using (UX 4400MV) Ultrasonic Flaw Detector, supplied by Roop Telsonic Ultrasonix Limited with an accuracy of ±0.01%. The instrument was calibrated by measuring the velocity of triple distilled water, acetone and dimethyl sulfoxide. The densities of the were determined using a 10ml specific gravity bottle with a permissible error of $\pm 0.1^0$C supplied by Jennson and a digital balance of accuracy $\pm 10^{-6}$ kg. Viscosity measurements were made with an Ostwald's viscometer in which the flow time for solutions was measured through a digital stop clock of accuracy ±0.01 s.

**Acoustical Measurements:** By using measured values of ultrasonic velocity (u), density (ρ) and coefficient of viscosity (η), various acoustical parameters were obtained from following equations[8-10].

Adiabatic compressibility

$\beta = 1/u^2 \rho$ …… (1)

Where, $u$ = velocity & $\rho$ = density

Intermolecular free length

$L_f = K \beta^{1/2}$ …… (2)

Acoustic impedance

$Z = u \rho$ …… (3)

The relaxation time

$\tau = 4\eta/3\rho u^2$ …… (4)

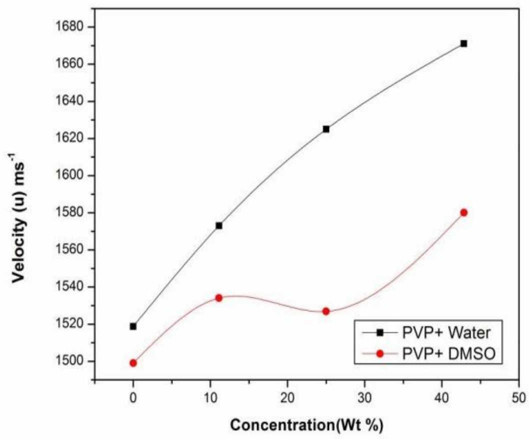
Absorption coefficient

$\alpha/f^2 = 2\pi^2 \tau /u$ …… (5)

**RESULTS AND DISCUSSION**: The experimentally measured values of density, viscosity and velocity of sound and other related parameters such as adiabatic compressibility ($\beta$), acoustical impedance (Z) free length ($L_f$), free volume ($V_f$), relaxation time (τ), absorption coefficient ($\alpha/f^2$) of the PVP-water and PVP-DMSO systems, as a function of concentration are obtained and graphs are plotted. The plotted graphs for different acoustical parameters, explains the interactions between polymer (PVP-40) and solvent (water and DMSO).

In fig.1, variations of ultrasonic velocity (u) in solution of PVP-water and PVP-DMSO for different concentrations are shown. Graph shows that ultrasonic velocity increases with increase in concentration of PVP in water and DMSO. For sound propagation, ultrasonic velocity increases on decrease of free length[11]. PVP-water system shows linear whereas PVP-DMSO system nonlinear increase in ultrasonic velocity. Variation in ultrasonic velocity explains interaction of PVP molecule with water and DMSO. The nonlinear behavior of PVP with DMSO may be due to presence of two methyl groups and double bonded oxygen which may interact complexly with polymer.

**Figure.1: Plots of Ultrasonic velocity with increasing concentration of PVP-40 in water and DMSO.**




The variation in adiabatic compressibility ($\beta$) in solution of PVP-water and PVP-DMSO for different concentrations is shown in fig. 2. The graph shows that, adiabatic compressibility decreases as concentration of PVP-40 in water increases. The higher compressibility value implies that the medium is loosely packed whereas the lower compressibility is an indication of maximum interaction. The gradual decreases in adiabatic compressibility with increase in concentration of polymer suggest that the medium become less and less compressible. The polymer in water tends to break the molecular clustering of water, which makes available dipoles for further interaction[12]. Due to these dipole interactions, solute-solvent molecules are coming close to each other and the space between them is decreases with rise in concentration of polymer. This supports to the strong solute-solvent interaction in the solution[13]. But the variations in adiabatic compressibility for PVP-DMSO system are not continuous. The nonlinear behavior of compressibility implies that polymer molecules shows complex behavior with DMSO. The same results can be observed by variation in free length. In fig. 3 graph shows exactly same variations as adiabatic compressibility. A continuous decrease in compressibility means more compact and pack structure is formed which reduces free length of the molecule.

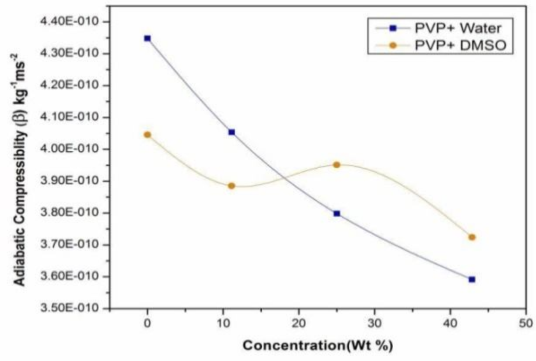



**Figure.2: Plots of Adiabatic Compressibility with increasing concentration of PVP-40 in water and DMSO.**

The variations in acoustic impedance for both the systems are shown in fig.4. It is observed from the graph that acoustic impedance of both the system increases with increase in concentration of polymer in solvent. PVP-DMSO shows nonlinear behaviour.

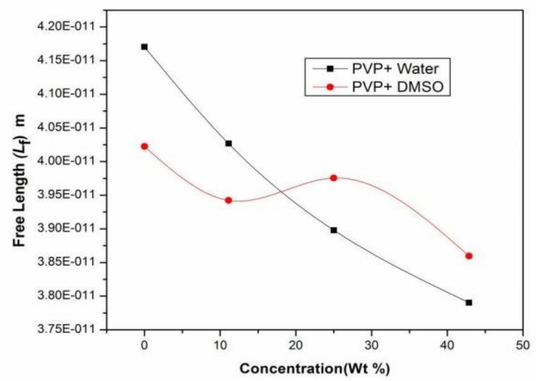
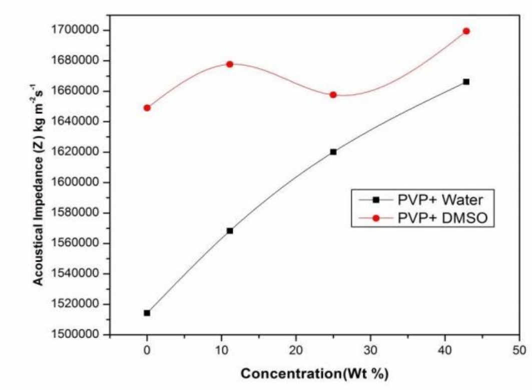



**Figure.3: Plots of Free length with increasing con-**




**centration of PVP-40 in water and DMSO.**

**Figure.4: Plots of Acoustical Impedance with increasing concentration of PVP-40 in water and DMSO.**

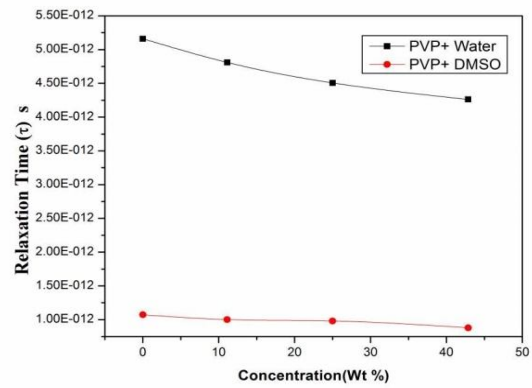



**Figure.5: Plots of Relaxation Time with increasing concentration of PVP-40 in water and DMSO.**

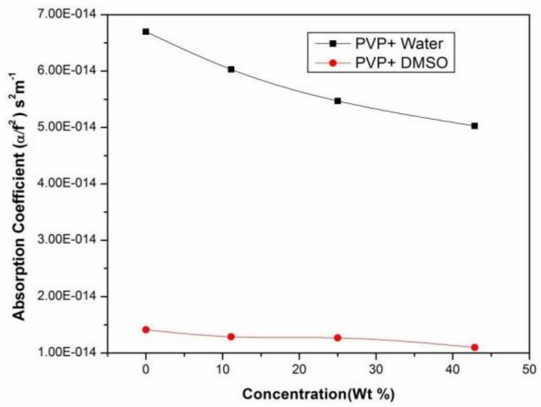



**Figure.6: Plots of Absorption Coefficient with increasing concentration of PVP-40 in water and DMSO**.

Acoustic impedance is a measure of opposition offered by the system to the acoustic flow. The increase in acoustic impendence shows that the molecular interactions in these solutions are associative[14,15]. It means molecular association increases with increase in concentration of polymer in solvent.

Relaxation time and absorption coefficient is observed to be decreasing with increase in concentration of PVP in water and DMSO consistently which is shown in fig.5 and fig.6 respectively. This decrease is observed more on PVP-water system compared to PVP-DMSO system, which suggest breaking of water molecule is more than DMSO molecule.

**CONCLUSION:** Ultrasonic velocity, density and viscosity of solutions of PVP-water and PVP-DMSO system for different concentrations are measured and acoustical parameters are calculated. The variations in some acoustical parameters such as ultrasonic velocity, adiabatic compressibility ($\beta$), acoustical impedance (Z) free length ($L_f$), free volume ($V_f$), relaxation time (τ), absorption coefficient ($\alpha/f^2$) with increase in concentration shows that solute-solvent interaction are present in the solution. The addition of polymer will break the bonds of solvent molecule which provide the free ions to interact with polymer molecules. These free ions interact with the polymer molecules in which partially negatively charged Oxygen atom of PVP may be attracted towards partially positively charged Hydrogen atom of water and methyl group of DMSO. This will increase association in polymer and solvent molecule and complex formation takes place between them. Also polymer-polymer interaction is a present in the system. Behaviour of PVP with DMSO is complex compared to water.

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