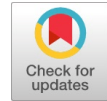


Intermolecular Interaction of Aqueous Dextran with Urea



Subhrraj Panda, Achyuta Prasad Mahapatra

Abstract: In this paper, the authors have given information regarding intermolecular interactions of aqueous dextran solution in urea. The behavior of dextran in urea has been examined by the help of ultrasonic interferometer working at frequency 5MHz at different temperatures ranging from 303 K to 323 K in 5K interval. Ultrasonic speed, density, viscosity measurements have been used for the evaluation of thermodynamic parameters like Gibb's free energy (ΔG) as well as acoustical parameters are acoustic impedance (Z), isentropic compressibility (β), intermolecular free length (L_f) and relaxation time (τ), etc. The results have been used to throw light on the nature of the interaction among solute and solvent, interpreted in the light of structural rearrangement occurs in the aqueous dextran and urea solution.

Keywords: Dextran, acoustic impedance, isentropic compressibility, and Gibb's free energy.

I. INTRODUCTION

The molecular interaction studies [1] of polymer in different solvents from acoustic measurements have assumed significant recently due to their commercial application in the field of medical science. In continuation of prior work on various solute and solvent [2-4], we have made further attempt to study systematically the physicochemical behavior of dextran in urea by evaluating different thermo-acoustic parameters are, acoustic impedance (Z), isentropic compressibility (β), intermolecular free length (L_f), relaxation time (τ) and Gibb's free energy (ΔG). From these values, we have assessed the nature and strength of the molecular interaction of dextran in urea. The ultrasonic speed (U) in a fluid is fundamentally identified with the coupling powers between the atoms or molecules and has been effectively utilized in understanding the idea of molecular interaction in the fluid [5].

The study of the propagation of ultrasonic waves in liquids as well as liquid solutions is well established for determining the nature of intermolecular interaction in these systems. The reason is molecular interactions are the key to understand the structure and properties of liquids, solids, and gases.

Molecular interactions give some comprehension idea of the problems concerned about the mechanism of chemical and biochemical catalysis and the ways of the chemical reaction. Hence ultrasonic investigations provide an extensive application in characterizing the thermodynamic and

physicochemical behavior of the liquids solutions. The measurement of U enables the accurate determination of some useful acoustical parameters which are highly sensitive to molecular interactions. The acoustical parameters give qualitative information regarding the physical nature and strength of the molecular interaction in the fluid solution [9-11] Dextran is a complex, branched polysaccharide made of numerous glucose atoms made out of chains of varying length (from 10 to 150 kilodaltons). Polymer Dextran is a water-soluble, an α -D-1, 6-glucose connected glucan with side chains 1-3 connected to the backbone units of the polymer. Urea is a mineral that is only stable in an arid environment. The structure of urea the carbon is attached to oxygen by a double bond whereas it is attached to two NH_2 with a single bond each. Urea is utilized in numerous multi-part strong manure formulations. Urea is exceptionally soluble in water and is therefore also very reasonable for use in manure solutions.

II. EXPERIMENTAL SECTION

A. Materials

The solution prepared in distilled water as a solvent for preparing the dextran solution at different concentrations. Dextran of M.W. 70,000 utilized as a solute, is of A R grade, made by HI Media Laboratories, India. Solvent 6(M) urea is an A R grade, made by Fisher scientific used in this state throughout the experiments.

B. Measurements

Speed

The speed of the ultrasonic wave in the solution has been measured utilizing an ultrasonic interferometer, working at 11 various frequency supplied by M/s Mittal Enterprises, New Delhi (Model M-84). The measuring cell of the interferometer is a specially structured twofold walled vessel with an arrangement for temperature constancy. An electronically worked advanced steady temperature shower provided by M/s Mittal Enterprises, New Delhi, (Model SSI-03spl) working in the temperature range -10°C to 85°C with a precision of $\pm 0.1\text{K}$ has been utilized to circulate water through the external jacket of the twofold walled estimating cell containing the test fluid.

Density (ρ)

The ρ of the solution were estimated using a 10 ml Pycnometer bottle.

The Pycnometer bottle with the investigational solution was submerged in a temperature-controlled water shower.

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The ρ was estimated using the equation

$$\rho_2 = \frac{w_2}{w_1} \rho_1$$

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

Viscosity (η)

The viscosities of the solution were estimated using Ostwald's viscometer standardized with distilled water. The Ostwald's viscometer with the investigational solution was submerged in a temperature-controlled water shower. The time of flow was measured using an advanced stopwatch with a precision of 0.01 s. The η was calculated using the equation,

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

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 = Time of flow of water, t_2 = Time of flow of investigational solution.

III. THEORETICAL ASPECT

The information of ultrasonic speed, ρ , and η lead to the determination of different thermo-acoustical parameters, using standard equation.

Acoustic impedance	$z = u \cdot \rho$
Isentropic compressibility	$\beta = \frac{1}{\rho u^2}$
Intermolecular free length	$L_f = \frac{KT}{u \rho^{3/2}}$
Relaxation time	$\tau = \frac{4 \eta}{3 \rho u^2}$
Gibb's free energy	$\Delta G = kT \ln \frac{kT\tau}{h}$

Where $KT = (93.875+0.375T) \times 10^{-8}$ 'T' is the absolute temperature; 'k' is the Boltzmann's constant and 'h' is the Planck's constant.

IV. RESULTS AND DISCUSSION

The experimental values of ρ , η and U of 6(M) urea with aqueous dextran and calculated acoustic parameters at temperatures ranging from 303 K to 323 K in 5K interval for 5 MHz frequency in various concentration of dextran have been presented in tables 1 to 4 and figures 1 to 16.

The increasing value of ρ and η with concentrations (Fig.1&Fig.3) shows that there is a strong attraction among polymer dextran and aqueous urea particles. The decrease in values of ρ and η with rise in temperature (Fig.2 Fig.4) demonstrates the diminishing in intermolecular powers because of the expanding warm vitality of the framework [3]. It is seen that U rises with rise in concentration of solute in

urea (Fig.5), showing their association. The rise of proposes is a structure-production capacity of dextran in solution. With rise in the temperature there happens a structural improvement because of solvation prompting a similarly progressively state so the U rises with rise in temperature [5].

$z = u \cdot \rho$. As ρ and speed both raise with the rise in concentration the z esteem likewise expands (Fig.8) .which shows a strong interaction among the dextran and urea particles at higher concentration, hence strong opposition to the propagation of an ultrasonic wave through the solution. z rises with rise in temperature (Fig.7) [8].

β decreases with rise in concentration (Fig.9) and temperature (Fig.10), because this depends on electron donor and acceptor capacity. Water is a polar solvent when urea is added, the association of solute and solvent molecules occurs resulting in close packing of molecules. The decreased values of isentropic compressibility indicate a strong intermolecular association between urea and water molecules. The compressibility of a solvent is complex than that of a solution and declines with rise in concentrations and temperatures of the solution.

L_f is the average separation among the surfaces of two neighboring particles, which is called intermolecular free length. Free length declines with rise in concentration (Fig.12) but rises with the rise of temperatures (Fig.11) indicating the dissociation of intermolecular forces because of rise in the thermal energy of the system which causes rise in volume expansion. It demonstrates that there is a significant interaction among solute and solvent particles.

With rise in temperature excitation energy rises and hence relaxation time diminishes (Fig.13).The rise in relaxation time with rise in concentration (Fig.14 shows that the arrangement is exceedingly ordered because of brilliant hydration.

ΔG decreases with rise in temperature (Fig.15) because the thermal energy is utilized in expansion and suggests the larger time for rearrangement of molecules in the solution. It is observed that (ΔG) rises with rise in concentration (Fig.16). This shows that the solution is highly ordered due to a strong association among the dextran and urea molecules. It suggests a smaller time for reshuffle of the dextran particles in the solution [9-10].

Table 1 Values of ρ and η of dextran in 6(M) urea.

T (K)	Concentration of dextran									
	0.10 %		0.25 %		0.50 %		0.75 %		1 %	
	ρ kg/m ³	$\eta \times 10^{-3}$ N s/m ²	ρ kg/m ³	$\eta \times 10^{-3}$ N s/m ²	ρ kg/m ³	$\eta \times 10^{-3}$ N s/m ²	ρ kg/m ³	$\eta \times 10^{-3}$ N s/m ²	ρ kg/m ³	$\eta \times 10^{-3}$ N s/m ²
303	1077.26	1.039	1078.00	1.059	1078.75	1.086	1080.04	1.105	1081.00	1.124
308	1075.25	0.965	1076.00	0.990	1076.75	1.036	1078.02	1.054	1079.21	1.073
313	1073.81	0.884	1074.00	0.920	1075.40	0.963	1076.19	0.980	1077.77	0.999
318	1071.38	0.820	1071.75	0.850	1072.57	0.900	1073.00	0.923	1074.54	0.941
323	1067.93	0.750	1068.50	0.783	1069.00	0.834	1069.91	0.851	1071.09	0.868

Table 2 Values of U and Z of dextran in 6(M) urea.

T (K)	U m/s					Z 10 ⁶ kg·m ² /s				
	0.10 %	0.25 %	0.50 %	0.75 %	1 %	0.10 %	0.25 %	0.50 %	0.75 %	1 %
303	1613.00	1617.00	1618.50	1620.50	1621.00	1.738	1.743	1.746	1.750	1.752
308	1616.50	1619.00	1621.00	1622.50	1623.00	1.738	1.742	1.745	1.749	1.752
313	1620.00	1622.00	1622.50	1624.00	1625.00	1.740	1.742	1.745	1.748	1.751
318	1623.00	1625.00	1625.00	1626.00	1626.50	1.739	1.742	1.743	1.745	1.748
323	1626.00	1628.00	1628.00	1629.50	1630.00	1.736	1.740	1.740	1.743	1.746

Table 3 Values of β and L_f of dextran in 6(M) urea.

T (K)	β (10 ⁻¹⁰ m ² /N)					L_f (10 ⁻¹⁰ m)				
	0.10 %	0.25 %	0.50 %	0.75 %	1 %	0.10 %	0.25 %	0.50 %	0.75 %	1 %
303	3.568	3.548	3.539	3.526	3.521	3.748	3.737	3.732	3.726	3.723
308	3.559	3.546	3.534	3.524	3.518	3.776	3.769	3.763	3.757	3.754
313	3.548	3.539	3.532	3.523	3.514	3.803	3.797	3.794	3.789	3.784
318	3.543	3.533	3.531	3.525	3.518	3.832	3.827	3.825	3.822	3.818
323	3.542	3.531	3.530	3.520	3.514	3.864	3.858	3.857	3.852	3.849

Table 4 Values of τ and ΔG of dextran in 6(M) urea.

T (K)	τ (10 ⁻¹³ s)					ΔG 10 ⁻²⁰ kJ/mol				
	0.10 %	0.25 %	0.50 %	0.75 %	1 %	0.10 %	0.25 %	0.50 %	0.75 %	1 %
303	4.943	5.008	5.126	5.196	5.275	206.78	209.16	213.36	215.83	218.58
308	4.578	4.680	4.883	4.954	5.033	199.05	203.12	210.96	213.61	216.52
313	4.182	4.341	4.533	4.606	4.681	188.31	195.33	203.45	206.43	209.46
318	3.875	4.005	4.237	4.340	4.415	179.81	186.08	196.83	201.41	204.69
323	3.542	3.687	3.922	3.992	4.067	168.27	176.02	188.01	191.43	195.04

Intermolecular interaction of aqueous dextran with urea

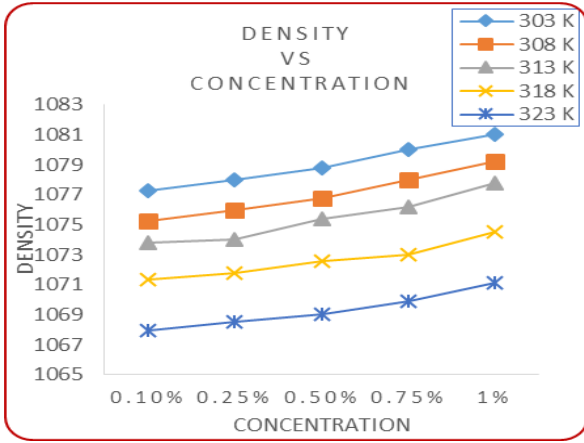


Fig: 1 Plots of density vs. concentration

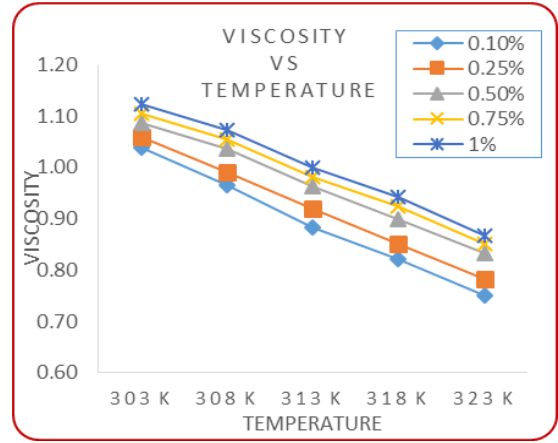


Fig: 4 Plots of viscosity vs. temperature

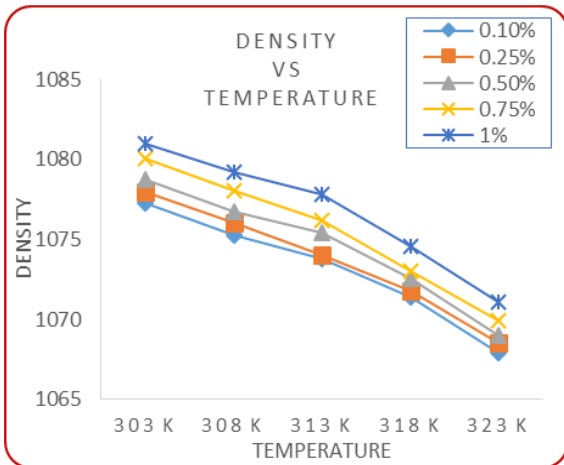


Fig: 2 Plots of density vs. temperature

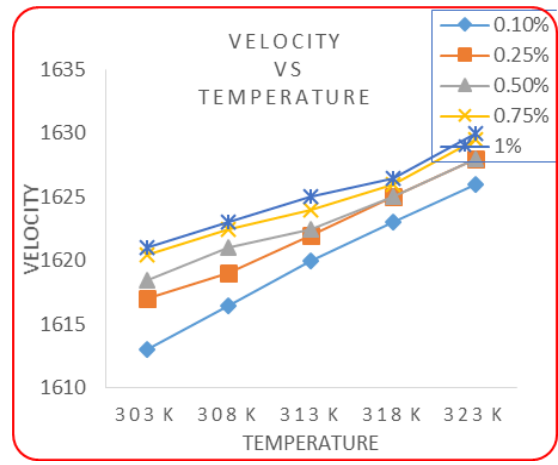


Fig: 5 Plots of speed vs. temperature

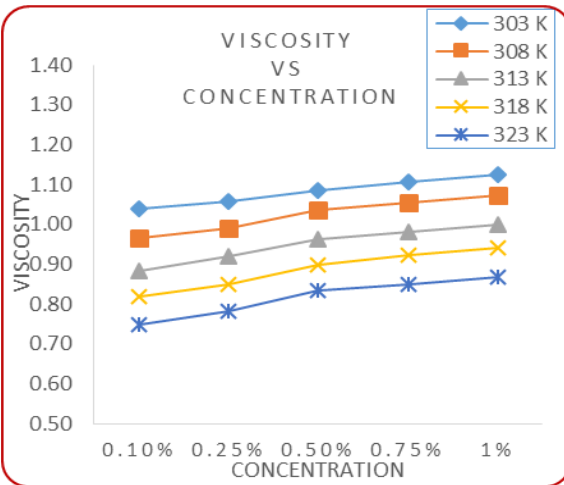


Fig: 3 Plots of viscosity vs. concentration

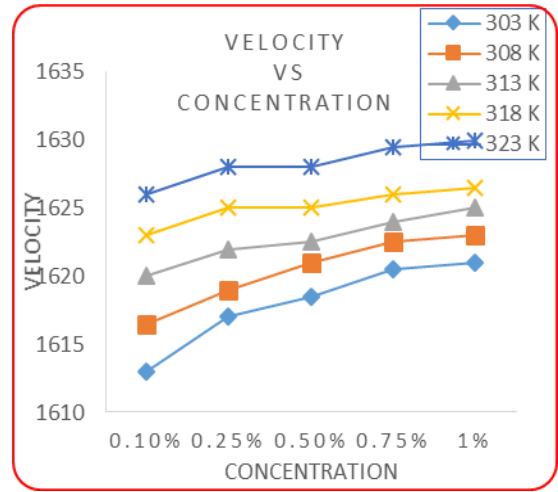
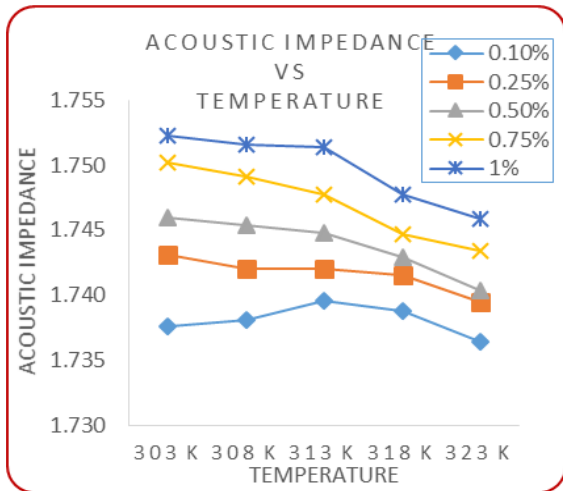
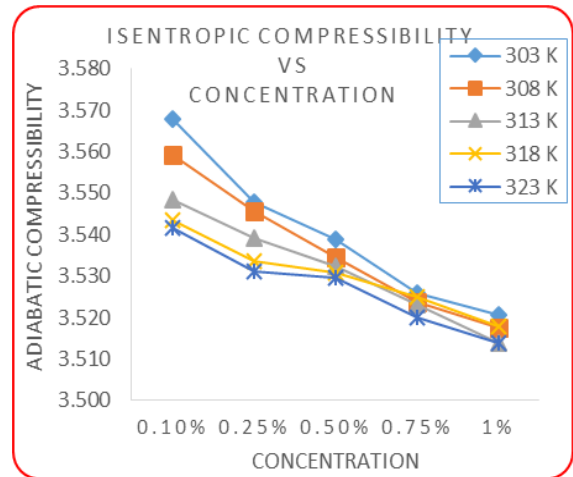


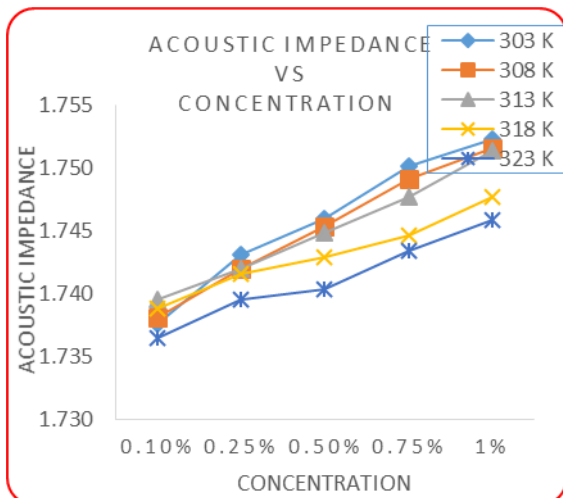
Fig: 6 Plots of speed vs. concentration



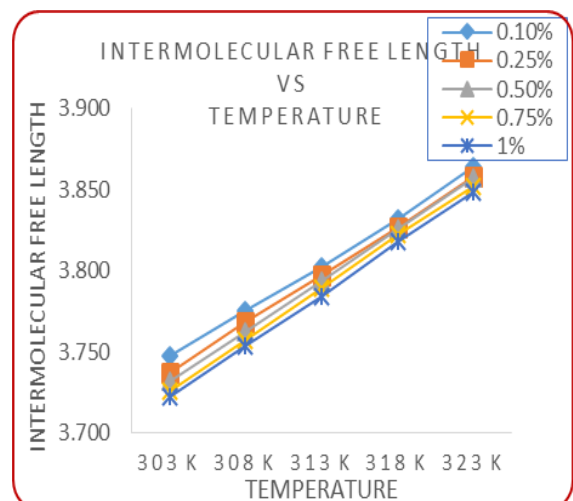
Fig; 7 Plots of acoustic impedance vs. temperature



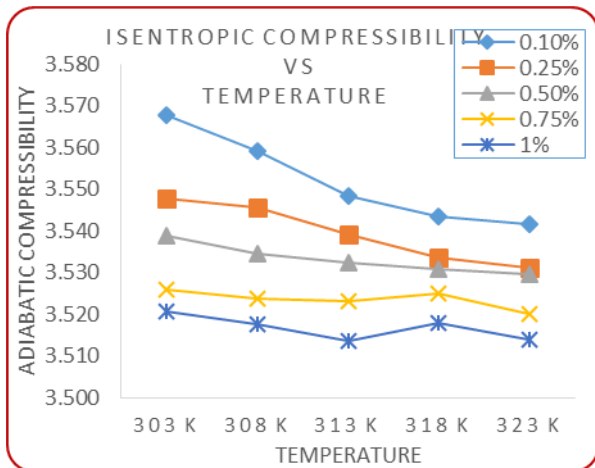
Fig; 10 Plots of isentropic compressibility vs. concentration



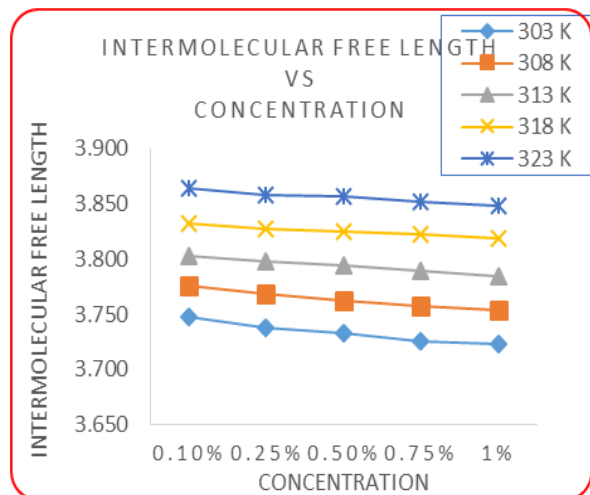
Fig; 8 Plots of acoustic impedance vs. concentration



Fig; 11 Plots of intermolecular free length vs. temperature



Fig; 9 Plots of isentropic compressibility vs. temperature



Fig; 12 Plots of intermolecular free length vs. concentration

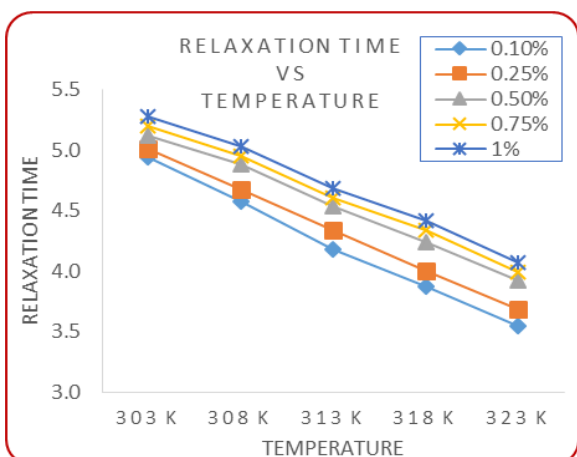


Fig: 13 Plots of relaxation time vs. temperature

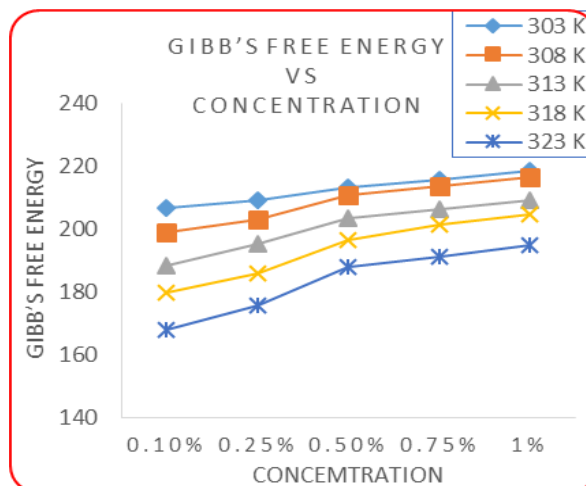


Fig: 16 Plots of Gibb's free energy vs. concentration

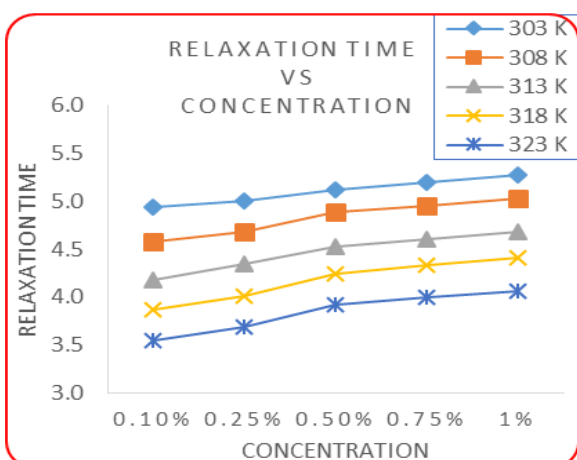


Fig: 14 Plots of relaxation time vs. concentration

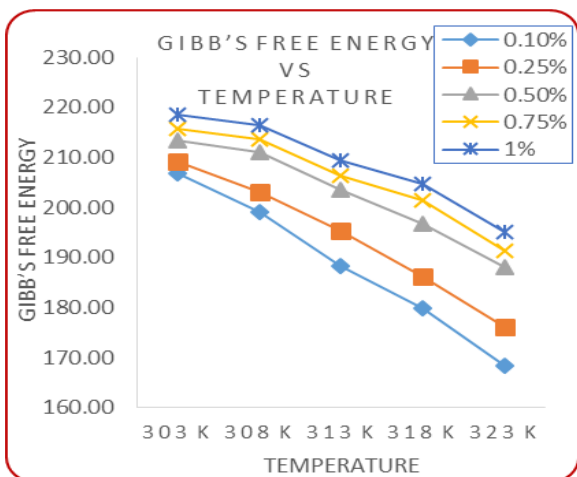


Fig: 15 Plots of Gibb's free energy vs. temperature

V. CONCLUSION

When a polymer dextran fragment is added to the solvent, forces of attraction or dispersion start acting between them depending on their polarity, chemical nature, and their solubility parameter. When this urea-dextran interaction becomes more powerful than the dextran-dextran attraction, the forces holding the polymer dextran segments together become weak. So the solvent urea molecule enters between the segments and breaks the segment-segment contact. They surround the individual segments and establish contact with them

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