Molecular Dynamics and Dielectric Behavior of Indole-3-Carbinol in Dimethyl Sulfoxide: A Spectroscopic Analysis of Structural and Thermodynamic Characteristics

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Abstract

This paper investigates the dielectric and thermodynamic behavior of Indole-3-carbinol (I3C) in dimethyl sulfoxide (DMSO) using time-domain reflectometry. It identifies two distinct relaxation processes: low-frequency (I3C-driven) and high-frequency (DMSO-driven). Key parameters such as permittivity, relaxation time, dipole moment, and thermodynamic factors (free energy, entropy, and enthalpy) reveal the dynamics of molecular interactions. The study shows that increasing I3C concentration leads to greater steric hindrance, longer relaxation times, and stronger solute-solvent interactions. Structural changes reduce the dielectric constant and effective dipole moment, while negative entropy values highlight an increasingly ordered system at low frequencies.

Keywords: Time-Domain Reflectometry, Thermodynamic, Dipole Moment

1. Introduction

A potent tool for comprehending molecular structures is spectroscopy, which is the study of material characteristics through interactions with radiated energy. The characteristics that are observed are highly sensitive to the frequency of the electromagnetic spectrum that is used to illuminate the substance. Modern spectroscopy has opened up a world of possibilities in the biological sciences and beyond, touching almost every part of the electromagnetic spectrum. Analytical tools that shed light on material structures include dielectric relaxation spectroscopy (DRS), nuclear magnetic resonance (NMR), ultraviolet (UV), and X-ray (XRD) images. Analytical chemists rely heavily on ultraviolet (UV) spectroscopy for studying UV-absorbing molecules like DNA and proteins and for determining the chemical makeup of substances. Biomolecules, like proteins, can have their atomic configurations revealed by X-ray spectroscopy. The molecular vibrations, which are studied by infrared spectroscopy, are commonly called the "fingerprint region." Molecular flexibility and rigidity are studied by dielectric spectroscopy (DRS), which provides information about electrical properties, biological and pharmacological activities across a wide range of magnitudes. The relaxation behavior of organic molecules, especially heterocyclic compounds, can be studied with great benefit using dielectric spectroscopy. It shows how phenyl and heterocyclic rings, among other molecular structures, affect molecular behavior. Spectroscopy is crucial for the study and development of novel molecular structures in biomolecular, organic, and polymeric systems due to its wide range of applications. The polar aprotic solvent dimethyl sulfoxide (DMSO) is indispensable in many fields, including biotechnology, medicine, and chemistry. Its polarity and hydrogen-bonding capability are associated with its distinctive characteristics, such as its capacity to cross biological membranes relatively unscathed. Due to its ability to form associations with various biological components, such as water, proteins, carbohydrates, nucleic acids, and more, DMSO is an intriguing material to study in relation to interactions with heterocyclic organic compounds.

The organic heterocyclic biomolecule indole-3-carbinol (I3C) comes from cruciferous vegetables like cabbage and broccoli. With antioxidant, anti-atherogenic, and anticancer properties, this molecule shows promise as a pharmacologically active agent. I3C in DMSO has not been studied structurally or dynamically, even though heterocyclic compounds have been studied extensively for their dielectric properties, especially in the GHz frequency range and at temperatures below room temperature. Using time-domain reflectometry (TDR), this study intends to fill that void.

2. Experiment

Materials: Hi Media Laboratories Pvt. Ltd. of Mumbai, India, supplied the indole-3-carbinol (I3C) and dimethyl sulfoxide (DMSO), both of which were ≥99% pure. We used the samples as-is, without purification, and accurately weighed them to create DMSO solutions of varying concentrations of I3C.

Measurements: Tektronix Digital Serial Analyzer (DSA8300) with sampling module 80E10B was used to measure dielectric. An impedance of 50 Ω was used by the system, which transmitted a 12 ps incident pulse and a 15 ps reflected rise time pulse via a coaxial line. Over a 5-ns time window, 2000 points were digitally recorded for the reflected pulses ($R_1(t)$) without a sample and ($R_x(t)$) with a sample. The complex permittivity spectra ($\varepsilon^*(\omega)$) were calculated using the least square fit method after data was transformed and analyzed using Fourier transform.

3. Results and Discussion: We computed a number of dielectric and thermodynamic parameters for various I3C concentrations in DMSO. Here are the parameters:

- Static permittivity (ε′)
- Dielectric loss (ε″)
- Relaxation time (τ)
- Correlation factor (g)
- Dipole moment (μ)
- Effective volume (V_{eff})
- Number of irrotationally bound DMSO molecules (Z_{ib})

These are the thermodynamic parameters: the molar activation free energy (ΔF), the molar activation entropy (ΔS), and the molar activation enthalpy (ΔH). The complex permittivity, which was measured across a range of concentrations and temperatures as a function of frequency, is defined as $\varepsilon^* = \varepsilon' - j\,\varepsilon''$. Figure 1 displays the dielectric dispersion and absorption curves for the I3C-DMSO system at different concentrations. It also compares the experimental spectra to the fitted ones. The results show that changes in concentration and temperature affect the dielectric behavior of I3C in DMSO, which gives valuable insights into its structural and dynamic properties.

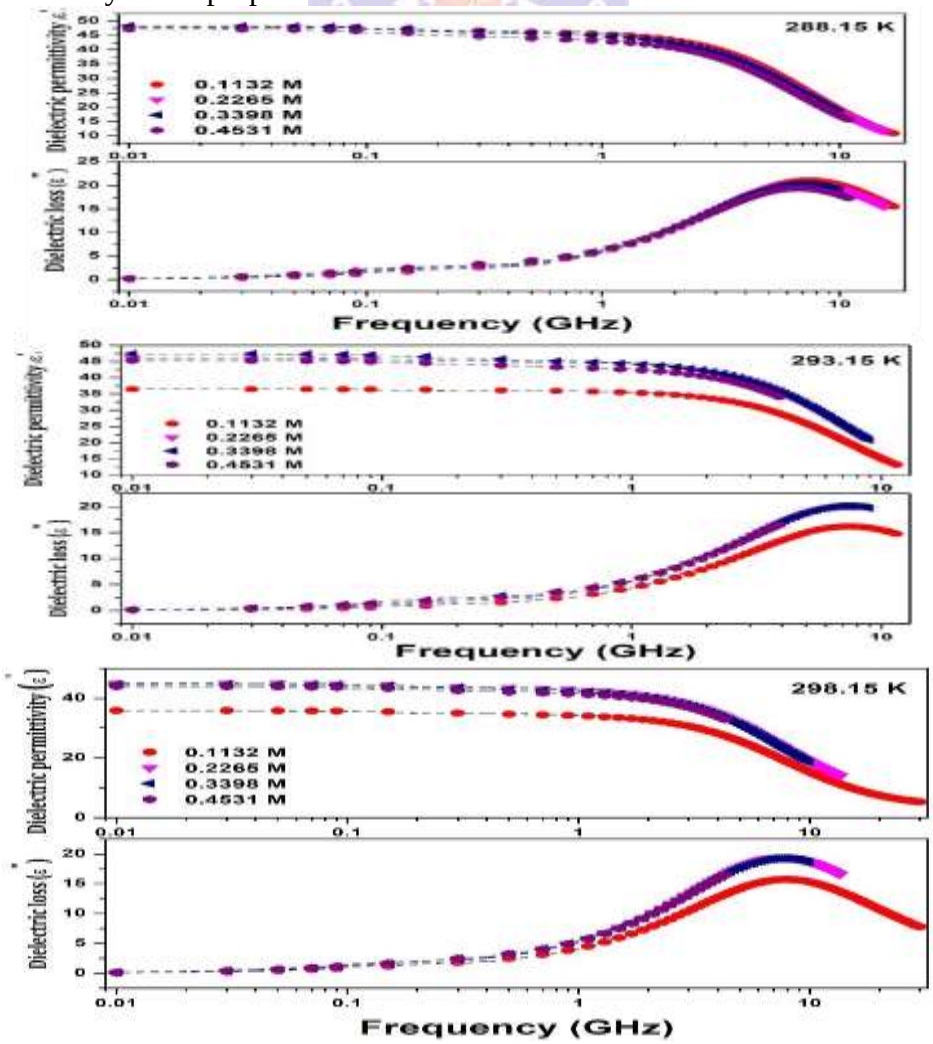

Fig. 1: Variation of complex permittivity spectra of Indole 3-Carbinol-DMSO with log frequency at different temperature and concentrations

As temperature increased, dielectric permittivity (ε") slightly decreased for all I3C concentrations in DMSO. Loss peaks shifted to lower frequencies, indicating solute-solvent interactions. Two relaxation peaks were observed: high-frequency relaxation (6-7 GHz) attributed to DMSO molecules, and low-frequency relaxation (80-100 MHz) dependent on I3C concentration. At lower temperatures, the I3C relaxation peak became more pronounced. The relaxation processes were effectively modeled using the S. Havriliak-Negami equation and fitted via the least square method.

$$\varepsilon^*(\omega) = \varepsilon_\infty + \frac{\Delta\varepsilon_i}{[1 + (j\omega\tau_i)^{1-\alpha}]^\beta} \quad (1)$$

For systems with two relaxation processes, the equation was extended as:

$$\varepsilon^*(\omega) = \frac{\Delta\varepsilon_1}{1 + (j\omega\tau_1)} + \frac{\Delta\varepsilon_2}{1 + (j\omega\tau_2)} + \varepsilon_\infty \quad (2)$$

- $\Delta\varepsilon_1$ and $\Delta\varepsilon_2$ are the relaxation strengths for the low- and high-frequency processes, respectively.
- $\varepsilon\infty$ is the high-frequency limiting static dielectric constant.
- ω is the angular frequency.
- τ_1 and τ_2 are the relaxation times for the low- and high-frequency processes, respectively.
- α ($0 < \alpha < 1$) is the distribution parameter that characterizes the broadness of the symmetric relaxation curve. According to the Cole-Cole dispersion model, the dielectric data of the I3C-DMSO system showed symmetric relaxation behavior. These results shed light on the temperature- and concentration-dependent molecular dynamics and interaction mechanisms in the I3C-DMSO system.

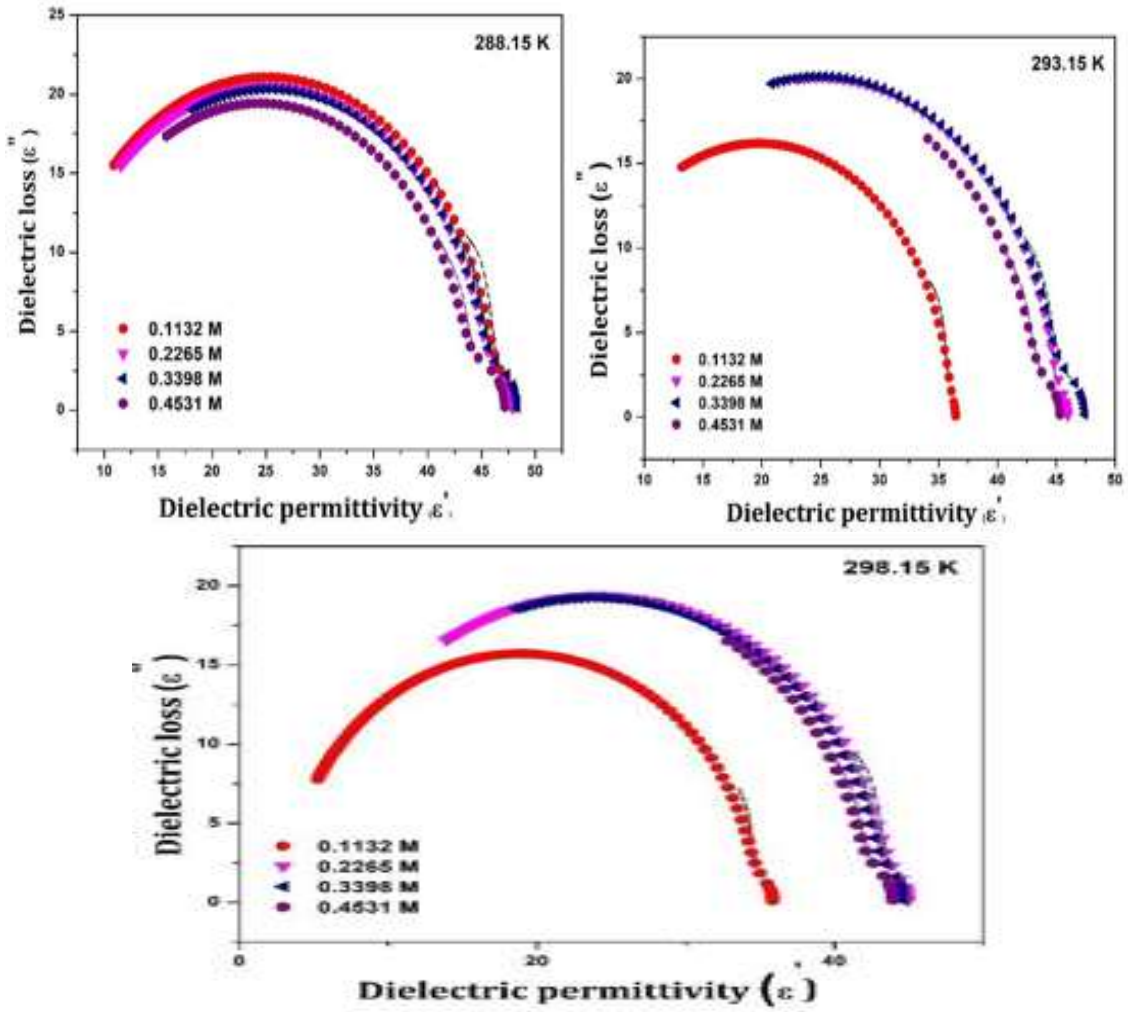

Fig. 2: Cole-Cole spectra for indole-3-carbinol+ DMSO for all temperature and concentrations

Static Dielectric constant:

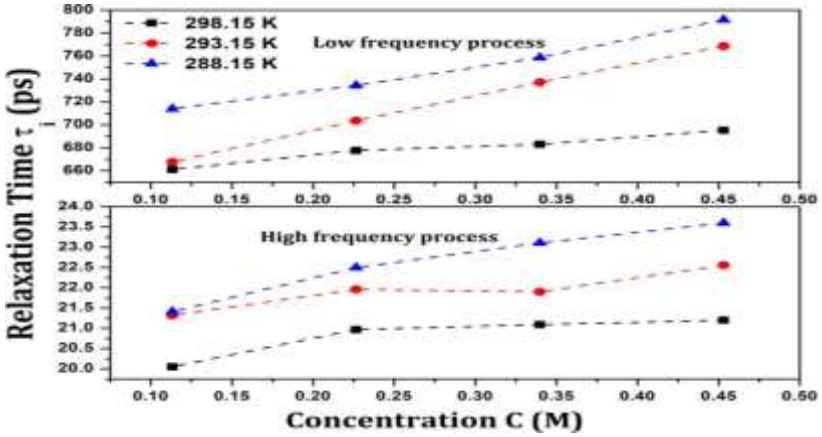

Fig. 3: Low- and high-frequency relaxation processes' static dielectric constants plotted against concentrations at various temperatures

As Indole-3-Carbinol (I3C) molecules form multimers by hydrogen bonding, their effective dipole-dipole antiparallel alignment rises. As the concentration increases, the correlation factor g (Table 1) drops, plainly indicating that the dipoles are not aligned in a parallel fashion. As the concentration of I3C increases and the temperature rises, the dielectric constant (ε2(c)) for the high-frequency relaxation process drops. The cooperative relaxation of I3C molecules coupled with DMSO is indicated by the concentration dependence of the high-frequency static dielectric constant (ε 2(c)) (Fig. 3). The larger relaxation time (τ 2) shown at lower DMSO concentrations, which correspond to higher solute concentrations, lends additional credence to this link (Fig. 4). The dielectric properties are also greatly affected by the structural properties of the I3C-DMSO combination, which vary with temperature. At lower temperatures, the static dielectric constant for the low-frequency relaxation process increases, perhaps because the thermal energy is reduced, which causes the dipoles to align. This arrangement highlights the robust shielding effect of DMSO surrounding the I3C molecules and reduces solute-induced interactions by weakening short-range dipole-dipole interactions. As a result, it is noted that at lower temperatures, the relaxation period (τ1) increases (Fig. 4). For all concentrations, the static dielectric constant for the high-frequency relaxation process increases as the temperature drops. The formation of a more ordered dipolar arrangement by a larger number of DMSO molecules associating with I3C molecules is responsible for this rise. Concentration and temperature interact dynamically to affect the dielectric behavior and structural properties of the I3C-DMSO system, as shown by these results.

Dielectric relaxation time:

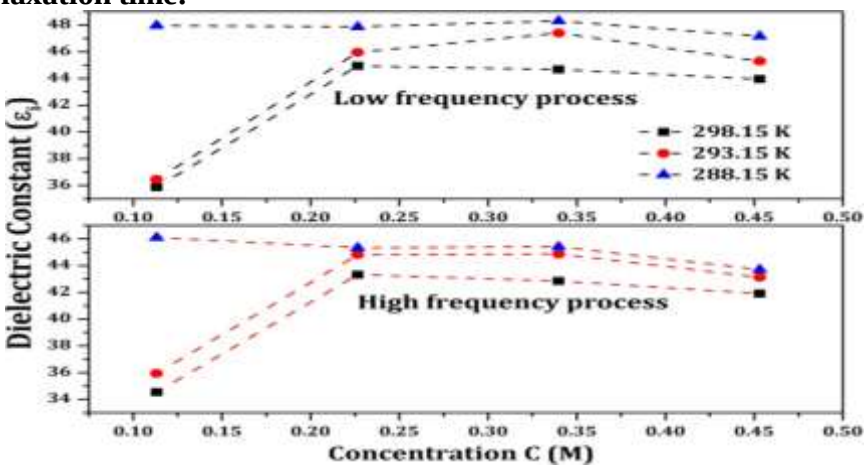

Fig. 4: The relaxation time of dielectrics at low and high frequencies in relation to concentration and temperature

Dipole Moment

Thermal motion constantly changes the orientation of dipoles in liquids, in contrast to gases or solids where dipoles are immobilized in stable geometric orientations or when dipole

interactions are weak because of big molecular distances. Liquids undergo dielectric alterations as a consequence of the ever-changing orientation and motion of molecular dipoles. Understanding the dispersion of electronic charges under different concentrations and temperatures can be greatly enhanced by calculating the dipole moment.

Using Cavell's equation, the effective dipole moment (μ_{eff}) was determined.

$$\Delta\varepsilon_j = \frac{\varepsilon_s}{3(\varepsilon_s + (1-\varepsilon_s)A_j)} \frac{N_A k_B T \varepsilon_0 \mu_{\text{eff},j}^2}{(1-\alpha_j f_j)^2} \quad (3)$$

- ε_s is the static permittivity.
- N_A is Avogadro's number.
- k_B is Boltzmann's constant.
- T is the temperature.
- A is the shape parameter of the reaction field (A=1/3 for spherical particles).
- f is the reaction field factor.
- α is the molecular polarizability.

The effective dipole moment (μ_{eff}) is related to the gas-phase dipole moment (μ_0) through the correlation factor (g_i):

$$\mu_{\text{eff},j}^2 = g_i \mu_{0,j}^2$$

$$\hat{\mu} = \frac{\mu_{\text{eff},j}}{(1-\alpha_j f_j)} = \frac{\sqrt{g_i}\mu_{0,j}}{(1-\alpha_j f_j)} \quad (4)$$

The correlation factor g_i (where i=1 for low-frequency and i = 2 for high-frequency processes) indicates the alignment tendencies of dipoles:

- gi = 1: No orientational correlation between dipoles.
- gi >1: Tendency toward parallel dipole alignment.
- gi<1: Tendency toward antiparallel dipole alignment.

Table 1: values of effective dipole moment (μ_{eff}), correlation factor (g), Number of irrotationally bound DMSO molecules (Z_{ib}), effective volume as a function of temp. at various concentrations.

Molar Conc./ Temp.(K)	288.15	293.15	298.15
	μ_{eff}		
0.1132 M	4.61	4.01	4.01
0.2265 M	3.25	3.21	3.20
0.3398 M	2.67	2.66	2.60
0.4531 M	2.28	2.25	2.23
Correlation factor g			
0.1132 M	0.81	0.79	0.79
0.2265 M	0.40	0.51	0.50
0.3398 M	0.27	0.35	0.33
0.4531 M	0.20	0.25	0.24
Number of irrotationally bound DMSO molecules Z_{ib}			
0.1132 M	1.93	3.26	4.85
0.2265 M	1.37	1.65	2.48
0.3398 M	0.87	0.70	1.80
0.4531 M	1.10	1.10	1.58
$V_{eff}*10^{-30}$ m^3			
0.1132 M	35.93	38.95	42.63
0.2265 M	36.77	40.31	43.72
0.3398 M	37.90	42.44	43.99

0.4531 M	39.37	44.35	44.71
	fsC		
0.1132 M	0.2788	0.3022	0.3308
0.2265 M	0.2853	0.3128	0.3393
0.3398 M	0.2941	0.3293	0.3414
0.4531 M	0.3055	0.3441	0.3469

Kirkwood Correlation Factor (g)

You can learn about the electric dipole orientation in a system from the Kirkwood correlation factor (g). The following expression can be used to compute the correlation factor for pure liquids:

$$g = \frac{\mu^2 \rho M}{9kTN\varepsilon_0} \cdot \frac{(\varepsilon_0 - \varepsilon_\infty)(2\varepsilon_0 + \varepsilon_\infty)}{\varepsilon_0(2 + \varepsilon_\infty)^2} \quad (5)$$

where:

- μ is the dipole moment.
- ρ is the density at temperature TTT.
- M is the molecular weight.
- k is Boltzmann's constant.
- N is Avogadro's number.
- ε_0 is the static permittivity

In order to assess how intermolecular interactions affected the dielectric relaxation time of the molecules under study, the values of g were calculated. We learn more about the molecule orientation and how hydrogen bonding defines the system's dielectric behavior from these data.

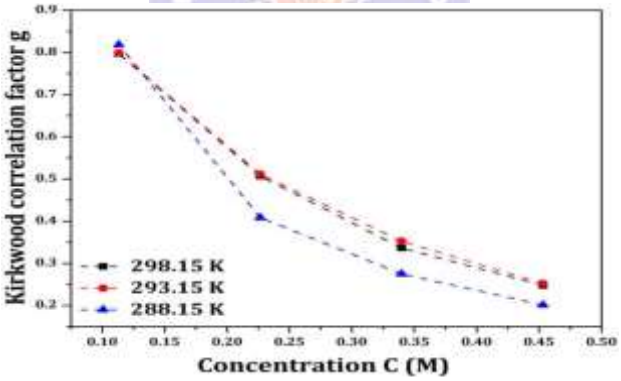

Fig. 6: Correlation factor (g) vs Concentration (M) of Indole 3-Carbinol-DMSO mixtures at different Temperatures

The dipoles are aligned antiparallel because the Kirkwood correlation factor (g1) is always smaller than 1 for all measured temperatures and concentrations. Multimer formation in the solution is quite probable, according to this. An increase in the concentration of a solute causes its effective dipole moment to decrease because of the increasing likelihood for antiparallel molecular dipole alignment. When the concentration of an indole-3-carbinol (I3C) molecule is infinitely diluted, there is no association between the molecules. For this study, we used the maximum concentration of I3C to determine the correlation factor. A molecule's orientational correlation with its closest neighbor can be measured using the Kirkwood correlation factor. Molecular interactions between solute and solvent molecules are shown as a divergence from unity. The correlation factor (g_1) for all concentrations and temperatures observed in the low-frequency relaxation process was less than 1. The effective dipole moment is further reduced when the concentration of I3C grows because the antiparallel dipole correlation becomes stronger. Changes in temperature caused the correlation factor (g1) to fluctuate slightly. At lower temperatures, the values of g_1 were somewhat greater, but they decreased marginally as they approached room temperature. At lower temperatures, the effective dipole moment is enhanced due to multimer formation and higher solute-solute interactions (I3C-I3C), as suggested by this pattern. The following

equation accurately describes the dependency of relaxation time on concentration and temperature using the molar fraction of the solute (X):

$\tau_1 = aX + b$ (6)

Here:

The equation takes a and b as parameters.

The regression coefficient, shown as R^2, shows how well the data fits the model.

Table 2 displays the computed parameters. Determined at infinite dilution was the relaxation time ($\tau 1$) from the intercept at the origin. The effective volume of rotation (V_{eff}) and other rotational dynamics features were computed using these parameters, which provided important information on the system's molecular behavior.

Table 2: Plotting the solute's relaxation time against its molar fraction X as a function of frequency for a low-frequency process

Temperature (K)	a	B	R^2	$\tau 1$ (10^{-12} Sec.)
288.15	0.0603	-9.1850	0.9574	653.13
293.15	0.1796	-9.1944	0.9977	639.14
298.15	0.1323	-9.1628	0.9906	687.38

Effective Volume of Rotation (V_{eff})

The effective volume of rotation (V_{eff}) of an ellipsoidal molecule is related to its geometrical volume (V_m) by the equation:

$V_{eff} = f_s C V_m$ (7)

Here:

f_s is a geometrical parameter accounting for the deviation of the molecular shape from an ideal sphere (fs = 1 for a perfect sphere).

C is the friction parameter, correcting for the differences between macroscopic and microscopic viscosities:

C=1: Stick limit.

$C = (1 - f^{-2/3})$: Slip motion.

Motifs of Irrotationally Bound DMSO (Z_{ib}): One important metric for measuring the strength of interactions between solutes and solvents is the quantity of irrotationally bound solvent molecules (Z_{ib}). It reflects the strength of the interactions between the solute molecules and the solvent by showing the effective number of solvent molecules that are dynamically locked or frozen. According to Figure 7, better solute-solute interactions are indicated by a decreasing Kirkwood correlation factor (g) as the concentration of I3C increases. One way to describe the apparent concentration of DMSO molecules is as follows:

$C_{app} = g_2(c) C_{DMSO}$ (8)

Here: $g_2(0)$ is the correlation factor for pure DMSO, and C_{DMSO} is the analytical concentration of DMSO in the Using Cavell's equation and considering DMSO as a spherical molecule (A2=1/3), the apparent concentration of DMSO is given by:

$$C_{app} = \frac{g_2(c)}{g_2(0)} C_{DMSO} \quad (9)$$

The number of irrotationally bound DMSO molecules (Z_{ib}) can then be calculated as:

$$Z_{ib} = \frac{C_{app}}{C_{DMSO}} \quad (10)$$

The formula Z_{ib} takes into account the ratio of the Kirkwood correlation factors, which are a measure of the effective solute-solvent interactions, which are $(g2(c))/g2(0)$. For tiny solutes and constrained concentration ranges, Z_{ib} depicts the number of DMSO molecules frozen or irrotationally bound to I3C, assuming $g\ 2\ (c)/g\ 2\ (0\ ) \approx 1$. This method emphasizes the vital role of Z_{ib} as an indicator of the strength of the solute-solvent interaction and the structural dynamics of DMSO molecules when I3C is present.

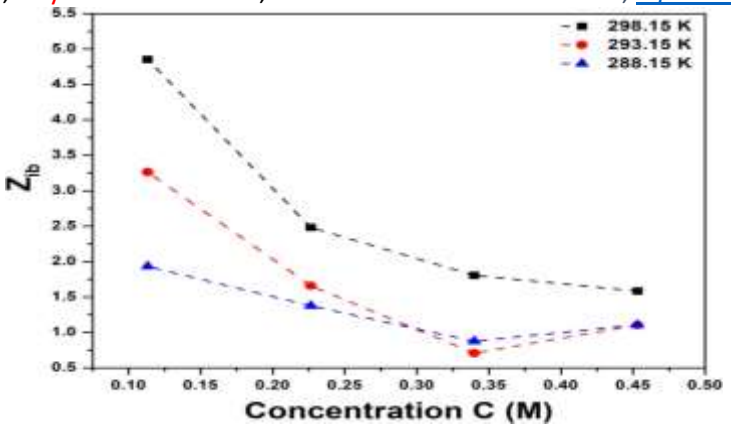

Fig. 7: Irrotationally bound DMSO molecules vs Concentration (M) of Indole 3-Carbinol-DMSO mixtures at different temperatures

Bound DMSO molecules that are twisted (Z_{ib}): The number of irrotationally bound DMSO molecules (Z_{ib}) at 298.15 K was 10.63 at low doses of Indole-3-Carbinol (I3C), according to Table 1. At 288.15 K, the number of Z_{ib} molecules increased slightly to 11.10. On the other hand, when the concentration of I3C was increased, the value of Z_{ib} dropped from 2.40 at 298.15 K to 2.38 at 288.15 K. At lower temperatures and higher I3C concentrations, there is less DMSO attached to each other, suggesting that I3C multimers are more likely to form. Due to the low number of solvent molecules that can associate with the solute, these multimers are the product of intense intermolecular interactions.

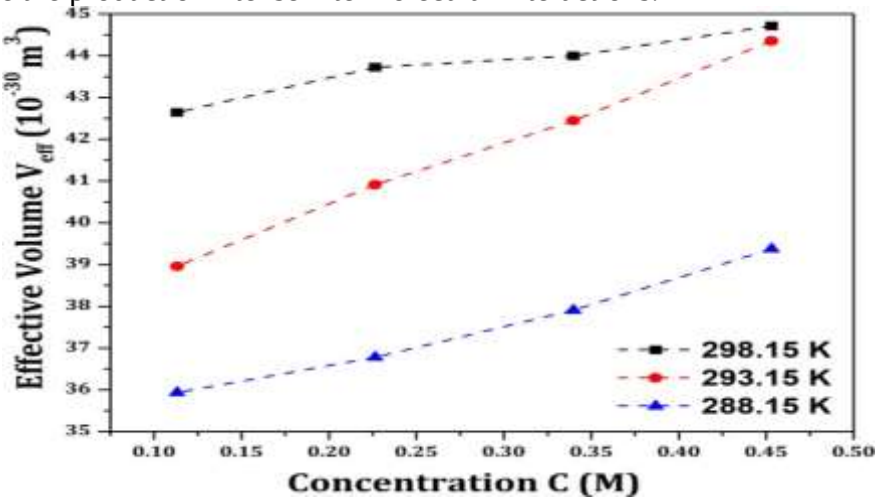

Fig. 8: Indole concentration in DMSO solutions at various temperatures and their effect on effective volume V_{eff}

4. Aspects of thermodynamics

Arrhenius plot: The Arrhenius plot, which displays the relationship between log (Tt_0) and 1000/T for all indole-3-carbinol concentrations, is shown in Figure 9. There is a near-linear relationship between the various temperatures.

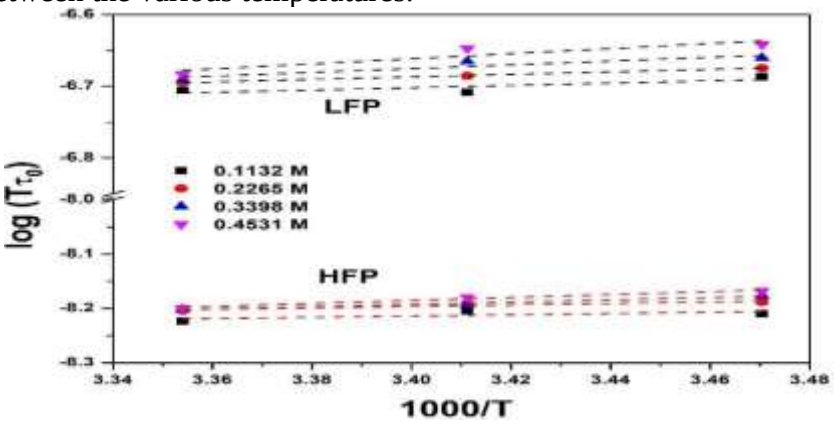

Fig. 9: Arrhenius plot of Log($T\tau_i$) vs reciprocal of temperature (K^{-1}) of Indole 3-Carbinol -DMSO mixtures at different concentration

Table. 3: Variations in concentration-dependent thermodynamic parameters

Molar Conc.(M)/ Temp. (K)	288.15		293.15		298.15	
	LFP	HFP	LFP	HFP	LFP	HFP
Free energy (ΔF)(Kcal/mol)						
0.1132	4.558	2.869	4.586	2.901	4.664	2.847
0.2265	4.963	2.913	4.647	2.915	4.693	2.877
0.3398	5.491	3.004	5.587	3.016	5.534	2.960
0.4531	5.293	2.987	5.420	3.001	5.572	3.009
Entropy (ΔS)(cal/mol.k)						
0.1132	-10.61	2.11	-10.52	1.96	-10.61	2.11
0.2265	27.20	3.58	27.82	3.51	27.21	3.57
0.3398	-4.40	4.39	-4.66	4.27	-4.41	4.39
0.4531	-27.87	-2.16	-27.82	-2.17	-27.87	-2.16
Enthalpy (ΔH)(kcal/mol)						
0.1132	1.50	3.47				
0.2265	12.80	3.94				
0.3398	4.21	4.27				
0.4531	-2.73	2.36				

Free energy of molecules: The activation molar free energy for dipole reorientation was calculated using Eyring's rate equation, with values ranging from 4.55 to 5.57 kcal/mol for the low-frequency relaxation process. While temperature had minimal influence on the DMSO-I3C system, the activation free energy was more dependent on I3C concentration. As I3C concentrations increased, so did the activation free energy, likely due to the formation of multimers or stronger solute-solute interactions. The small rise in free energy with increasing temperature may reflect enhanced thermal agitation, although this effect is counterbalanced by the weakening of hydrogen bonds in the mixture. This balance results in little to no significant change in free energy values as temperature rises. For I3C molecules associated with DMSO via weak hydrogen bonding or DMSO self-association, the activation free energy for dipole orientation was estimated at 2–3 kcal/mol for the high-frequency relaxation process.

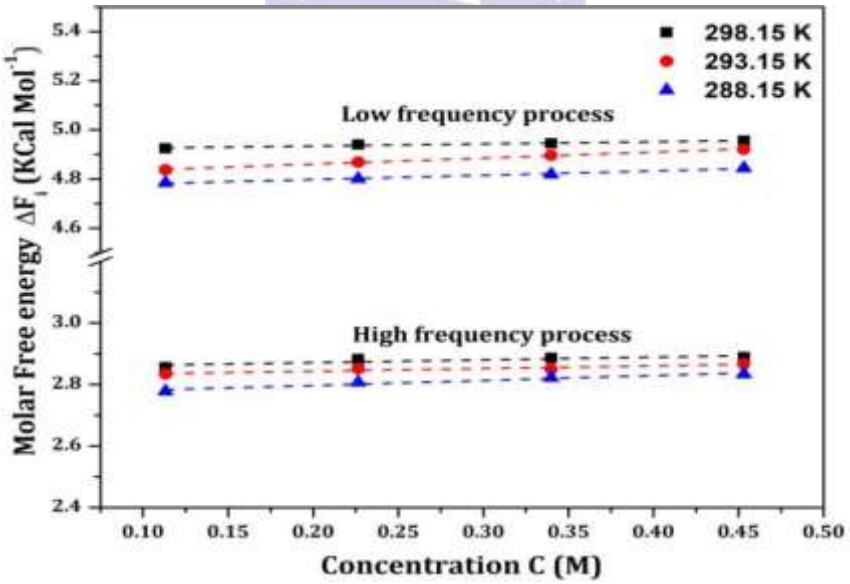

Fig. 10: Molar free energy as a function of temperature (K) of Indole 3-Carbinol- DMSO mixtures at different concentration.

Molar Entropy: If a system is chaotic, its entropy will be high. The system's stability is enhanced compared to a regular system if the local environment or surrounding entities cooperate with the active process. Negative entropy change characterizes the typical system. The activated system is in an unstable, more disordered state if the system's entropy is positive, which suggests a non-cooperative environment.

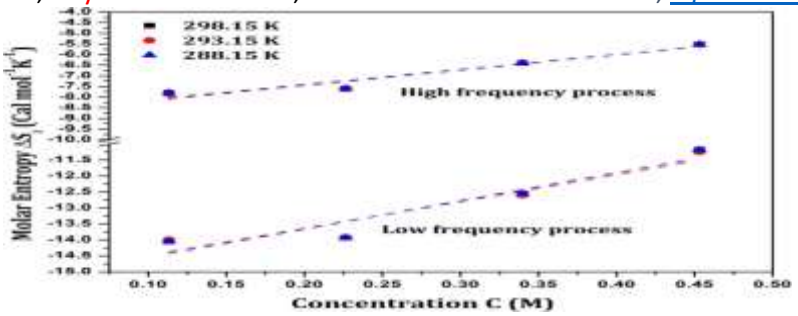

Fig. 12: Entropy($\Delta S\tau_i$) as a function of temperature (K) of Indole 3-Carbinol- DMSO mixtures at different concentration

5. Conclusion

I3C is responsible for the low-frequency relaxation process, whereas DMSO is responsible for the high-frequency relaxation process, both of which are observed in the analysed system. Various dielectric relaxation parameters might be derived from the complicated permittivity spectra by fitting them with the Cole-Cole model. The results show that the structural changes in the system are responsible for a drop in the dielectric constant for both the frequency process and the effective dipole moment, as revealed by the analyzed system. The relaxation period got longer as the concentration got higher in the high-frequency process, which could have been caused by a change in configuration or an increase in steric hindrance. Consequently, free energy likewise rose when concentration and temperature rose. The activation energy needed to break and establish hydrogen bonds is equal to the free energy discovered for low- and high-frequency processes. If the entropy value is very negative, it means the system is much more organized than in its typical state.

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