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Dielectric Relaxation and Thermodynamic Study of Caffeine-Chloroform Solution using TDR

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***Abstract:** The Complex permittivity of caffeine – Chloroform solution for different temperature and various concentrations have been measured in the range of 10MHZ to 30 GHz using Time Domain Reflectometry. From complex permittivity spectra, Static dielectric constant (ε_o) and relaxation time (τ) were determined using nonlinear least square fit method. Using Erying rate equation, for different molar concentration of caffeine Enthalpy of Activation ΔH and Entropy of Activation ΔS were determined.*
***Keywords:** Caffeine, Static dielectric constant, relaxation time, thermodynamic parameter.*

I. INTRODUCTION

Caffeine is natural stimulant, most commonly found in tea, coffee. It works as stimulating brain and nervous system [1]. In 1827 a scientist named Oudry discovered caffeine in tea [2]. Caffeine is colourless compound in silky needles. Caffeine is nitrogenous compound. It is used for nerve and heart stimulant as a medicine [3]. Caffeine is extracted using chloroform from tea. Extraction process depends upon plants and solvent selected [4]. The pure caffeine is extremely toxic and must be handled with mask and groves.

The present paper reports the static dielectric constant (ε_o), relaxation time (τ), Enthalpy and Entropy of activation for different molar concentration in the frequency range 10 MHz to 30GHz using Time Domain Reflectometry.

II. EXPERIMENTAL DETAILS

A. Material

Caffeine was purchased from OTTO chemie India. Using chloroform as a Solvent, different concentrations in molar fraction were prepared.

B. Experimental Setup and Procedure

The Tektronics model No. DSA8200 sampling oscilloscope with 30 GHz bandwidth with TDR module 80E08 with Step generator unit was used. The experimental setup is as shown in Fig. 1

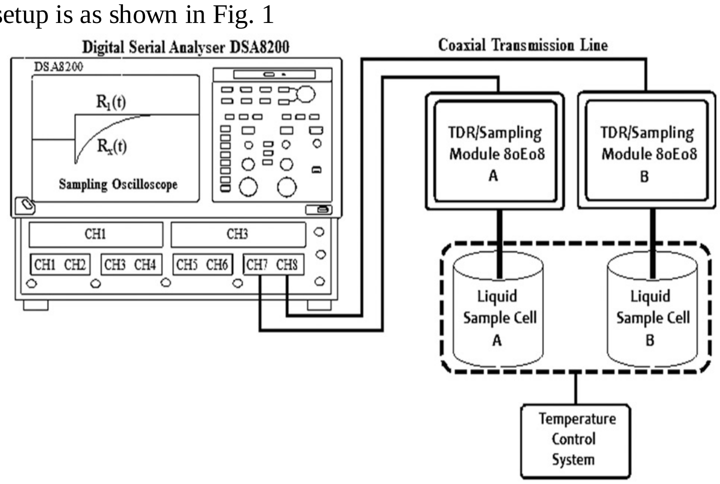

Fig. 2 Experimental setup of TDR

The complex permittivity spectra were studied using TDR method [5-7]. The complex permittivity of solution was observed in frequency range 10 MHz to 30 GHz at different temperature.

III. RESULT AND DISCUSSION

The time dependent data were processed to obtain complex reflection coefficient Spectra ρ*(ω) over the frequency range 10 MHz to 30 GHz using fourier transformation [8,9] as

$$\rho*(\omega) - \frac{c \quad p(\omega)}{j\omega d\, q(\omega)} \qquad \text{-- (1)}$$

The complex permittivity spectra ε*(ω) were obtained from ρ*(ω)by applying a bilinear Calibration method [10].

The Caffeine – Chloroform solution at all molar concentration could fit Debye type dispersion [11]. Experimental values of ε*(ω) were fitted to Debye equation.

$$\varepsilon*(\omega) = \varepsilon_{\infty} + \frac{\varepsilon_0 - \varepsilon_\infty}{(1+jw\tau)} \qquad \text{-- (2)}$$

A. Static Dielectric Constant (ε_o) and Relaxation Time (τ)

Using non linear least square fit method [12] with Debye equation 2, Static dielectric constant (ε_o) and relaxation time (τ) are obtained. These dielectric parameters for different temperatures and different concentration of caffeine are listed in table 1.

Table 1 (A) Dielectric relaxation parameters for solution of Caffeine – Chloroform at different concentration at temperature 25ºC

25^{0}C			
Concentration of Caffeine in Molar (M)	ε_0	τ(ps)	ε_∞
0	4.82(1)	6.87(4)	2.00(1)
0.1	4.97(1)	7.15(5)	2.00(1)
0.2	4.96(1)	7.9(5)	2.00(1)
0.3	4.92(1)	8.65(8)	2.00(1)
0.4	5.03(1)	8.94(9)	2.00(1)
0.5	5.07(2)	9.34(11)	2.00(1)

Table 1 (B) Dielectric relaxation parameters for solution of Caffeine – Chloroform at different concentration at temperature 20ºC

20^{0}C			
Concentration of Brucine in Molar (M)	ε_0	τ(ps)	ε_∞
0	4.98(6)	7.33(11)	2.22(7)
0.1	5.08(1)	7.56(5)	2.00(1)
0.2	5.08(8)	8.43(4)	2.00(1)
0.3	5.08(1)	8.23(6)	2.00(1)
0.4	5.21(1)	8.42(9)	2.00(1)
0.5	5.20(2)	9.91(12)	2.00(1)

Table 1 (C) Dielectric relaxation parameters for solution of Caffeine – Chloroform at different concentration at temperature 15ºC

15^{0}C			
Concentration of Brucine in Molar (M)	ε_0	τ(ps)	ε_∞
0	5.53(2)	5.83(6)	2.02(3)
0.1	5.52(1)	6.37(2)	2.00(1)
0.2	5.53(8)	6.95(3)	2.00(1)
0.3	5.55(1)	7.78(4)	2.00(1)
0.4	5.68(2)	8.39(15)	2.00(1)
0.5	5.42(2)	8.38(12)	1.88(1)

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Variation of static dielectric constant (ε_o) with molar concentration of caffeine – chloroform at various temperature is as shown in fig.2

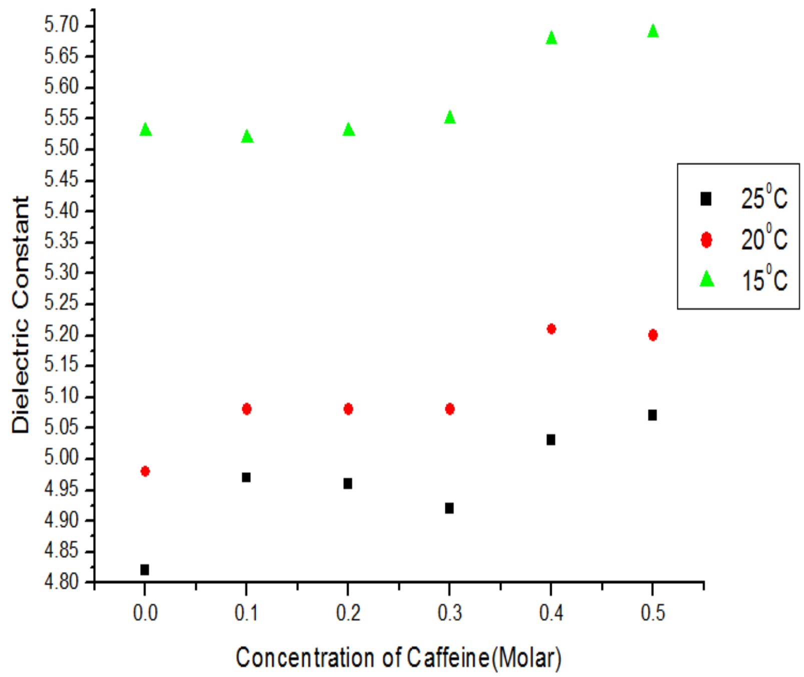

Fig. 2 Variation of static dielectric constant with molar concentration of Caffeine - Chloroform at various temperatures

Variation of relaxation time with temperature at different concentration is shown in fig.3

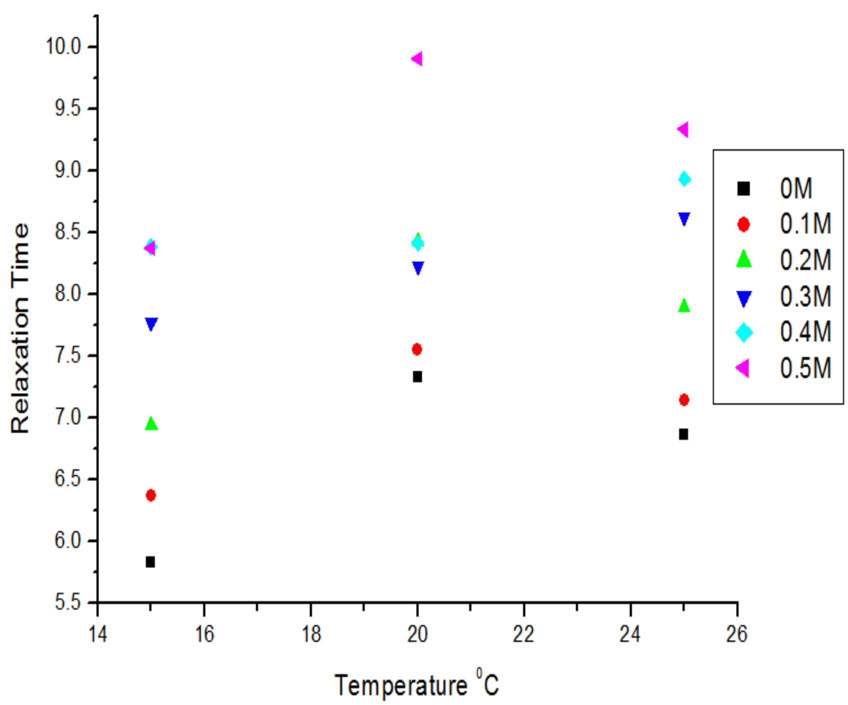

Fig. 3 Variation of relaxation time with molar concentration of Caffeine - Chloroform at various temperatures

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B. Determination of Thermodynamic Parameters

Using Erying equation, the energy of activation of relaxation process can be determined from relaxation time (τ), the Enthalpy of activation (ΔH) and Entropy of activation (ΔS) are calculated from Erying rate equation[13,14].

$$\tau = \frac{h}{kT} \exp \frac{\Delta H - T\Delta S}{RT} \quad \text{-- (3)}$$

The Arrehenius plot of log (τT) versus 1000/T is as shown in fig.4

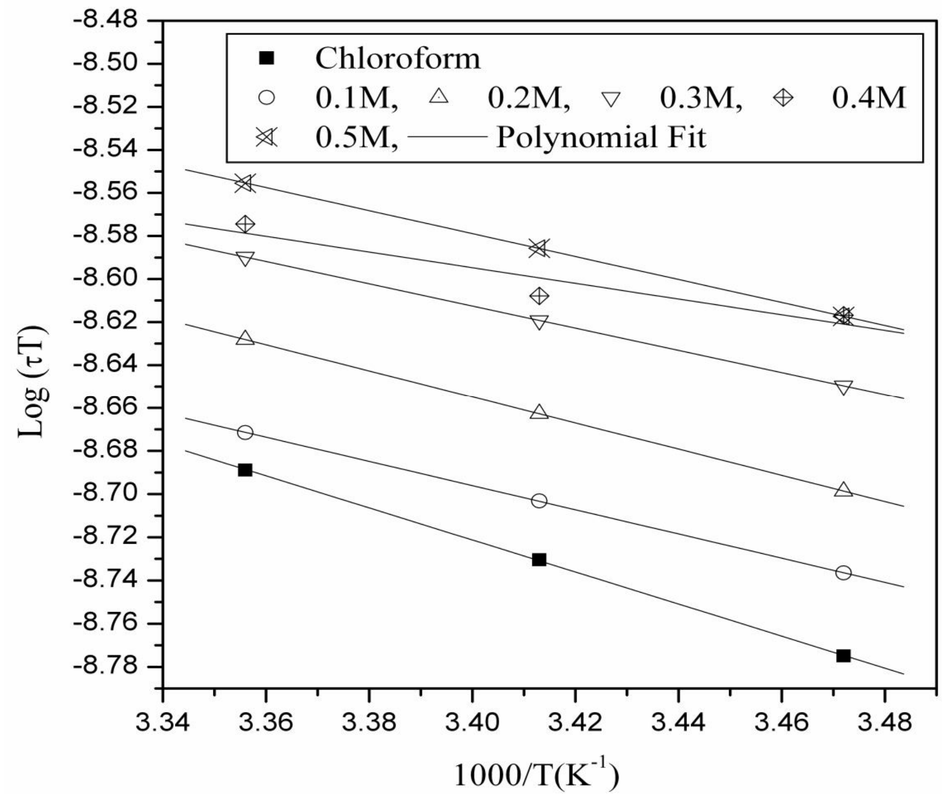

Fig. 4 The Arrehenius plot of log(τT) versus 1000/T for Caffeine – Chloroform solution

The values of Enthalpy of activation (ΔH) and Entropy of activation (ΔS) are obtained from Erying equation. These values are reported in table 2

Table 2 – Enthalpy and Entropy of activation for Caffeine - Chloroform solution

Concentration of Caffeine (M)	Enthalpy of Activation ΔH (KJ $mole^{-1}$)	Entropy of Activation ΔS (J $mole^{-1}$ J^{-1})
0M	-14.26(11)	0.150(4)
0.1 M	-10.76(9)	0.161(3)
0.2 M	-11.68(10)	0.157(3)
0.3 M	-9.86(1)	0.163(3)
0.4 M	-6.94(2)	0.173(8)
0.5 M	-10.26(9)	0.161(3)

IV. CONCLUSION

Static dielectric constant (ε_o increases with increase concentration of Caffeine, It also increases with decreases in temperature. Relaxation time (τ) increases with increase in concentration of Caffeine. Enthalpy of activation (ΔH) is negative i.e. heat energy is released. Such reactions are called Exothermic reaction [15].

V. ACKNOWLEDGEMENT

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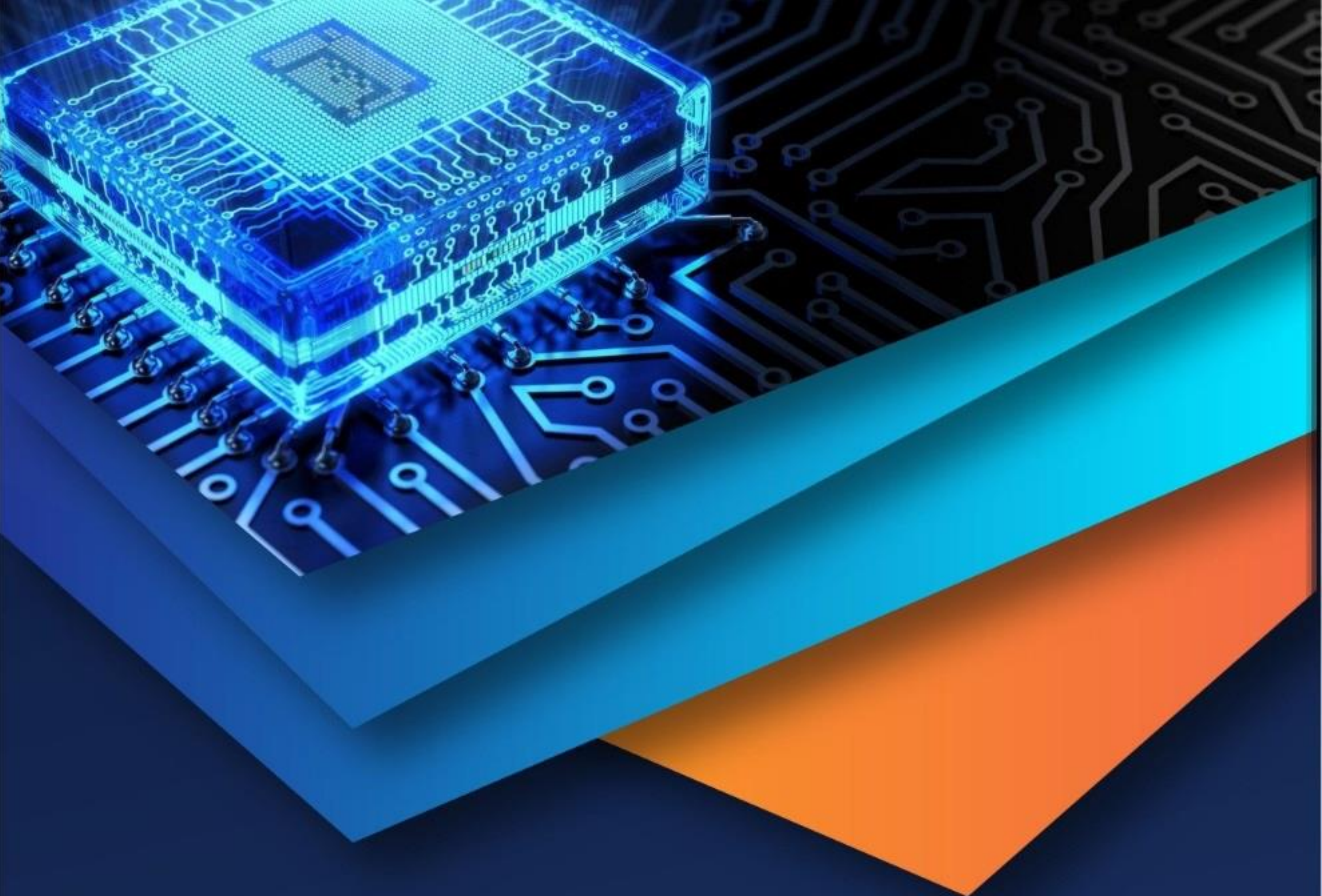

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