Thermodynamic behaviour and Dielectric Relaxation Study of 2-3 Dimethoxy Strychnine – Chloroform solution using Time Domain Reflectometry (TDR)

[1]**A. R. Lathi** [2]**S M. Yenorkar**

1 Associate Professor, A.E.S. College, Hingoli,- 341531 Maharashtra, India,
2 Associate Professor, Shri Shivaji College, Parbhani, - 431401 Maharashtra, India.

Abstract: The Complex permittivity of 2-3 Dimethoxy Strychnine – Chloroform solutions for various concentrations and for different temperatures have been measured in the range of frequency 10MHz to 30GHz using Time Domain Reflectometry Technique (TDR). Static dielectric constant (ε_0) and relaxation time (τ) were obtained from complex permittivity spectra using nonlinear least square fit method. Thermodynamic Parameters Enthalpy of activation Δ H and Entropy ΔS was determined from Erying rate equation for different molar concentration of 2-3 Dimethoxy Strychnine in Chloroform.

Keywords: **2-3 Dimethoxy Strychnine Dielectric constant , Relaxation Time , Enthalpy , Entropy.**

1. INTRODUCTION

2-3 Dimethoxy Strychnine is a natural Alkaloid. It comes under Indole II Group [1] . Brucine is used in pesticides [2, 3]. It also used as antitumor in Cancer treatment [4]. It founds in bark and seeds of Strychnine tree [5]. It also used in Chinese Medicine as analgesic agent [6]. It is soluble in chloroform and alcohol but less solubility in water.

I present Thermodynamic behaviour and Dielectric relaxation study of 2-3 Dimethoxy Strychnine – Chloroform solution for different molar concentration and different temperature between frequency range 10 MHz to 30 GHz using Time Domain Reflectometry Technique (TDR). Dielectric relaxation study is related to Molecular interaction in liquid. The Dielectric relaxation behaviour of this solution is explained by Cole-Davidson Model [7].

2. EXPERIMENTAL METHOD

2.1 Material and sample preparations:

2-3 Dimethoxy Strychnine (Brucine) was purchased from OTTO chemie India, and used without further purification. Molecular mass 2-3 Dimethoxy Strychnine is 394 gm/mole. Its Molecular formula is $C_{23}H_{26}N_2O_4$. Considering Molecular mass and its solubility in chloroform, the solutions of different molar concentration were prepared. Chloroform is nonpolar solvent.

2.2 Experimental Setup:

The setup consists of sampling oscilloscope Tektronics DSA 8200. Bandwidth of this oscilloscope is 50 GHz . TDR module 80E08 with step generator and co-axial cable was used. To keep temperature constant, a temperature control system was used. The Experimental set up TDR]8,9] is as shown in Fig.

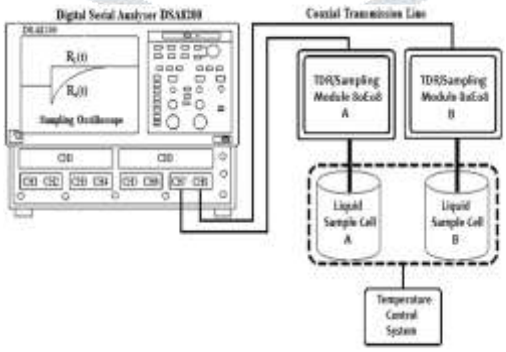

Fig.1 Experimental setup of TDR

The Complex permittivity spectra were studied using TDR method [10-12] for various concentrations solutions and different temperature in frequency range 10MHz to 30 GHz.

3. RESULT AND DISCUSSION

Reflected pulse without sample $R_1(t)$ and with sample $R_x(t)$ were recorded by oscilloscope for various concentration and temperature in the window 5ns and digitized in 2000 points. The difference and sum of reflected pulse $p(t) = [R_1(t)-R_x(t)]$ and $q(t) = [R_1(t)+R_x(t)]$ respectively . The Fourier transform of $p(t)$ and q(t) was obtained by a summation method and Samulon method [13,14]

$$p(\omega) = T \sum_{n=0}^{N} \exp(-i\omega nT)p(nT) \qquad \text{-- (1)}$$

$$q(\omega) = \frac{T}{1-\exp(-j\omega T)} \left[\sum_{n=0}^{n}(q(nT) - q(n-1)T)\exp(-j\omega nT)\right] \qquad \text{-- (2)}$$

The complex reflection coefficient $\rho^*(\omega)$ over a frequency range 10MHz to 30GHz were determined as per the equation (3)

$$\rho * (\omega) = \frac{c}{j\omega d}\frac{p(\omega)}{q(\omega)} \qquad \text{-- (3)}$$

The Complex permittivity spectra $\varepsilon^*(\omega) = \varepsilon' - j\,\varepsilon''$ was obtained from reflection coefficient spectra $\rho^*(\omega)$, by applying the bilinear calibration method suggested by Cole [15].

Frequency dependance dielectric permittivity (ε') and dielectric loss (ε'') for various Brucine chloroform solution at 25° C is shown in Fig. 2.

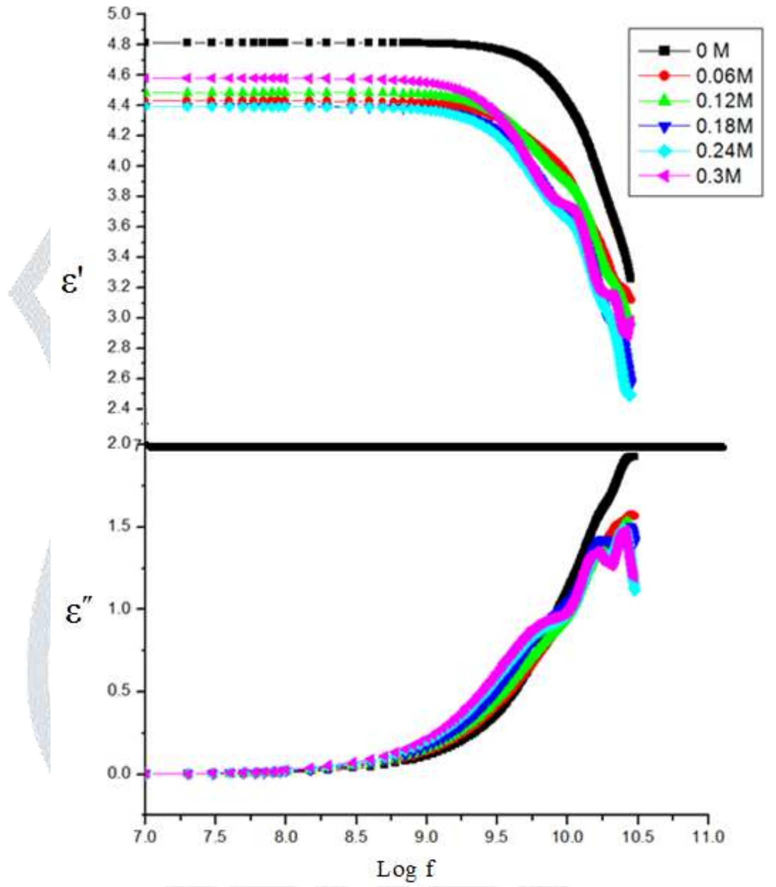

Fig.2 Complex permittivity spectra for Brucine-Chloroform solution for various concentrations at 25^{0}c

3.1 Static Dielectric constant and Relaxation time:

To determine static dielectric constant (ε_0), relaxation time (τ) and distrubution parameters (α, β). The complex permitivity $\varepsilon^*(\omega)$ data were fitted by the non linear least square method to the Harviliak – Negami expression [16].

$$\varepsilon * (\omega) = \varepsilon_\infty + \frac{\varepsilon o - \varepsilon \infty}{[1+(j\omega t)1-\alpha]\beta} \qquad \text{--- (4)}$$

The Brucine – chloroforma solutions for all concentration could fit Debye type dispersion i.e. $\alpha = 0$ & $\beta=1$ [17]. Experimental Values $\varepsilon^*(\omega)$ were fitted to Debys equation

$$\varepsilon^*(\omega) = \varepsilon_\infty + \frac{(\varepsilon_0 - \varepsilon_\infty)}{(1+jw\tau)} \quad \text{--- (5)}$$

The Static dielectric constant (ε_0) and relaxation time (τ) for different temperatures and concertrations are listed in Table -1

Table1. Dielectric relaxation parameters for solution of Brucine – chloroform at different concentration at temperature 25ºC, 20 ºC, 15ºC

25^0C			
Concentration of Brucine in Molar (M)	ε_∞	ε_0	τ(ps)
0	2 (1)	4.82 (1)	6.87 (4)
0.06	2.30 (3)	4.41 (3)	9.12 (7)
0.12	2.04 (5)	4.43 (4)	10.08 (9)
0.18	2.03 (3)	4.36(3)	11.04 (7)
0.24	2.04 (7)	4.34 (8)	12.28 (15)
0.3	2.62 (1)	4.31 (3)	13.52 (29)

20^0C			
Concentration of Brucine in Molar (M)	ε_∞	ε_0	τ(ps)
0	2.22 (7)	4.98 (6)	7.33 (11)
0.06	2.36 (3)	4.64 (3)	8.97 (6)
0.12	2.18 (4)	4.72 (4)	9.83 (8)
0.18	2.09 (5)	4.56(5)	10.51 (9)
0.24	2.19 (3)	4.61 (3)	11.16 (17)
0.3	2.22 (6)	4.65 (7)	12.7 (13)

15^0C			
Concentration of Brucine in Molar (M)	ε_∞	ε_0	τ(ps)
0	2.02 (3)	5.53 (2)	5.83 (16)
0.06	2.12 (1)	5.23 (1)	7.5 (1)
0.12	2.14 (4)	5.23 (4)	8.06 (6)
0.18	2.18 (6)	5.1 (6)	9.2 (10)
0.24	2.05 (7)	5.18 (6)	10.57 (10)
0.3	2.42 (7)	5.11 (8)	11.95 (13)

Variation of Static Dielectric constant with concentration at various temprature is shown in Fig. 3. and varation relaxation time with conscentration of brucine at various temprature is shown in Fig. 4

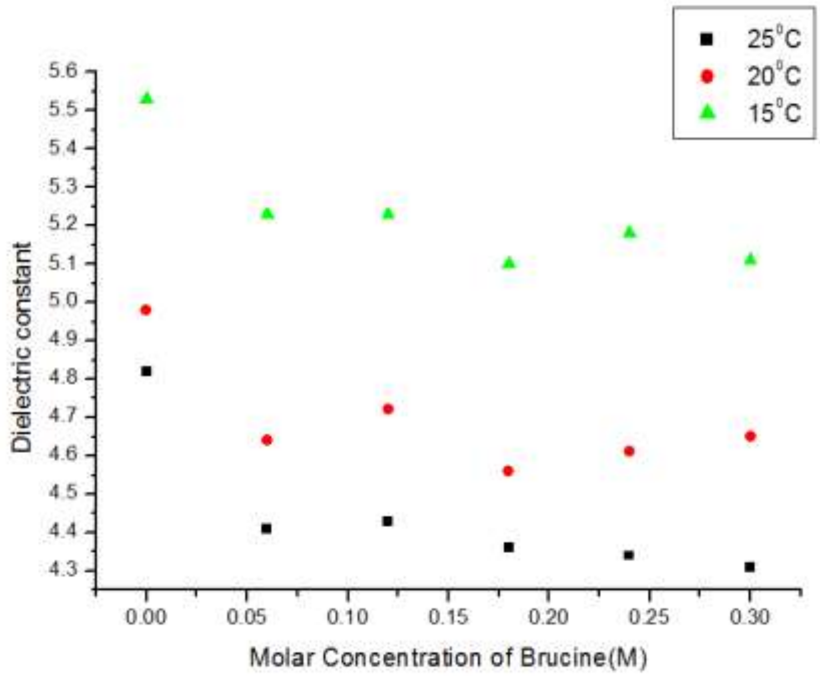

Fig.3 Variation of static dielectric constant with molar concentration of Brucine in Chloroform at various temperatures

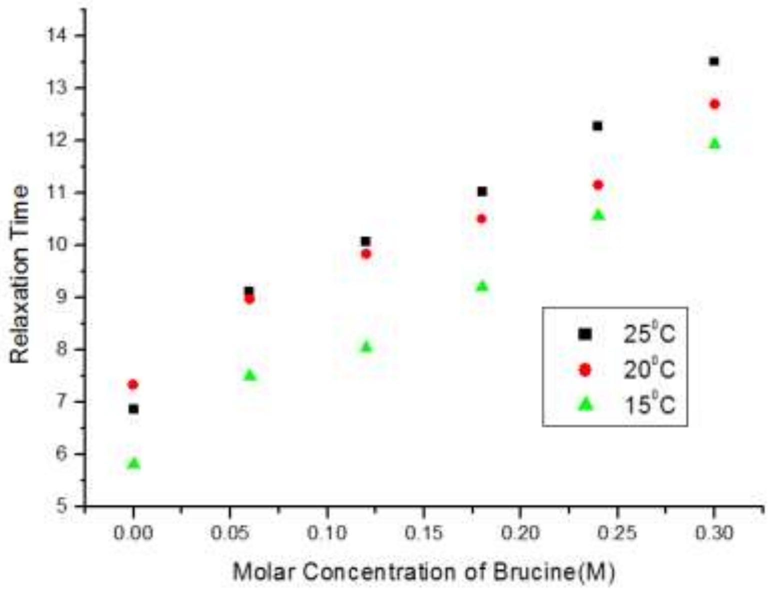

Fig.4 Variation of relaxation time with molar concentration of Brucine in Chloroform at various temperatures

3.2 Thermodynamic Parameter :

The energy of activition of dielectric relaxation process can be calculated from relaxation time using Erying equation[18]. The Enthalpy of activation Δ H and entropy of activation ΔS are determined from Erying rate equation.

$$\tau = \frac{h}{kT} \exp \frac{\Delta H - T\Delta S}{RT} \qquad \text{--- (6)}$$

Where h Is Planck's constant , K is Boltzmann's constant , T absolute temprature , τ is relaxation time and R is gas constant. The relaxation time depends on temprature which is described by Arrehenius plot log (τ T) versus 1000/T is shown in Fig.5

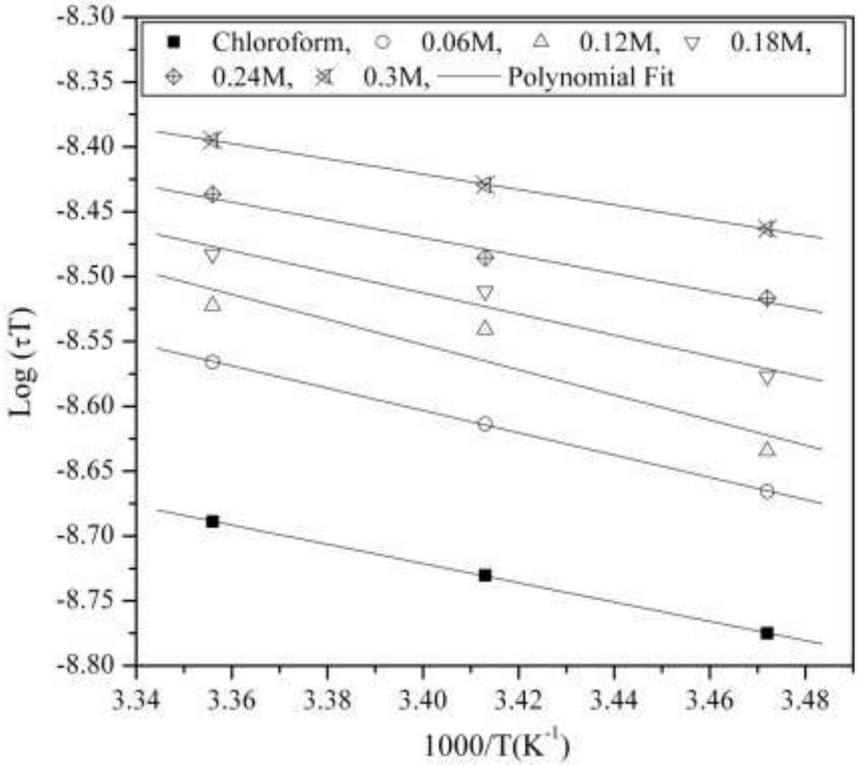

Fig.5 The Arrehenius plot of log (τT) versus 1000/T for Brucine-Chloroform solution

The values of Enthalpy of activation Δ H and entropy of activation ΔS are determined. These values are reported in Table-2.

Table2. Enthalpy and Entropy of activation for Brucine – chloroform solution

Concentration of Brucine(M)	Enthalpy of Activation ΔH (KJ $mole^{-1}$)	Entropy of Activation ΔS (J $mole^{-1}$ J^{-1})
0 M	-14.26 (11)	0.150 (4)
0.06 M	-16.45 (6)	0.140 (2)
0.12 M	-18.46 (6)	0.133 (2)
0.18 M	-15.47 (3)	0.142 (1)
0.24 M	-13.11 (1)	0.149 (6)

When an amount of Brucine is added to chloroform, enthalpy of activation Δ H, increases (Negative Values) to maximum for 0.12 M solution. Negative sign indicates exothermic reaction i.e. in such reaction heat energy is released[19], where entropy ΔS is minimum for 0.12M.

4. CONCLUSION

It is observed that Static dielectric constant (ε_0) decreasess with increasing concentration and temprature. Relaxation time (τ) increases with increasing concentrations of Brucine, it also increases with temperature. Static Dielectric Constant (ε_0) and relaxation time (τ) are temprature dependant. Enthalpy of activation Δ H is negative which indicates exothermic reaction i.e. in such reaction heat energy is released.

5. ACKNOWLEDGEMENT

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