

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor, Monthly, Peer Reviewed Journal)

Visit: www.ijirset.com

Vol. 6, Issue 12, December 2017

Molecular & Structural Interaction Study of Chlorobenzene-Xylene Binary Mixture Using X-Band Dielectric Technique

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ABSTRACT: The study of molecular interaction in binary mixtures of Chlorobenzene (CB) with Xylene has been carried out at room temperatures for 11 concentrations using X-band microwave technique. The molecular interaction of solute-solvent mixture in the microwave frequency 8.845 GHz gives information about the interaction between the molecules of the given binary mixtures. The structural parameters such as dielectric constant, dielectric loss, relaxation time penetration depth, loss tangent and conductivity have been obtained to know the intermolecular interactions between the solute solvent.

KEYWORDS: Dielectric constant, dielectric loss, loss tangent, Microwave Conductivity, Penetration depth & X-band microwave technique.

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I. INTRODUCTION

In past few years frequency domain and time domain spectroscopy has achieved best results in the experimental as well as theoretical properties of binary liquid mixtures. This technique plays an important role in understanding the molecular effects and intermolecular interactions in binary liquids [1-3]. The molecular interaction of liquids mixture gives information about structural properties. In this work, we report the structural properties at room temperature and concentrations of Chlorobenzene with Xylene binary mixture.

Dielectric relaxation study of Chlorobenzene with Xylene provides important information regarding molecular interactions because of dipole-dipole interactions and bonding between the two different molecules [4-5]. The Chlorobenzene (CB) is a non-associative liquid. Chlorobenzene is chlorine group molecule & Xylene is mixed isomer of P, M & O-Xylene. Xylene (mixed isomer of dimethylbenzene) is an aromatic hydrocarbon, colorless, flammable liquid. It is used as a solvent, it has applications in medical field, in printing, rubber and lather industries [6].

In the present work, we report a dielectric relaxation study of CB with non polar solute (Xylene) at various concentrations at room temperatures employing X-Band microwave technique in the frequency range of 8.845 GHz. It is interesting to see the effect of chlorine group molecule in the Xylene system. The dielectric constant, dielectric loss, Loss tangent, penetration depth and microwave conductivity has been obtained.

II. EXPERIMENTAL DETAILS

2.1 Materials

Chlorobenzene, (LR grade, s d fiNE-CHEM LIMITED, Bombay) and Xylene, (AR grade Himedia Laboratories Pvt. Ltd. Mumbai) were used without further purification. The solutions were prepared at 11 different volume fractions of CB from 0% to 100% in Xylene binary mixtures.

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2.2 Measurements

The dielectric constant, dielectric loss and other parameters were studied using an X-band microwave technique [1]. The X-band microwave technique consists of a microwave bench with klystron power supply, liquid dielectric cell (X-910) with plunger and digital multi-meters for power output measurement. The CRO is used to calibrate the input and output power.

3. Data Analysis

The experimental values for forward and reflected output that is I_f and I_r are used to calculate ϵ' and ϵ'' by putting these values in the following equations [1],

$$VSWR = \frac{I_f + I_r + 2\sqrt{I_f I_r}}{I_f - I_r} \quad (1)$$

The complex relative permittivity of the material is expressed as [5,7-9],

$$\epsilon = \epsilon' - j\epsilon'' \quad (2)$$

where,

ϵ' - is the dielectric constant and

ϵ'' - is the dielectric loss.

To eliminate the losses, a graph is plotted between several mean values of ρ_n versus n . The slope of this graph gives the

value [7-8] of $\frac{d\rho_{mean}}{dn}$.

The dielectric constant, dielectric loss and the relaxation time are given by the following equations [1]

$$\text{Dielectric Constant} = \epsilon' = \left(\frac{\lambda_0}{\lambda_c}\right)^2 + \left(\frac{\lambda_0}{\lambda_d}\right)^2 \quad (3)$$

$$\text{Dielectric Loss} = \epsilon'' = \frac{2}{\pi} \left(\frac{\lambda_0}{\lambda_d}\right)^2 \left(\frac{\lambda_g}{\lambda_d}\right) \left(\frac{d\rho_{mean}}{dn}\right) \quad (4)$$

The loss tangent, Conductivity and Penetration depth can be calculated using the following equations [1,7-9]

$$\text{Tan } \delta = \frac{\epsilon''}{\epsilon'} \quad (5)$$

$$P_d = \frac{\lambda \sqrt{\epsilon'_r}}{2\pi \epsilon'_r} \quad (6)$$

where, λ_0 is the free space wavelength, λ_d is the wavelength in the dielectric cell, λ_g wavelength of waveguide and λ_c is the cut-off wavelength which is equal to $2a$, n_D is the refractive index of the liquid material and $\omega = 2\pi f$.

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Figure 1. X-Band Microwave Technique Experimental Setup with Liquid Dielectric Cell.

Table 1. Dielectric parameters for CB-Xylene binary solutions at room temperatures.

Volume fraction of CBZ	ϵ'	ϵ''	Tan δ	P_d
0.0	2.6427	0.1853	0.3877	0.3871
0.1	3.2497	1.2602	0.2552	0.3784
0.2	3.4015	0.8680	0.2248	0.3784
0.3	3.4015	0.7648	0.1570	0.3606
0.4	3.7451	0.5883	0.0723	0.3606
0.5	3.7451	0.2709	0.0112	0.3516
0.6	3.9401	0.0443	0.0401	0.3424
0.7	4.1530	0.1666	0.0547	0.3239
0.8	4.6425	0.2542	0.1268	0.3145
0.9	4.9247	0.6247	0.2170	0.3145
1.0	4.9247	1.0691	0.3877	0.3871

4.1 Dielectric Constant and Loss

The values of dielectric parameters such as dielectric constant (ϵ'), dielectric loss(ϵ'') obtained by putting the experimental data into the equations (1), (2), (3), (4) & (5). The change in dielectric constant of the mixtures indicates the heterogeneous interaction [3-4] in CB-Xylene mixtures. As the volume fraction of CB increases in Xylene, the dielectric constant of the mixture goes on increasing which shows the more parallel alignment of dipoles [5] in mixture, shown in Table 1. The larger values of dielectric constant of Chlorobenzene are due to presence of Cl group and its

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molecular size. The values of dielectric constant increases with increasing CB in Xylene. The dielectric constant values for CB are greater than Xylene. This means molecular size of CB is greater than the Xylene system.

4.2 Penetration depth and Loss tangent

The values of loss tangent and penetration depth are given in table 1. As shown in table, the tangent loss is minimum for 0.5 volume fraction of CB and it is maximum for pure liquids. Also in penetration depth, the value goes on decreasing as the volume fraction of CB increases in Xylene.

V. CONCLUSION

Study of molecular interaction of CB in Xylene has been studied using X-Band microwave technique in the frequency range of 8.845GHz. As the volume concentration of CB increases in Xylene, static dielectric constant. Values of theoretical dielectric constant are in good agreement with the experimental values.

Acknowledgements

The Department of Chemistry, Department Zoology for providing chemicals & Department of Physics and Electronics, Maharashtra Udayagiri Mahavidyalaya, Udgir for providing all the research facilities are gratefully acknowledged.

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