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Dielectric Relaxation Studies of Paracetamol Using X-Band Microwave Bench at Different Temperature

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Abstract: The dielectric parameters of paracetamol for four different temperature (30°C, 40°C, 50°C and 60°C) at a microwave frequency 9.265 GHz have been observed in the dilute solutions of carbon tetrachloride with the help of X-band microwave bench. The dielectric parameters like dielectric constant (ε), dielectric loss (ε "), static permittivity (ε 0) and optical permittivity (ε 0) are calculated for five different weight fractions of paracetamol in the dilute solutions of carbon tetrachloride. The values of ε 0 and ε 0 are calculated by using Dipole meter and Abbe's refractometer. The analysis shows that the values of dielectric parameters increase with the increase in the weight fraction of paracetamol whereas these values decrease as the temperature increases. This study suggests that there are both intermolecular and intramolecular orientation exist in the solutions.

Key Words: dielectric constant, dielectric loss.

1. INTRODUCTION

Paracetamol is one of the most popular and most commonly used [1] analgesic and antipyretic drugs around the world and is manufactured in huge quantities [2]. It is also known as acetaminophen. It is a first line treatment which can be used without any prescription. Many diseases like headache, muscle aches, arthritis, backache, toothaches, colds, fevers etc are treated by it. Its chemical formula is CH₃CONHC₆H₄OH. Its molecular weight is 151.17[g/mol]. [3] It is available in the form of white crystalline powder. It is soluble in water. Its IUPAC name is N-(4-hydroxyphenyl) and represented by the symbol:

Figure: 1 Symbol of Paracetamole

The study of dielectric parameters gives important information about structural behavior of polar molecules. It is also useful in finding intermolecular and intramolecular interaction between the molecules. The dielectric parameters which are related with inter molecular association and internal rotations also help to find the structural behavior of the molecules. Madhulika and Gandhi [4] have investigated the dielectric relaxation

behaviour of n-butyl acrylate, allyl-methacrylate, isobutyl-methacrylate and isobutyl-acrylate in non-polar solvent for various temperatures. The relaxation studies of polar liquids and their binary mixtures in dilute solution of non polar solvent gives significant information about solute-solute and solute-solvent interaction. The dielectric studies of binary mixtures of polar molecules are useful to know the intermolecular interactions in the mixture arising due to the dipole-dipole interaction, hydrogen bonding etc.[5] Dielectric characterization is really very useful to analysis the phenomenon like, H-bond interactions, dipolar alignment, hydrogen bond connectivity etc.

Gedam and Suryavanshi [6] concluded that the dielectric studies deals with weak forces between the molecules which is useful to know the intermolecular reorientation dynamics of the solute. For the polar liquids in dilute solution of benzene, ε' and ε " increase with the concentration of polar substance.. Sahoo [7] observed that the simple Debye model of polar and non polar liquids can satisfactorily explain the dielectric behavior of amides and acetone under static and high frequency electric fields. Jain and Bhargava [8] studied the dielectric relaxation behavior of the binary mixture of nicotinamide and 1-butanol at four different temperatures viz. 303K, 313K, 323K and 333K in dilute solutions of benzene at a constant frequency of 9.385 GHz. The values of different dielectric parameters were calculated by using standard methods. This study suggests the existence of both the intermolecular and overall molecular rotation in the binary mixture.

2. EXPERIMENTAL

Paracetamol used in this study is purchased AR grade from Central Drug house, Delhi, India. Carbon tetrachloride is also purchased from General scientific compony, Jaipur, India. CCl_4 is used as a solvent in this investigation. The samples are made by dissolving different mole fraction of paracetamol (0.01, 0.015, 0.02, 0.025, 0.03) in the dilute solution of 1 mole of carbon tetrachloride. The values of dielectric constant and dielectric loss were determined at constant microwave frequency 9.265 GHz by using X-band microwave bench. The double minima method for low loss liquid given by Heston et. al.[9] is used to determine ε and ε ". According to this method the values of ε and ε " are given as follows:

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$$\varepsilon = \left(\frac{\lambda_o}{\lambda_c}\right)^2 + \left(\frac{\lambda_o}{\lambda_d}\right)^2 \tag{1}$$

$$\varepsilon'' = \left(\frac{\lambda_g}{\lambda_d}\right) \left(\frac{\lambda_o}{\lambda_d}\right)^2 \left(\frac{d\rho}{dn}\right) \tag{2}$$

where

$$\rho = \frac{\sin\theta}{(2 - \cos^2\theta)^{1/2}} \tag{3}$$

and

$$\theta = \frac{\pi \Delta x}{\lambda_q} \tag{4}$$

where λ_o , λ_g , λ_c and λ_d are the free space wavelength, the guided wavelength, the cutoff wavelength and the wavelength in the dielectric medium respectively. Parameter ρ is the inverse voltage standing wave ratio (VSWR), n is the number of minima and dp/dn is the slope of the curve drawn between ρ and n. The precision of measurement of wavelength with the available X-band microwave test bench is ± 0.001 cm. Corresponding to this value of accuracy, the estimated error by using the conventional method of error analysis in the measurement of ε and ε " are about $\pm 1\%$ and $\pm 5\%$ respectively. The refractive indices of the solutions are measured by using Abbe's refractometer which gives the value of optical permittivity. The static permittivity of the solutions are calculated by using a Dipole meter supplied by M/s Mittal Entreprises, New Delhi.[10]

For the dilute solutions in non polar solvents ε , ε ", ε ₀, and ε _{\infty} can be expressed [11-12] as a linear functions of concentrations in the following manner:

$$\varepsilon' = \varepsilon_1' + a'W_2 \tag{5}$$

$$\varepsilon'' = a'' W,$$
 (6)

$$\varepsilon_0 = \varepsilon_{10} + a_0 W_2 \tag{7}$$

$$\varepsilon_{\infty} = \varepsilon_{I_{\infty}} + a_{\infty} W_{2}$$
 (8)

Here subscript 1 refers to the pure solvent, 2 to the solute, while 0 refers to the static or low frequency case and ∞ refers to the infinite or optical frequency case, W_2 is taken as the weight fraction of the solute. a', a", a_0 and a_∞ are the slopes of above mentioned linear equations.

3. RESULTAND DISCUSSION

In the present paper X-band microwave bench have been used to calculate ε ' and ε " for different mole fractions of paracetamol using carbon tetrachloride as a solvent at four different temperatures. The value of ε_0 is determined by using dipole meter whereas the value of ε_∞ is determined by using Abbe's refractometer at different temperature for the same samples as mentioned above. Different values of dielectric parameters with weight fraction and temperature is listed out in the given

table. From the table it is clear that ε' , ε'' , ε_0 and ε_∞ increases linearly with the increase in the weight fraction. This behavior suggests that there is no change in the nature [13] of the rotating molecules entities in the CCl₄ solutions. This may possibly be due to increase in the molar volume [14] and also may be due to the dipole-dipole interaction of pure liquid. [15]

This table also shows that the values of all the dielectric parameters decrease as the temperature increases. It indicates the existence of inter molecular and intra molecular association in the solution. To minimize the solute-solute interaction the concentrations of the solution were made sufficiently dilute [6]. By using the values of ε_0 and ε_∞ we can further calculate different relaxation times and free activation energy of molecules. Thus the relaxation studies can provide useful information about the nature of molecular orientation process [16]

Table 1. Values of different dielectric parameters (ε ', ε ", ε_0 and ε_∞) for different mole fraction of paracetamol at four different temperature

Weight Fraction	Temp. 303 K.			
	€'	€"	\mathcal{E}_0	\mathcal{E}_{∞}
0.009198	2.28	0.1975	2.29	2.096
0.013734	2.31	0.2013	2.31	2.098
0.018234	2.33	0.2101	2.34	2.099
0.022688	2.34	0.2243	2.38	2.101
0.027102	2.36	0.2281	2.41	2.102
	Temp. 313 K.			
	ε'	€"	\mathcal{E}_0	\mathcal{E}_{∞}
0.009198	2.187	0.1813	2.26	2.088
0.013734	2.199	0.1831	2.3	2.089
0.018234	2.229	0.1907	2.38	2.091
0.022688	2.269	0.1938	2.32	2.092
0.027102	2.313	0.2007	2.34	2.094
	Temp. 323 K.			
	arepsilon'	arepsilon''	\mathcal{E}_0	\mathcal{E}_{∞}
0.009198	2.181	0.1642	2.2543	2.0808
0.013734	2.194	0.1807	2.3028	2.0822
0.018234	2.205	0.1809	2.3056	2.0836
0.022688	2.249	0.1922	2.3106	2.0851
0.027102	2.295	0.1821	2.3356	2.0865
	Temp. 333 K.			
	€'	arepsilon"	\mathcal{E}_0	\mathcal{E}_{∞}
0.009198	2.133	0.1563	2.2501	2.0635
0.013734	2.134	0.1675	2.2932	2.2932
0.018234	2.144	0.1677	2.2981	2.2981
0.022688	2.172	0.1789	2.3024	2.3024
0.027102	2.209	0.1891	2.3187	2.3187

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4. CONCLUSION

In this paper different dielectric parameters (ε ', ε ", ε_0 and ε^∞) are determined for different weight fractions of paracetamol in the dilute solutions of carbon tetrachloride. The values of dielectic loss and dielectric constant are measured by using X-bench whereas the static and optical permitivitty was calculated using standard methods. From the present study it is concluded that these values of dielectric parameters provide information about the structural behaviour as well as about the intermolecular and intramolecular association of molecules. These values of dielectric constant and dielectric loss [17] of paracetamol is important during microwave heating for mathematical description of the pharmaceutical product temperature history.

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