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Microwave and Refractive Index Studies on Propyl *P*-Hydroxy Benzoate and Isopropanol Binary System in Benzene for Various Concentrations

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ABSTRACT: Microwave dielectric permittivity, high frequency (optical) dielectric permittivity and static dielectric permittivity Plunger method, Abbe's refractometer and LCR bridge were used respectively in the binary system of Propyl *p*-hydroxy benzoate and Isopropanol as solute and benzene as solvent at various concentrations to obtain relaxation times. Applying Higasi method dipole moments were measured. Relaxation time increased with the increase of concentration of benzoate while dipole moment decreased. The results indicate the formation of hydrogen bond between the systems through molecular interactions.

KEYWORDS; Plunger Technique, Dielectric Permittivity, Cole-Cole Plot, Dipole Moment, Relaxation Time

I. INTRODUCTION

Materials are characterized through dielectric permittivity and loss. It has contributions from the dipolar polarization, ionic polarization and electronic polarizability which are functions of frequency and temperature [1]. The characterization of dielectric materials may include the measurement of complex dielectric permittivity, dipole moment and relaxation times [2]. Dielectric investigations of solutions containing varying amounts of interacting molecules help in detecting the formation and composition of complexes in them.. The present trend is of liquid mixtures leading to formation of hydrogen bonding in the system due to solute-solvent interactions. Hydrogen bonding is a complex in the liquid state because of the uncertainty in identifying the particular bonds and the number of molecules involved. One of the physical parameters used for conformational analysis of any resultant structure is the net dipole moment, relaxation time and thermodynamic parameters such as enthalpy, etc [3,4].

II. RELATED WORK

Dielectric Studies were carried out on hydrogen Bonded Polar Binary Mixtures of Alkyl *p*-Hydroxy Benzoates and Isopropanol by Sreehari Sastry et al. [5]. Using cavity perturbation technique dielectric studies were carried out on heptyl *p*-hydroxyl benzoate [6], on nonyl *p*-hydroxy benzoate by Radha Krishna et al. [7], by plunger method by Parvateesam et al. [8] and on pentyl *p*-hydroxy benzoate by Kiran et al. [9]. The importance of these compounds, propyl *p*-hydroxybenzoate and alcohols are used in various applications like food preservatives, cosmetics [10] and various applications like medical, etc. [11] respectively. In continuation of our dielectric work on Alkyl *p*-hydroxy benzoates, the present study is to know the dielectric behavior of binary system of propyl *p*-hydroxy benzoate and isopropanol in benzene which provide useful information about the formation of complex in the mixture and formation of hydrogen bond.

III. EXPERIMENTAL

Butyl *p*-Hydroxy benzoate (3HB or PHB) of 99.5% purity was supplied by M/s Frinton Laboratories Inc, USA. It is colorless/white powder and odorless. Its molecular weight is 166.18. Its structure is shown in Fig. 1

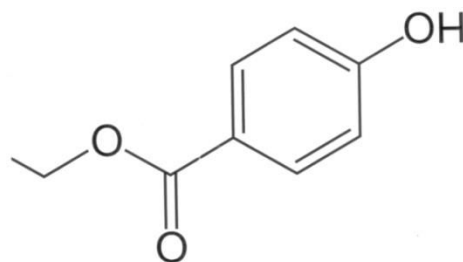


Fig. 1 Structure of 3HB

Excelsior grade Isopropanol and Benzene were obtained from Qualigens, India and were double distilled. Benzene is used as solvent, the binary system of Propyl p-hydroxy benzoates (3HB) and Isopropanol is used as solute in the preparation of solution. 3HB is dissolved in Isopropanol in various concentrations, the various weights of 3HB for each concentration is given for 26.5 ml of Isopropanol, the mole fraction of 3HB in isopropanol is given in Table 1

Table 1: Mole fraction of 4HB in 26.5 gms of isopropanol corresponding to 3HB weight

Mole fraction of 4HB in isopropanol	0.01%	0.02%	0.03%	0.04%	0.05%	0.06%	0.07%	0.08%	0.09%
Weight of 4HB (gms)	0.6539	1.3210	2.002	2.6971	3.4069	4.1317	4.8722	5.6288	6.4020

A single pan electronic balance Dhona make, model 100 DS with an accuracy of 0.01 mg was used to measure weights. Each concentration of solute is diluted with benzene in volume fractions of 90% benzene and 10% solute, 80% benzene and 20% solute, 70% benzene and 30% solute, and 60% benzene and 40% solute. The dielectric studies are carried out using LCR Bridge (static dielectric permittivity at 1kHz), the microwave bench adopting plunger [8] method (in X-band at 10GHz) and Abbe's refractometer for refractive index (high frequency using sodium D-line) at 300 K temperature. The relaxation time τ can be found [12] from the arc plot using

$$\omega\tau = \left(\frac{v}{u} \right)^{1-\alpha} \quad \text{--1}$$

where ω is the angular frequency, v and u are as shown in the figure 2 (in results and discussion part). The dipole moments are calculated from Higasi method [13].

$$\mu^2 = \frac{27 k T M_2 (a_0 - a_\infty)}{4 \pi N d_1 (\epsilon_1 + 2)^2}$$

where M_2 is molecular weight of solute, d_1 is density of solvent, ϵ_1 is the dielectric constant of solvent (benzene), a_0 and a_∞ are respectively the slopes of ϵ_0 and ϵ_∞ with respect to the concentration.

IV. RESULTS AND DISCUSSION

Dielectric permittivity

Various concentrations of solute system (PHB + Isopropanol) are dissolved in non-polar solvent benzene at various volume concentrations. The dielectric permittivity of each concentration is measured at optical frequency, low frequency and microwave frequency at room temperature. The representative dielectric data at microwave frequency for different concentrations of the solute are carried out. By varying uniformly the plunger the readings are noted and as a representative case 0.02 % of Propyl p-Hydroxy Benzoate (3HB) in Isopropanol taken as solute and benzene as solvent for concentration of 90% benzene and 10 % solute. Is represented in fig. 2.

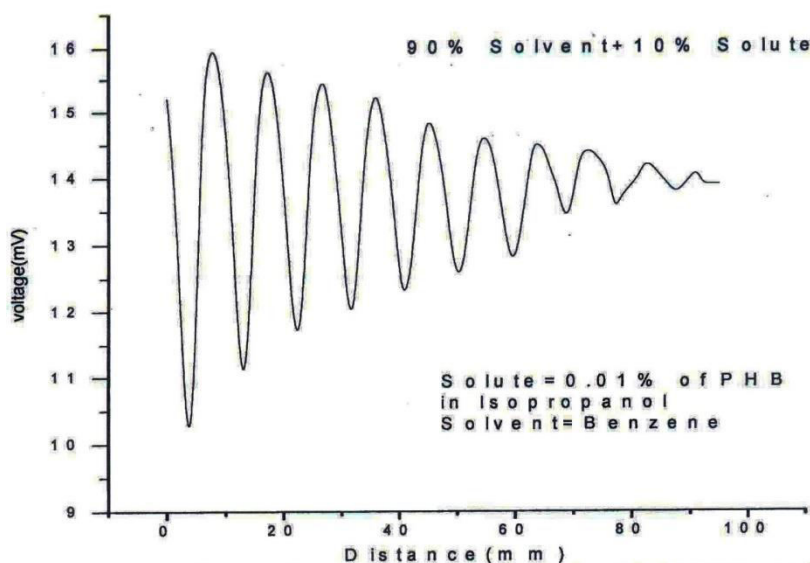


Fig 2: Voltage Vs Length of liquid in dielectric cell Cole – Cole plots and Relaxation time

All the dielectric permittivity data were used to fit in an Argand diagram (ϵ' versus ϵ'') to obtain the relaxation times. It is observed that a distribution of relaxation times as witnessed from Cole-Cole arc plot. Cole-Cole equations [14] signify the distribution of relaxation times. Eventually a macroscopic relaxation time (predominant relaxation time) is computed. Cole-Cole plots are shown in Fig. 3. The comprehensive data is given in Table 2.

Table.2: Data on Dielectric constant, Relaxation time, Dipole moment for various concentrations of (PHB+Isopropanol) in Benzene

% of PHB in Isopropanol	Volume fraction of solute+solvent	ϵ_{static}	$\epsilon_{\text{microwave}}$	n^2 (optical frequency)	Relaxation time τ pico sec	Dipole moment μ (Debye)
0.01	90+10	3.8	3.40-j0.30	2.214	3.86	3.37
	80+20	3.9	3.36-j0.74	2.16	9.68	
	70+30	4	3.39-j0.47	2.13	7.41	
	60+40	5.285	3.72-j0.72	2.10	15.08	
0.02	90+10	3.6	3.09-j0.35	2.22	8.10	3.45
	80+20	3.7	3.08-j0.61	2.18	14.81	
	70+30	3.8	3.38-j0.51	2.15	7.21	
	60+40	5.2	4.06-j1.41	2.12	11.44	
0.03	90+10	3.75	3.08-j0.46	2.22	13.41	4.10
	80+20	3.9	3.38-j0.57	2.19	8.20	
	70+30	4.13	3.39-j0.43	2.15	6.96	
	60+40	6.07	3.66-j1.15	2.12	27.23	

0.04	90+10	3.75	3.09-j0.33	2.22	10.22	3.90
	80+20	3.9	3.36-j0.70	2.19	9.13	
	70+30	4	3.71-j0.80	2.16	8.43	
	60+40	5.92	4.14-j0.81	2.12	14.66	
0.05	90+10	3.8	2.91-j0.77	2.20	17.82	3.68
	80+20	3.95	3.24-j0.35	2.18	8.66	
	70+30	4.71	3.40-j0.32	2.14	15.92	
	60+40	5.53	3.75-j0.42	2.11	20.52	
0.06	90+10	4.25	2.27-j0.29	2.211	14.29	3.70
	80+20	3.92	3.36-j0.54	2.184	11.79	
	70+30	4.71	3.49-j1.60	2.152	14.80	
	60+40	6.00	3.82-j1.01	2.131	16.9	
0.07	90+10	3.50	3.15-j0.36	2.214	12.84	4.22
	80+20	4.28	3.37-j0.72	2.184	15.84	
	70+30	5.14	3.87-j0.64	2.15	13.6	
0.08	90+10	3.5	2.83-j0.3	2.2	17.54	4.5
	80+20	4.83	3.50-j0.90	2.185	15.56	
	70+30	5.42	3.70-j2.71	2.16		
0.09	90+10	4.2	2.93-j0.40	2.226	16.93	2.8
	80+20	5.2	3.35-j0.77	2.202	21.75	
	70+30	4.92	3.72-j0.77	2.164	12.92	

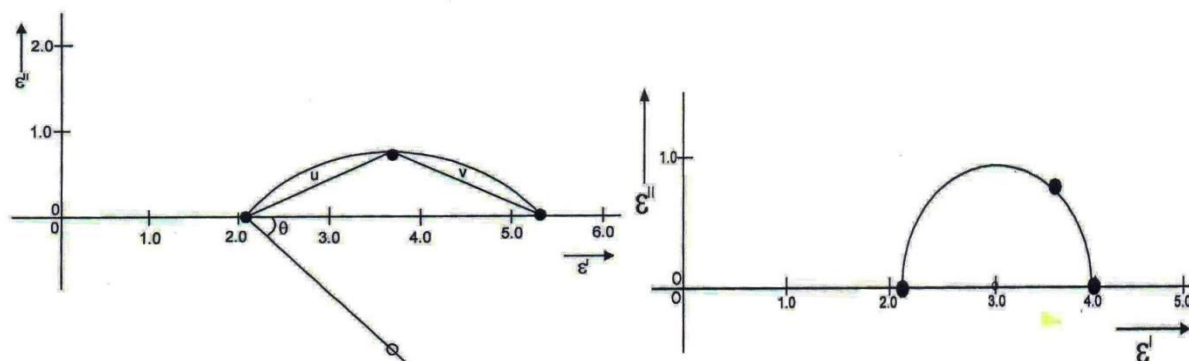


Fig.3. Cole-Cole plot for Solute=0.07MF of BHB in Isopropanol Solvent=Benzene, 65% Solvent+35% Solute

Dipole moment

The data required for calculating dipole moment are given along with the dipole moment at each concentration in Table

2. The values of a_0 and a_∞ are found from the graphs of ϵ_0 (static dielectric constant) and ϵ_∞ Vs concentration respectively which are shown in Figs. 3 and 4. ϵ_0 (static dielectric permittivity) is measured at 1 kHz using LCR meter. ϵ_∞ is the dielectric permittivity measured at optical frequency using Abbe refractometer. It is evident from the data given in the Table 3, the dielectric permittivity increases with the increased frequency. The microwave data show that these compounds are polar in nature and correspondingly the dielectric permittivity is a complex quantity. The relaxation time is found to increase in magnitude for a given concentration of BHB in Isopropanol with the increase of dilution in benzene which shows that the molecules are free to rotate as benzene concentration increases.

The same tendency is also seen for different concentrations of BHB in Isopropanol. The dipole moment values decrease with increase of BHB in Isopropanol which is probably due to the hydrogen bonding in the system. However from the present study the dipole moment is varied from 3.28 to 4.5 for various concentrations of BHB in Isopropanol. From the table 2, it can be said that, the static dielectric permittivity (ϵ_{static}) increases with the increase of concentration of solute. Comparing the static dielectric permittivity of EHB [15], and BHB, it can be concluded that when concentration of solute increases static dielectric permittivity also increases in the microwave region also the dielectric permittivity increases with the increase of concentration of BHB in binary system. But at optical frequency region the dielectric permittivity decreases when the concentration of solute increases in the binary system. It is due to dipolar polarization contribution decreases at high frequency. At high frequency the dipolar polarization disappears and only atomic polarization or electronic polarization is present. The dielectric permittivity decreases with the increase of frequency (from static (low frequency) to optical (high) frequency). It means frequency increases the dipolar polarization contribution decrease and vanishes. At static frequency all polarizations are present. The relaxation time increases with the increase of concentration of solute up to certain concentration (0.06%) and after that concentration the relaxation time decreases. This behaviour may be attributed to the formation of hydrogen bond between isopropyl alcohol and 3HB. The phenomenon of dielectric relaxation of the binary mixture of polar molecules in non-polar solvents at microwave frequencies has been attempted by many research workers. Raman Kumar and Rangra [16] also calculated the binary mixture of N- Methylacetamide and acetonitrile in benzene using microwave plunger technique(X-Band). They concluded that some molecular interactions exist in the binary mixture. The same may attributed to the present case that is, forming of hydrogen bond between BHB and isopropanol. The strength of hydrogen bond reflects in the corresponding relaxation time and dipole moment value.

Table.3: Data on u , v , θ , α and Relaxation time values of parameters for dipole moment.

Mole fraction of PHB in isopropanol	Volume fraction of solvent+solute	U	V	$\Theta = \pi\alpha/2$	Distribution parameter (α)	Relaxation time τ (pico-sec)
0.01	90+10	2.4	1.3	51°	0.5666	3.86
	80+20	2.8	1.8	10°	0.11	9.68
	70+30	6.6	4	31°	0.344	7.41
0.02	90+10	1.8	1.2	36°	0.4	8.10
	80+20	2	1.9	26°	0.28	14.81
	70+30	2.8	1.5	19°	0.21	7.21
0.03	90+10	2	1.8	35°	0.38	13.40
	80+20	2.7	1.6	19°	0.21	8.20
	70+30	2	1.8	35°	0.53	6.96
0.04	90+10	1.9	1.5	42°	0.46	10.22
	80+20	2.7	1.7	15°	0.16	9.13
	70+30	3.4	1.8	0°	0	8.43
0.05	90+10	2	2.2	14°	0.15	17.82

	80+20	2.4	1.6	30 ⁰	0.33	8.66
	70+30	2.6	2.6	54 ⁰	0.6	15.92
0.06	90+10	2.5	2	44 ⁰	0.488	14.29
	80+20	2.8	1.9	19 ⁰	0.21	11.77
	70+30	3.8	3.5	8 ⁰	0.89	14.9
0.07	90+10	1.9	1.2	47 ⁰	0.52	12.84
	80+20	2.3	2.1	37 ⁰	0.41	18.5
	70+30	3.8	2.7	49 ⁰	0.54	13.6
0.08	90+10	1.7	2	36 ⁰	0.4	17.54
	80+20	3.5	3.4	20 ⁰	0.22	15.56
0.09	90+10	1.9	2.2	52 ⁰	0.5782	16.93
	80+20	3.2	4.5	32 ⁰	0.356	19.47
	70+30	3.8	2.7	35 ⁰	0.389	12.92

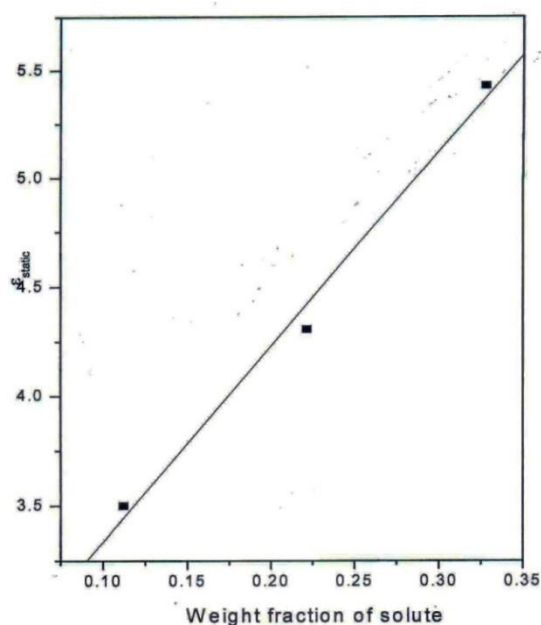


Fig.3 ϵ_{static} vs weight fraction of solute
0.02 MF BHB in isopropanol

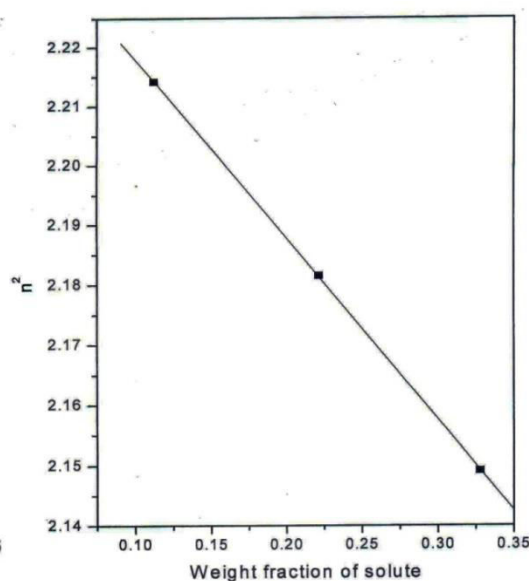


Fig.4 n^2 vs weight fraction of solute

V. CONCLUSIONS

The refractive index value in the optical frequency decreased with increase in the concentration of the solute binary system (benzoate and alcohol) in non polar solvent benzene at room temperature while at the optical, microwave and low frequency static dielectric permittivity increased with increase in the concentration of the solute binary system in non-polar solvent benzene at room temperature. There is an increase in the relaxation time as the concentration of the benzoate is increased but dipole moment is decreased in solute system in different concentrations of non-polar solvent benzene which is due to the formation hydrogen bond in the solute system. It is due to the formation hydrogen bond between the solute systems. The dipole moment values of PHB increased when compared to the corresponding values of Ethyl HB.



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