

# DIPOLE MOMENT STUDIES OF SOME SUBSTITUTED BENZALDEHYDE WITH 1- OCTANOL

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**Abstract** - The experimental values of the complexes of the dipolar increment of Benzaldehyde, 2-Fluorobenzaldehyde, 4-Fluorobenzaldehyde with 1-Octanol in Carbontetrachloride were studied at 303K. The dipole moment of the complexes has determined by Huysken's and Debye's polarization based on the Onsager theory. The results shown that complexation is used to discuss the molecular interaction. The increment of the dipole moment were obtained from bond angles data.

**Keywords** - *H-Bonding, substituted Benzaldehyde, o-Fluoro benzaldehyde, p-Fluorobenzaldehyde Huysken's method, dipolar increment.*

## I. INTRODUCTION

Dielectric studies provide meaningful information about the intra and intermolecular interaction. This method used to investigation of Benzaldehyde and its derivatives have shown antitumor activity mice [1-2]. The dielectric constant of a few alcohols carbonyls mixtures is studied by shanmugasundaram and Mohan [3]. Alcohols are excellent proton donors. In the recent years several author [4-8] studies the complex of ketones, ester, amides, aldehyde, and amines with phenol and alcohols using the dielectric method. The review of Davie's [9] Zenger's -Huysken's and [10] Muller et al [11] can be importance of this type of complex. In this present works, it is aimed to investigation the dipole moment for binary and complex system by using mixture of Benzaldehyde, o-Fluoro benzaldehyde, p-Fluorobenzaldehyde with 1-Octanol in CCl<sub>4</sub> at 303K from polarization [12] and Huysken's method [13].

## II. EXPERIMENTAL

### A. Materials

The Benzaldehyde o-Fluorobenzaldehyde, p-Fluorobenzaldehyde, 1- Octanol compounds were purified by standard procedures and checked against their literature value.

### B. DIELECTRIC CONSTANT ( $\epsilon_0$ )

Dipole meter is an instrument that is used to measure the dielectric constant of liquids. In the equipment a particular circuit has been developed for audio oscillator that produce stabilized wave and experiment dielectric cell is standardized using reference liquid. The known dielectric constant by immersing the dielectric cell assembly in to reference liquid. Then unknown liquid whose dielectric constant has to be determining as taken and assembly is immersed into liquid into resulting in change in frequency. The resulting shift capacitance of cell in unknown of liquid is calculated ( $c_x$ ).

## III. THEORY

These methods have been to understand the merits of determined the dipole moment of the solute.

Using the limiting polarization method [13] the dipole moment of the solute ( $\mu_b$ ) in a non-polar solvent can be calculated from the relation.

Debye's methods:

The dipole moment  $\mu$

$$\mu_b = \sqrt{\frac{9K}{4\pi N}} [(P_{2\infty} - R_D) T]^{1/2} \quad (1)$$

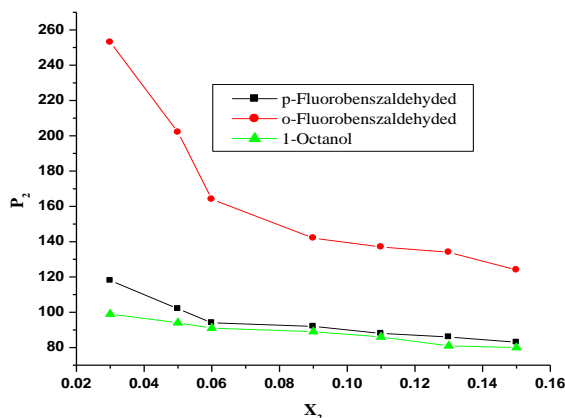


Fig. 1. Variation of polarization (P) with concentration (Mol/L) of solute in CCl<sub>4</sub>

Where K is the Boltzmann constant,

N is Avogadro's number is the absolute temperature

P<sub>2∞</sub> molar polarization at infinite dilution and

R<sub>D</sub> is mole fraction of the solute

$$R_D = \frac{(n_2^2 - 1)}{(n_2^2 - 2)} \frac{M_2}{d_2} \quad (2)$$

Here n<sub>2</sub>, d<sub>2</sub> and M<sub>2</sub> are the refractive index, density and molecular weight of the solute.

### Dipole moment of the complex by Huysken's method

The dielectric constant ε and the refractive index for the sodium line n<sub>D</sub> of a ternary solution with formal concentrations C<sub>A</sub> of proton donor and C<sub>B</sub> proton acceptor of base in CCl<sub>4</sub> solution are measured first. The quantity Ω<sub>B</sub> is then computed from the experiment data [14]

$$\Omega_B = \frac{9KTX 10^{22}}{4\pi N_A} \frac{1}{C_B} \left[ \frac{(\epsilon - n_D^2)(2\epsilon + n_D^2)}{\epsilon(n_D^2 + 2)^2} - \frac{C_A(\epsilon_s - n_{D_s}^2)(2\epsilon_s + n_{D_s}^2)}{C_B^2 \epsilon_s(n_{D_s}^2 + 2)^2} \right] \quad (3)$$

C<sub>s</sub><sup>0</sup> is the formula concentration of the solvent in the pure state

C<sub>s</sub> its actual concentration in the pure solvents refers to the pure solvent.

If the internal index of refraction of the dissolved entities can be approximated as n<sub>D</sub> the theories of Onsager [15] and Froehlich [16].

This serves as a criterion for choosing the proper concentration of C<sub>A</sub> and C<sub>B</sub> of the proton

donor and proton acceptor for 1:1 complexation. If the formal concentration C<sub>A</sub> of the proton acceptor is far greater than the formal concentration C<sub>B</sub> of the proton donor such that,

$$C_B - C_A \gg k-1 \quad (4)$$

Where K is the equilibrium constant for 1:1 complexation Eq (4) is valid. Thus, for the experimentally observed values of ε<sub>o</sub>, n<sub>D</sub>, ε<sub>s</sub>, and n<sub>Ds</sub>, it is possible to obtain the values of Ω<sub>B</sub> for different C<sub>A</sub>/C<sub>B</sub> along the x-axis and Ω<sub>B</sub> along the Y-axis. Intercept of the curve in the Y-axis gives (μ<sub>ab</sub><sup>2</sup> - μ<sub>b</sub><sup>2</sup>).

Table. 1

Variation of dielectric constant, refractive index, density and Ω<sub>B</sub> with the formal concentration of different aldehydes

Benzaldehyde+ 1-Octanol+CCL <sub>4</sub>					
C <sub>B</sub>		Refractive index	Density	C <sub>A</sub> /C <sub>B</sub>	Ω <sub>B</sub>
.1	2.2170	2.1304	1.400	0.5	7.4648
.2	2.2749	2.0272	1.394	0.25	6.3062
.3	2.3263	2.1257	1.390	0.166	5.68078
.4	2.3619	2.1243	1.386	0.125	5.0245
.5	2.4195	2.1228	1.376	0.100	4.9836
.6	2.4526	2.1213	1.366	0.0833	4.6196
.7	2.5215	2.1199	1.348	0.0714	4.5235
o-Fluorobenzaldehyde+ 1-Octanol+CCL <sub>4</sub>					
C <sub>B</sub>		Refractive index	Density	C <sub>A</sub> /C <sub>B</sub>	Ω <sub>B</sub>
.1	2.1301	2.1301	1.426	0.5	17.5687
.2	2.4244	2.1286	1.412	0.25	12.4083
.3	2.5627	2.1257	1.394	0.166	12.0204
.4	2.6137	2.1243	1.390	0.125	10.0523
.5	2.6796	2.1228	1.374	0.100	9.0878
.6	2.7405	2.1199	1.368	0.0833	8.3959
.7	2.8162	2.1170	1.346	0.0714	8.0070
p-Fluorobenzaldehyde+ 1-Octanol+CCL <sub>4</sub>					
C <sub>B</sub>		Refractive index	Density	C <sub>A</sub> /C <sub>B</sub>	Ω <sub>B</sub>
.1	2.3520	2.1272	1.416	0.5	19.0514
.2	2.4244	2.1257	1.402	0.25	12.5427
.3	2.4919	2.128	1.390	0.166	12.0409
.4	2.5726	2.1213	1.384	0.125	9.3212
.5	2.6384	2.1184	1.370	0.100	8.5378
.6	2.7092	2.1170	1.362	0.0833	8.0426
.7	2.7631	2.1155	1.348	0.0714	7.4776

#### IV. RESULTS AND DISCUSSION

The experiment values of the density ( $\rho$ ) refractive indices ( $n_D$ ) dielectric constant ( $\epsilon$ ) and  $\Omega_B$  for varying concentration of the proton donor are recorded in Table (1). The slope and the intercept of the straight line graph is plotted by  $C_A/C_B$  vs  $\Omega_B$ . Using least square fitting methods from values of  $\mu_{ab}$  and  $\mu_b$  are calculated.

**Table. 2**

Dipole moment of the components and their 1:1 complex and dipolar increments of the complex system

System	$\mu_a$ (D)	$\mu_b$ (D)	$\mu_{ab}$ (D)	$\Delta\mu$ (D)
1Octanol+Benzaldehyde	1.70	3.50	4.63	1.57
1-Octanol+o-Fluorobenzaldehyde	1.70	4.50	4.61	3.50
1-Octanol+p-Fluorobenzaldehyde	1.70	3.90	5.952	5.76

Huysken's method based on Onsager Theory is determined the dipole moment of the donor and acceptors were using carbon tetrachloride as solvent. The results are closely agreed with the solution data. The dipole moment of the complex and dipolar increment are discussed by Huyskens [17] is given in Figs. 2-4.

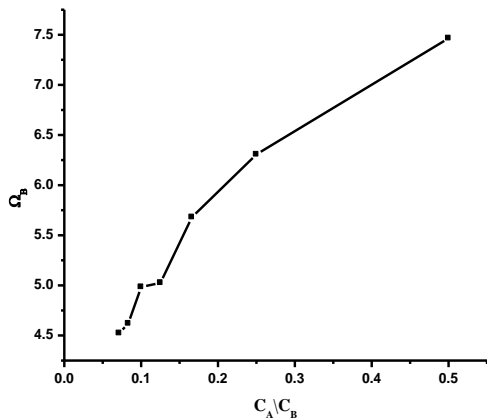
If a single H- bond is formed between the partners, it can be presumed that  $\Delta\mu$  has the direction of the hydrogen bond. The vector equation can be transformed in from.

The dipole increment is given by

$$\Delta\mu = (\mu_{ab}^2 - \mu_a^2 \sin^2 \theta_a - \mu_b^2 \sin^2 \theta_b - 2\mu_a \mu_b \sin \theta_a \sin \theta_b \cos \Phi)^{1/2} - \mu_a \cos \theta_a - \mu_b \cos \theta_b$$

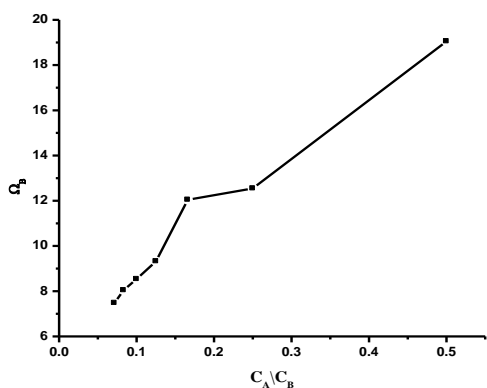
From the computed values of  $\mu_{ab}$  and  $\mu_b$ , the dipolar increments were obtained using eq (5).there values are given in Table 2 for all systems. The values of  $\theta_a$  and  $\theta_b$  were taken from the literature.

When a proton donor of dipole moment  $\mu_a$ ,  $\mu_b$ ,  $\mu_{ab}$ ,  $\theta_a$  and  $\theta_b$  values are shown the Table 1. The dipole moment may be enhanced by an amount  $\Delta\mu$ . The dipolar increment  $\Delta\mu$  determines the nature of complexes in the system studied only due to polarization effects and not due to charge transfer effect.



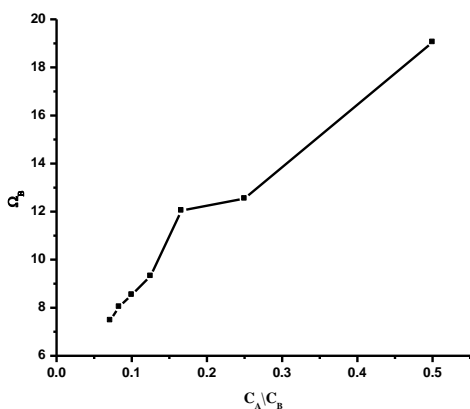
**g. 2. Plot  $C_A/C_B$  vs  $\Omega_B$  for given 1- Octanol with Benzaldehyde in  $CCL_4$ .**

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**g. 3. Plot  $C_A/C_B$  vs  $\Omega_B$  for given 1- Octanol with o-fluorobenzaldehyde in  $CCL_4$ .**

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**Fig. 4. Plot  $C_A/C_B$  vs  $\Omega_B$  for given 1- Octanol with p-fluorobenzaldehyde in  $CCL_4$ .**

For experimental values of concentrations studied, the plot of  $\Omega_B V_s C_A/C_B$  is a straight line indicates the formation of a 1: 1 complex. The values of  $\mu$  are reported in Table 2. The dipole moments for all system are in the order of  $5.76 > 3.50 > 1.57$ , dipole increment in all the system  $\Delta\mu$  is less than 10D due to polarization effects and it is not due to charge transfer. The dipole moment of the complex and dipole increment is donor (1-Octanol) p-Fluorobenzaldehyde as one of the acceptor [18, 19]. Similar conclusions were drawn [20] for the mixture of phenols with substituted piperidines. Similar results were reported by Thenappan [21] and Sabesan [22] for the alcohol mixtures.

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