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Optical Studies on Liquid crystalline mixture of Benzoic acid and amino phenyl benzoate

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Abstract - *In the present studies we have carried out the measurements of refractive indices and densities on 4- butoxy benzoic acid, Butyl4-({4-[(E)-{[4-dimethylamino)phenyl)methyliden}amino]phenyl]carbonyloxy) benzoate and their mixture. The molecular polarizabilities are calculated from the above measurements using the well known internal field models by Vuks and Neugebauer. The orientational order parameter were estimated by using Vuks and Neugebauer methods and the values obtained in both the methods are very close to each other.*

***Key Words*: Molecular Polarizability, refractive indices, densities and internal field models, orientational order parameter(OOP).**

1. INTRODUCTION

Liquid crystal (LC) devices are indispensable elements of modern life because of ubiquity of their application like spatial light modulator, optical antennas, and flat panel display devices [1–2]. The mixing of different liquid crystals is a unique technique to tailor their properties for specific applications. In particular, the mixing of two mesogens that are quite different from each other can strongly change the properties and the phase behavior of the mixtures compared to the pure compounds. For application of any liquid crystal in a practical device it must retain suitable values of certain parameters like dielectric permittivity, dielectric loss, conductivity, refractive index, birefringence and viscosity etc. with varying conditions like temperature and electric field [4-5]. Usually it is very difficult to fulfill these conditions with a single liquid crystal sample. Hence liquid crystal mixtures have come to play an important role in device applications.

In the present investigation the benzylidene amino phenyl benzoate and benzoic acid are mixed with appropriate ratios and their optical properties like refractive index, molecular polarizability and orientation order parameters are reported.
The molecular structures of the above liquid crystals is shown in figure 1.

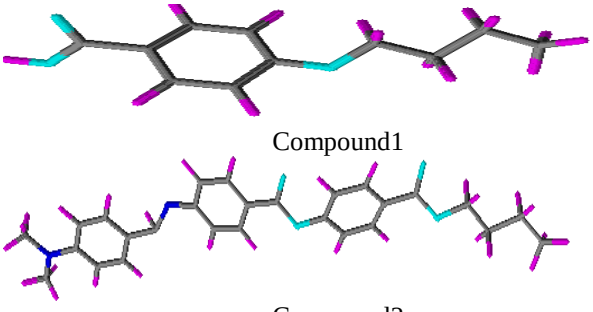

Fig -1: Molecular Structures of Liquid Crystals

2. EXPERIMENTAL

2.1 Refractive indices measurments

The refractive indices of the liquid crystalline compounds were measured with wedge shaped glass cell similar to the one used to obtain birefringence by Haller et al [6-7] and modified spectrometer. A wedge shaped glass cell was prepared with two optical flat rectangular glass plates (50mm x 25mm) sandwiched with glass slide of 0.05mm thick which acts as a wedge spacer. The cell is filled with the liquid crystal material. The liquid crystal material in the cell acts as a uniaxial crystal with its optic axis parallel to the edge of the spacer glass plate. The accuracy in the measured refractive indices was ± 0.0005.

2.2 Density measurments

The U-shaped bi-capillary pyknometer in conjunction with cathetometer was used for the density measurements at various temperatures. The absolute error of the measurement of the densities is $\pm 10^{-4}$ gm/cm^3. The cooling rate during the measurement was 0.5K/hr.

2.3 Estimation of Polarizabilities

For the estimation of the molecular polarizabilities of liquid crystalline compounds, the authors have considered Vuks and Neugebauer models. The relevant equations of the two models are given below.

2.3.1 Vuk's Method

Many authors [10-12] applied this method to estimate molecular polarizabilities and the equations used in this method are

$$\alpha_e = \left[\frac{3}{4\pi N}\right]\frac{n_e^2-1}{\bar{n}^2-1} \quad (1)$$

$$\alpha_o = \left[\frac{3}{4\pi N}\right]\frac{n_o^2-1}{\bar{n}^2-1} \quad (2)$$

Where N is the number of molecules per unit volume, n_e and n_o are the extraordinary and ordinary refractive indices of the LC molecule.

$\bar{n}^2 = \left[\frac{n_e^2+2n_o^2}{3}\right]$ and N = $N_A\rho/M$ where N_A is the Avogadro number, ρ is the density and M is the molecular weight.

2.3.2 Neugebauer Method

Subramanyam et al. [13] applied this method to estimate mean molecular polarizabilities. The equations used in this method are

$$\alpha_e = (AB - 3 \pm \sqrt{(AB-3)^2 - 4AB})/2A \quad (3)$$

$$\alpha_o = (AB + 3 \pm \sqrt{(AB+3)^2 - 16AB})/4A \quad (4)$$

Where $A = \left[\frac{4\pi N}{3}\right]\left[\frac{n_e^2+2}{n_e^2-1}\right] + \left[\frac{2(n_o^2+2)}{n_o^2-1}\right]$

and $B = 9(\bar{n}^2-1)/[(4\pi N_i)(\bar{n}^2+2)]$

N_i is the number of molecules per unit volume in the isotropic phase.

2.4 Estimation of Orientation Order Parameter

In the Vuks method the order parameter is given by [14-16]

$$S = \left(\frac{\alpha}{\alpha_\parallel - \alpha_\perp}\right)\frac{n_e^2-n_o^2}{\bar{n}^2-1} \quad (5)$$

Where $\bar{n}^2 = \left[\frac{n_e^2+2n_o^2}{3}\right]$

The order parameter in case of Neugebauer method [17, 18]

$$S = \left[\frac{\alpha}{\alpha_\parallel - \alpha_\perp}\right] f(B) \quad (6)$$

Where

$$f(B) = \left(\frac{9}{4AB}\right)\left[\left(B^2 - \left(\frac{10}{3}\right)B + 1\right)^{1/2} + \frac{B}{3} - 1\right]$$

and $B = \frac{n^2-1}{n^2+1}\left(\frac{n_e^2+2}{n_e^2-1} + \frac{2(n_o^2+2)}{n_o^2-1}\right)$

3. RESULTS AND DISCUSSION

For the above mesogenic mixture, the refractive indices are measured using modified spectrometer with small angled prism which houses the liquid crystalline compound. The small angled prism is placed in a heating block for measurement of refractive indices with temperature and a monochromatic source of wavelength 589.3nm is used. During isotropic-nematic phase transformation the incident light splits into two one higher and the other lower than the isotropic value called extraordinary ne and ordinary no refractive indices. In the nematic region the value of n_e increases where as the value of n_o decreases with temperature and both attains saturation deep in nematic region. The variation of refractive indices with temperature in isotropic and nematic region is illustrated in figures 2, 3 and 4.

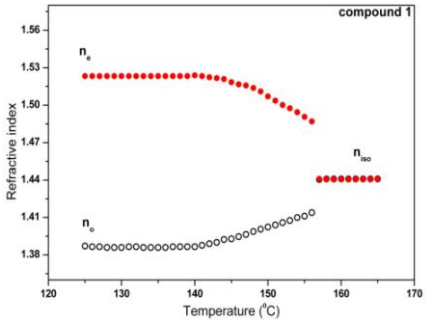

Fig -2: Temperature variation of Refractive index in compound 1

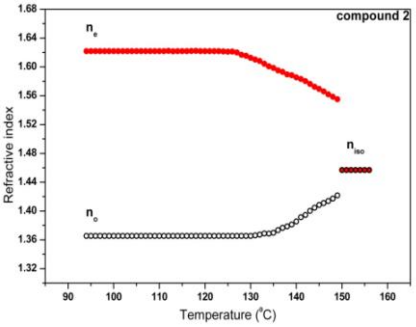

Fig-3: Temperature variation of Refractive index in compound 2

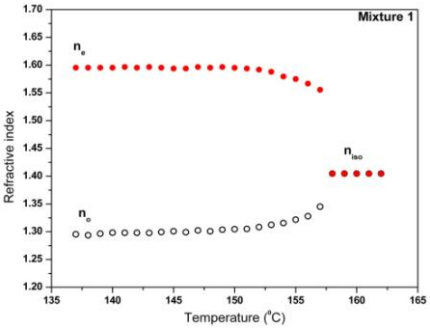

Fig-4: Temperature variation of Refractive index in Mixture

The temperature variation of density is measured by dilatometer attached with U-shape bicapillary pyknometer and represented in Figures 5, 6 and 7. It is found that with rise in temperature density decreases and at phase transformations there is density jumps.

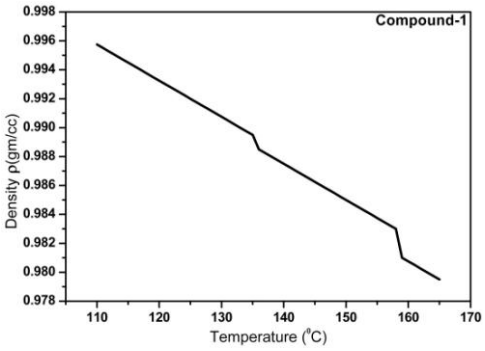

Fig-5: Temperature variation of Density in Compound1

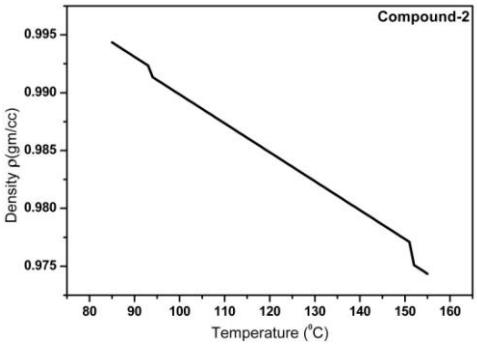

Fig-6: Temperature variation of Density in Compound2

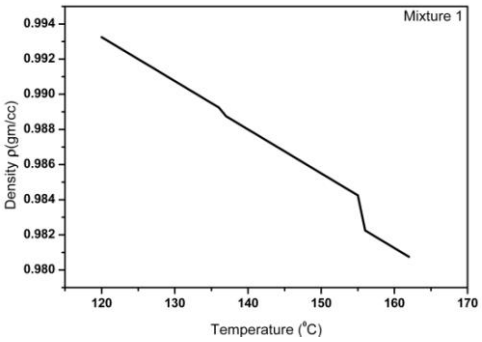

Fig-7: Temperature variation of Density in Mixture-1

The molecular polarizabilities are estimated by Vuks and Neugebauer internal field models and are presented in table-1. The order parameter is evaluated for both Vuks and Nuegauber model and shown in figures 8, 9 and 10.

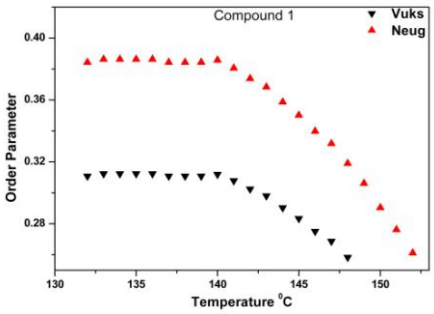

Fig-8: Variation of OOP with temperature in Compound-1

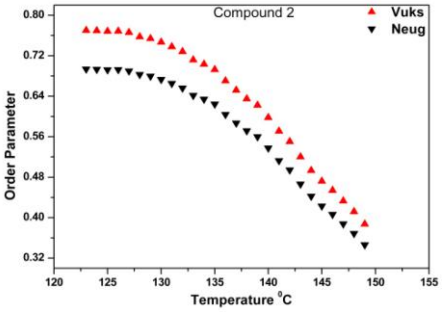

Fig-9: Variation of OOP with temperature in Compound-2

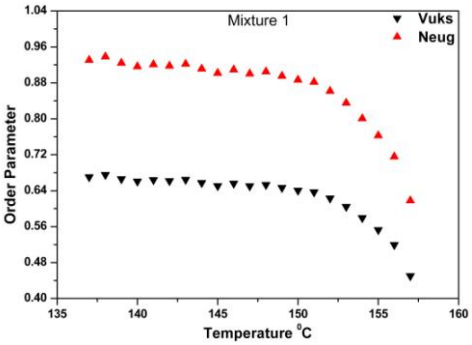

Fig-10: Variation of OOP with temperature in Mixture 1

Table -1: Mean molecular polarizabilities obtained in the liquid crystalline compounds by different methods [$10^{-24}cm^3$]

Compound	Vuks model	Neugebauer model
	α_M	α_M
Compound-1	20.04	20.38
Compound-2	24.46	24.42
Mixture	25.37	25.37

4. CONCLUSIONS

- The ordinary and extraordinary refractive indices attain saturation deep in the nematic phase.
- The mean molecular polarizabilities obtained from birefringence data using the internal field models due to Vuks and Neugebauer are in reasonably good agreement with each other.
- The orientational order parameter evaluated using both the models shows decrease with increase of temperature.
- The orientational order parameter estimated by Vuks and Neugebauer method is in between 0.3 to 0.7 which is in accordance with literature data available.

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