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# ORDER PARAMETER AND DISTRIBUTION FUNCTIONS FOR NEMATOGENIC OBA AND NBA

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*Abstract* Using refractive index and density data for nematogenic compounds Octyl benzoic acid (OBA) and Nonyl benzoic acid (NBA), orientational order and hence distribution function has been determined. From this, the higher order parameter $<P_4>$ has been estimated for these two compounds. The physical interpretation of these parameters $<P_2>$ and $<P_4>$ has been given in terms of statistical quantities like *variance* and *kurtosis*.

## *INTRODUCTION*

Alkyl benzoic acids are the simplest type of liquid crystals and the nematic phase in these compounds have been reported earlier[1]. These compounds are used to form synthetic media in electro-optic devices. There is a continued interest in the nematic liquid crystals due to their wide range of exquisite optical and physical properties [2–11]. One such property is the orientational order parameter, which determines the applicability of the nematics in electro-optic devices or displays. To explain the temperature dependence of the orientational order parameter, the molecular field theory of the nematics using anisotropic dispersion forces was given by Maier and Saupe [12] which is essentially an extension of London theory [13,14].

In this paper we report the results of the experimental measurements of the refractive indices and densities of OBA and NBA compounds at different temperatures. Using these data, the orientational order parameter has been estimated employing Neugebauer relations. By considering the orientational order parameter corresponding to the nematic-isotropic transition temperature and based on an empirical relation, we have determined the distribution function and hence the higher order parameter $< P_4 >$ for OBA and NBA. The fundamental concept of order parameter $< P_2 >$ and higher order parameter $< P_4 >$ has been discussed in terms of distribution function.

## *EXPERIMENTAL*

The compounds (Octyl benzoic acid (OBA) and Nonyl benzoic acid (NBA)) were obtained from M/s Merck Ltd., U.K. For use in our experiments, they were purified by recrystallization from their solutions in benzene. The nematic-isotropic transition temperatures ($T_c$) were determined using a polarizing microscope and a

specially constructed hot stage. The observed values are in good agreement with the reported values. The refractive index measurements were made using a goniometer spectrometer and a hollow glass prism of small angle ($3\text{-}5^0$) for the wavelengths 4358,5461 and 5780 A. The technique of measurement has been described in an earlier paper [10]. The densities at different temperatures in the nematic and isotropic phases were determined by using capillary tube technique [10]. The measured refractive index and density data are given in Table 1. The measurements of the temperature, refractive index and density are estimated to be accurate to within $\pm 0.1^0 C, 0.001$ and $0.001 gm/cm^3$ respectively.

## *RESULTS AND DISCUSSION*

Madhusudana [15] has analysed the various approaches used to calculate the principal polarizabilities $\alpha_e$ and $\alpha_o$ and has suggested that when reliable density data exist, it is more meaningful to use Neugebauer relations. Also, it has been found by various investigators that the polarizabilities obtained by Neugebauer's approach can be accounted for using bond polarizability data [10,15,16]. Hence we have used Neugebauer's relations for the calculations of $\alpha_e$ and $\alpha_o$. Using Haller's extrapolation procedure [17] and also from bond polarizability data, we have estimated the polarizability anisotropy $(\alpha_\parallel - \alpha_\perp)$ of the molecule and hence the orientational order parameter. It has been observed that the macroscopic techniques like magnetic and optical birefringence of obtaining the order parameter are more significant than the scattering methods like X-ray which gives informations which are in between the local (NMR) and macroscopic ones (magnetic and optical birefringence) [18]. Normally this difference is not considered while comparing the distribution function with that of Maier-Saupe model.

In accordance with the Maier-Saupe model, the distribution function $f(\theta)$ of a nematogenic system can be assumed to form a Gaussian distribution around the director and can be written as[19]

$$f(\theta) = \frac{1}{\sigma}[exp(-\frac{\theta}{2\sigma^2}) + exp\{-\frac{(\theta-\pi)^2}{2\sigma^2}\}] \qquad (1)$$

where $\sigma$ is the deviation. The orientational order parameter or the second moment is given by

$$< P_2 >= \frac{\int_0^{\pi/2} P_2(\cos\theta) f(\theta) \sin\theta d\theta}{\int_0^{\pi/2} f(\theta) \sin\theta d\theta} \qquad (2).$$

Using this expression and the order parameter obtained from the refractive index data we have estimated the parameter $\sigma$ by employing the one-dimensional minimization programe of SIMPLEX [20] at various temperatures. Now using this

$\sigma$ value we have determined the distribution functions which are given in Figure 1(a and b) for OBA and NBA at various temperatures. Higher order parameter $< P_4 >$ is given by

$$< P_4 >= \frac{\int_0^{\pi/2} P_4(\cos\theta) f(\theta) \sin\theta d\theta}{\int_0^{\pi/2} f(\theta) \sin\theta d\theta} \tag{3}$$

and the values are given in Table 1. These values are of the same order of magnitude as reported earlier for different nematogenic compounds from X-ray intensity data [18].

Table 1(a). Refractive index, density and orientational order parameter for OBA

| $T_c$-T | $\lambda$ 4358 | | $\lambda$ 5461 | | $\lambda$ 5780 | | $\rho$ | <$P_2$> | <$P_4$> |
|---|---|---|---|---|---|---|---|---|---|
| °C | $n_e$ | $n_o$ | $n_e$ | $n_o$ | $n_e$ | $n_o$ | (gm/cc) | | |
| 12.0 | 1.602 | 1.472 | 1.573 | 1.460 | 1.568 | 1.457 | 0.911 | 0.578 | 0.161 |
| 10.0 | 1.699 | 1.472 | 1.570 | 1.460 | 1.565 | 1.457 | 0.907 | 0.539 | 0.127 |
| 8.0 | 1.595 | .1.472 | 1.566 | 1.460 | 1.561 | 1.457 | 0.904 | 0.518 | 0.112 |
| 6.0 | 1.591 | 1.473 | 1.562 | 1.461 | 1.557 | 1.458 | 0.901 | 0.489 | 0.092 |
| 4.0 | 1.586 | 1.474 | 1.558 | 1.462 | 1.553 | 1.459 | 0.897 | 0.439 | 0.064 |
| 2.0 | 1.582 | 1.476 | 1.554 | 1.464 | 1.549 | 1.461 | 0.894 | 0.389 | 0.044 |
| -1.0(iso) | 1.512 | | 1.493 | | 1.489 | | 0.887 | | |

Table 1(b). Refractive index, density and orientational order parameter for NBA

| $T_c$-T | $\lambda$ 4358 | | $\lambda$ 5461 | | $\lambda$ 5780 | | $\rho$ | <$P_2$> | <$P_4$> |
|---|---|---|---|---|---|---|---|---|---|
| °C | $n_e$ | $n_o$ | $n_e$ | $n_o$ | $n_e$ | $n_o$ | (gm/cc) | | |
| 15.0 | 1.617 | 1.472 | 1.593 | 1.461 | 1.585 | 1.455 | 0.899 | 0.518 | 0.112 |
| 13.0 | 1.609 | 1.473 | 1.585 | 1.463 | 1.577 | 1.456 | 0.898 | 0.509 | 0.105 |
| 11.0 | 1.601 | .1.474 | 1.577 | 1.464 | 1.569 | 1.458 | 0.896 | 0.499 | 0.098 |
| 9.0 | 1.593 | 1.475 | 1.569 | 1.465 | 1.563 | 1.459 | 0.893 | 0.469 | 0.079 |
| 7.0 | 1.587 | 1.477 | 1.563 | 1.466 | 1.556 | 1.461 | 0.891 | 0.444 | 0.071 |
| 5.0 | 1.581 | 1.478 | 1.556 | 1.466 | 1.551 | 1.461 | 0.887 | 0.439 | 0.064 |
| 3.0 | 1.575 | 1.479 | 1.552 | 1.467 | 1.546 | 1.462 | 0.884 | 0.379 | 0.039 |
| 1.0 | 1.566 | 1.482 | 1.544 | 1.469 | 1.538 | 1.463 | 0.880 | 0.349 | 0.029 |
| -1.0(iso) | 1.512 | | 1.493 | | 1.489 | | 0.878 | | |

It is to be noted here that the distribution function $f(\theta)$ is more fundamental than the parameters $< P_2 >$ and $< P_4 >$ . In fact the orientational order parameter $S$ $(or < P_2 >)$ is directly related to the measure of variance (or width)

of the distribution function of $f(\cos\theta)$. Higher order parameter $< P_4 >$ which is a measure of *Peakedness* of the distribution function $f(\cos\theta)$ and it is called the *kurtosis*. With increase in temperature the variance as well as the kurtosis decrease showing that there is a decrease in the ordering of the molecules in the nematic phase.

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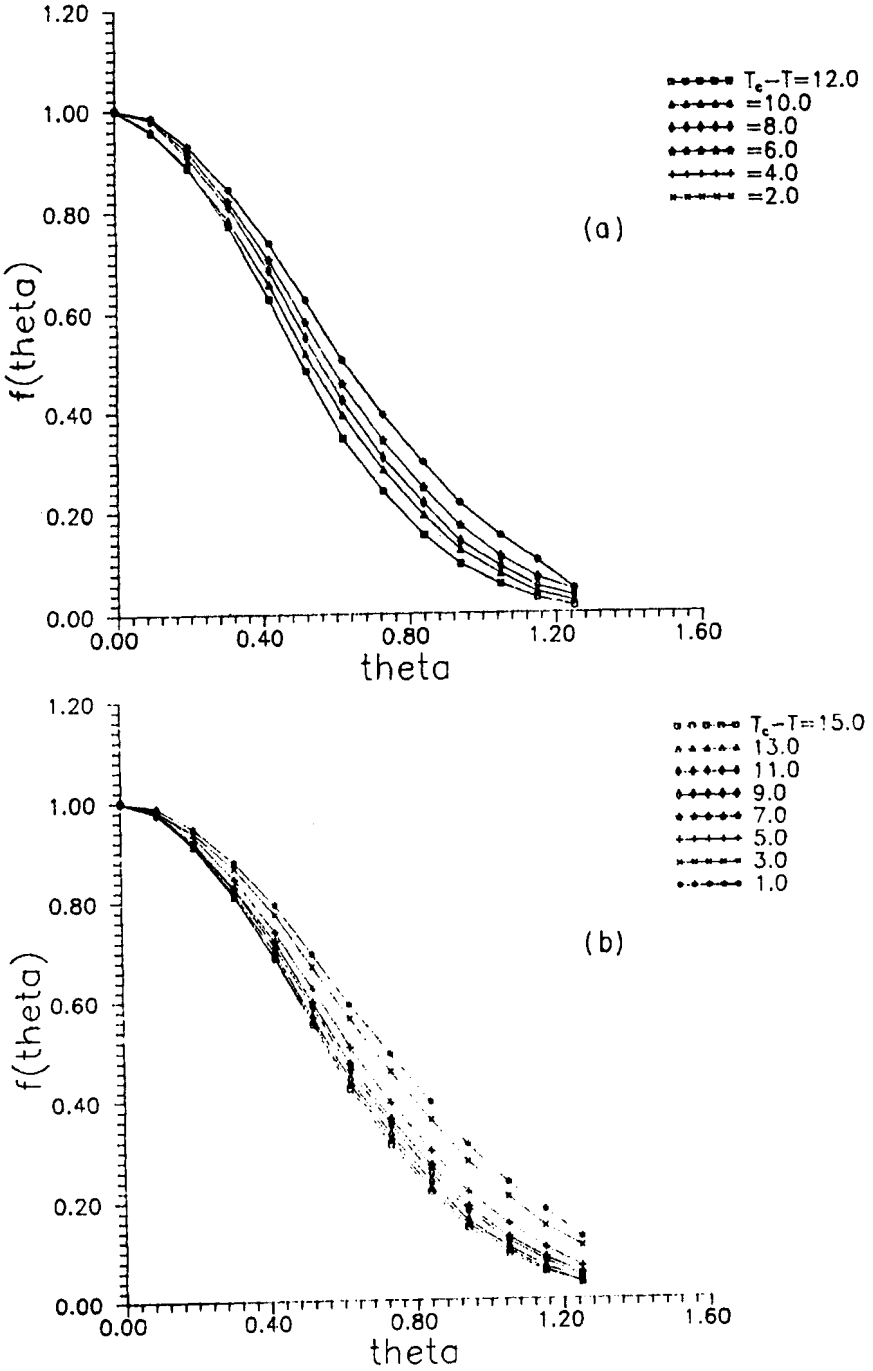


Figure 1. Distribution functions for OBA(a) and NBA(b).