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ABSTRACT

Orientational order parameter, S and effective geometry, α_g are calculated from the refractive index in three nematic room temperature liquid crystal mixtures, blOO3, blOO6, and blO38. The method due to Kuczynski et al. used to determine S from birefringence. The effective geometry parameter is $\alpha_g = n_o/n_e$. (n_o and n_e are the ordinary and extraordinary refractive indices of the liquid crystal material.) The behavior of α_g as a function of temperature and order parameter has also been reported. The S value calculated from α_g is identically equal to the value obtained from Kuczynski et al method, i.e., from birefringence, δn. Finally, dn_e/dT and dn_o/dT are obtained and the crossover temperatures, T_{CO} the characteristic temperature, which is in fact the temperature of minimum in the ordinary index of refraction in three mixtures for different wavelengths are calculated from dn_o/dT.

KEYWORDS

Effective geometry parameter; nematic room temperature LC mixtures; orientational order parameter; refractive indices; S; α_g

1. Introduction

The liquid crystal (LC) material possesses both the anisotropic and flow properties [1]. Therefore, these LCs can be very useful in applications such as displays, etc. [2]. Use of these materials in different applications depend on the properties these compounds posses. In order to use these LC materials in displays, one should know the properties of the compounds regarding the electrical and optical properties [2]. Hence, the knowledge of the refractive indices and in turn the birefringence, the order parameter, *S* and the dielectric constant are of great importance to decide the materials for the display technology and of course in the photonics.

The birefringence is influenced by the operating wavelength, the molecular structure, and the temperature. In literature, different theoretical models are developed showing the temperature and wavelength dependence of the birefringence. In this manuscript, the author presents the order parameter estimation from the macroscopic order parameter, *Q* from Kuczynski et al. method and how it represents the microscopic order parameter defined as $S = < 3\mathrm{Cos}^2\theta - 1 > /2$, where θ is the angle director and the long molecular axis in the case of Vuks isotropic model. Further, the effective geometry parameter is important to understand the light propagation in the LC compounds. Satiro et al. [3,4] used effective geometry parameter, $\alpha_g = n_o/n_e$ to explain from the geometrical properties the propagation of light near the disclamation lines. Light passing through these topological defects in LC compounds is

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deflected in a direction determined by the orientation of the director associated with such defects [5,6]. The degree of deflection depends on α_g and in turn it depends on the operating wavelength and temperature [6].

In the present study, three room temperature LC mixtures are chosen and they are blOO3, blOO6, and blO38. The refractive index of these compounds between 15°C and 55°C is taken from literature [7] and the analysis is carried out.

2. Theory involved

2.1. *Estimation of order parameter "S" from birefringence δn*

de Gennes et al. [8] pointed out the anisotropy of any physical quantity can be a measure of orientational order parameter. In the case of uniaxial LC, this parameter can be defined as

$$Q = \frac{\delta A}{\Delta A}, \tag{1}$$

where δA is the anisotropy of any arbitrary physical quantity $\Delta A = (A_{\parallel} - A_{\perp})$ and ΔA is the hypothetical anisotropy of A in the case of perfect order.

Kuczynski et al. [9,10] proposed a simple procedure for the determination of order parameter S from the birefringence measurements δn without considering the local field experienced by the molecule in a LC phase. The birefringence δn which is a function of temperature is fitted to the following equation:

$$\delta n = \Delta n \left(1 - \frac{T}{T*}\right)^{\beta}, \tag{2}$$

where T is the absolute temperature, $T*$ and β are constants. ($T*$ is about 1–4 K higher than the clearing temperature and the exponent β is close to 0.20.) This procedure enables one to extrapolate δn to the absolute zero temperature.

In practice, the three adjustable parameters $T*$, Δn and β were obtained by fitting the experimental data for δn to the following equation written in the logarithmic form

$$\log \delta n = \log \Delta n + \beta \log \left(\frac{T* - T}{T*}\right) \tag{3}$$

Thus, Q is given by

$$Q = \frac{\delta n}{\Delta n}. \tag{4}$$

Following the procedure of Kuczynski et al. [9,10], the author demonstrated that Q determined in this way describes well the nematic order parameter and is a good approximation of the order parameter S given by equation $S = 1/2 < (3\cos^2\theta - 1) >$, where θ is the angle between the long axis of the molecule and the director n. In general, the order parameter S, defined by Eq. (4), must not necessarily be identical with that defined through other tensorial properties and could be different from the order parameter S defined by the above equation. However, one can expect that within a given local field model, there should be a relation between macroscopic and microscopic order parameters and following Kuczynski et al. [9,10] the author also demonstrated it using the example of the Vuks model. Therefore $Q = S$.

The regression analysis is employed to get the best fit for the three parameters, viz., T^* or T_C, Δn and β and the values are given in Table 1 for the compounds studied. The log–log plots of $(1 - T^*/T)$ and δn are shown in the Figs. 1 and 2 for the compounds blOO3 and blO38 as

Table 1. Parameters for the best fit through linear regression for the equation $\log \delta n = \log \Delta n + \beta . \log \left(\frac{T* - T}{T*} \right)$

Compounds	Wavelength (nm)	T^*	T^*+	$\beta \pm 0.002$	Δn	R
blOO3	450	≤363.8	364.0	0.199	0.412	0.9951
	486	≤363.8	364.0	0.200	0.387	0.9999
	546	≤363.8	364.0	0.200	0.360	0.9999
	589	≤363.8	364.0	0.200	0.348	0.9999
	633	≤363.8	363.8	0.199	0.341	0.9997
	650	≤363.8	363.8	0.195	0.335	0.9998
blOO6	450	≤388.0	391.0	0.198	0.423	0.9972
	486	≤388.0	390.0	0.204	0.417	0.9991
	546	≤388.0	388.0	0.212	0.376	0.9990
	589	≤388.0	388.0	0.211	0.362	0.9996
	633	≤388.0	388.0	0.210	0.352	0.9998
	650	≤388.0	388.0	0.208	0.347	0.9991
blO38	450	≤367.0	367.0	0.197	0.438	0.9995
	486	≤367.0	367.0	0.197	0.401	0.9999
	546	≤367.0	367.0	0.194	0.369	0.9998
	589	≤367.0	367.0	0.199	0.359	0.9997
	633	≤367.0	367.0	0.197	0.348	0.9997
	650	≤367.0	367.0	0.196	0.343	0.9995

representative cases. The advantage of this method is that the S value can be obtained in other liquid crystalline phases like cholesterics and smectics also as no internal field is considered in evaluating the Δn, the birefringence in perfect order. From the study it is also observed that the clearing temperature of the compound can be estimated, if it is not known previously, from the β and regression coefficient, R. Kuczynski et al. [9,10] stated that β can be about 0.2 and regression coefficient can be as close as to 1.000. ($T*$ is about 0.001–4 K higher than the clearing temperature and the exponent β is close to 0.2.) Following this procedure, T^* can be obtained and the same procedure is adopted for the compounds and the clearing temperatures are about 90.8°C, 115.0°C, and 94.0°C, respectively. Table 1 gives the values that have been obtained through regression analysis for the three mixtures at different wavelengths. Figure 3 presents the value of δn at perfect order in the cases of the compound blO38 and the Fig. 4

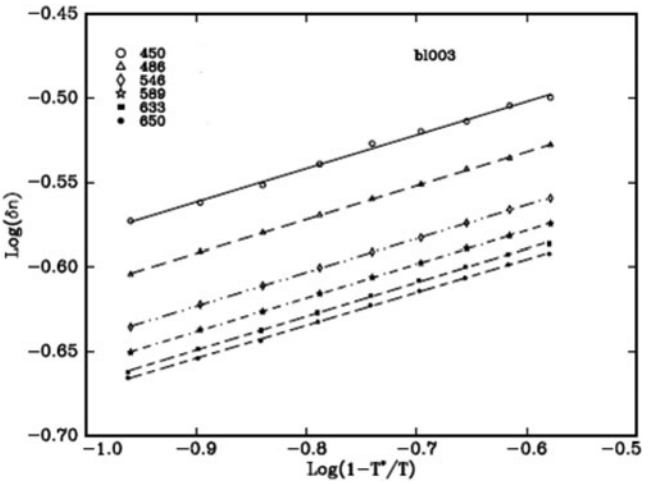

Figure 1. The log–log plot of birefringence δn versus reduced temperature for the blOO3 compound at different wavelengths (nm).

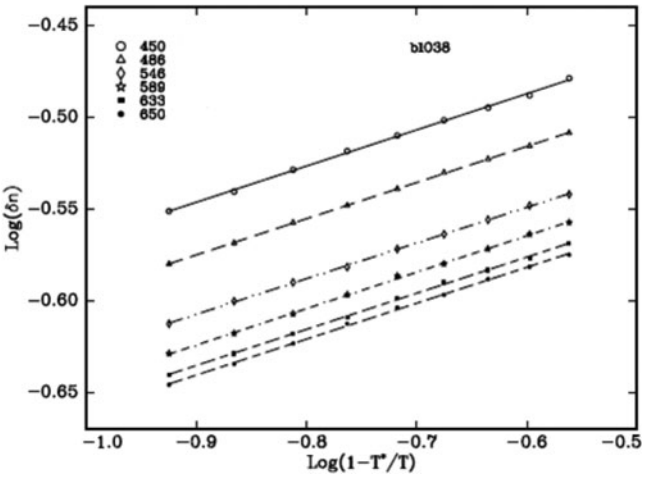

Figure 2. The log–log plot of birefringence δn versus reduced temperature for the blO38 compound at different wavelengths (nm).

shows the variation of δn with the temperature in the case of blO38. The Fig. 5 shows the variation of Δn estimated from regression analysis with the wavelength in the three mixtures.

Using equation (4) the order parameter, S is estimated for all the compounds and for different wave lengths. For the case of blOO3 is shown in Fig. 6 as representative one. This figure shows the order parameter, S is same within the experimental error for all the wavelengths for the compound. This is the case with the other two mixtures also.

However, one can expect that within a given local field model, there should be a relation between Q and S. It can be demonstrated by using the example of the Vuks model. The analysis and the relevant equations are given reference [8]. The author is not able to show here due to the non availability of the data in isotropic phase.

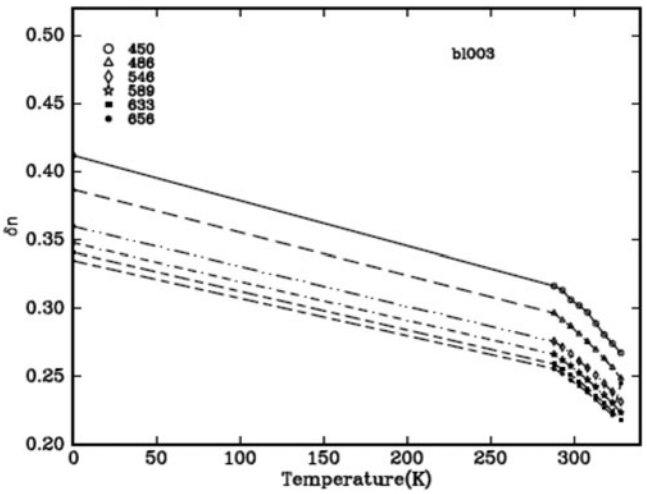

Figure 3. Variation of δn with temperature in blOO3 compound at different wavelengths (nm).

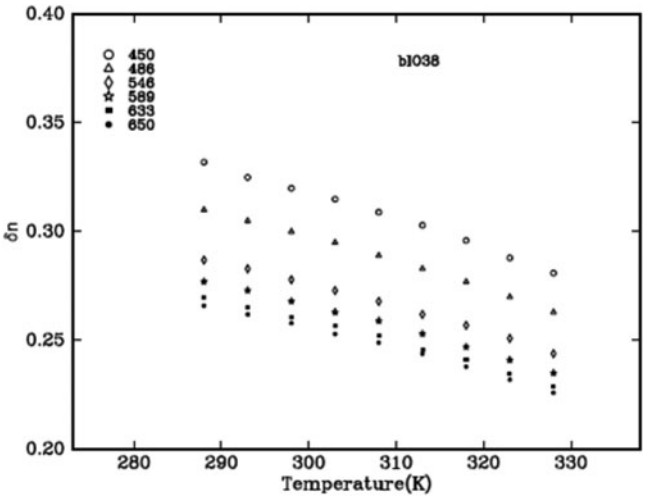

Figure 4. Variation of δn with temperature in blO38 compound at different wavelengths (nm).

2.2. *Estimation of S from α_g*

The equation for the determination of the order parameter S involving effective geometry parameter [11] $\alpha_g = n_o/n_e$ is given by

$$S = 3\sqrt{< n^2 > (1 - \alpha_g)}\ [2\alpha_g + 1]\ (\Delta n)_0, \tag{5}$$

where is the average refractive index obtained from the following equation

$$< n^2 > = 1/3(n_e^2 + 2n_o^2),$$

which slightly decreases linearly (the decrease is very small) with increase of temperature as follows:

$$\sqrt{< n^2 >} =< n >= C - DT. \tag{6}$$

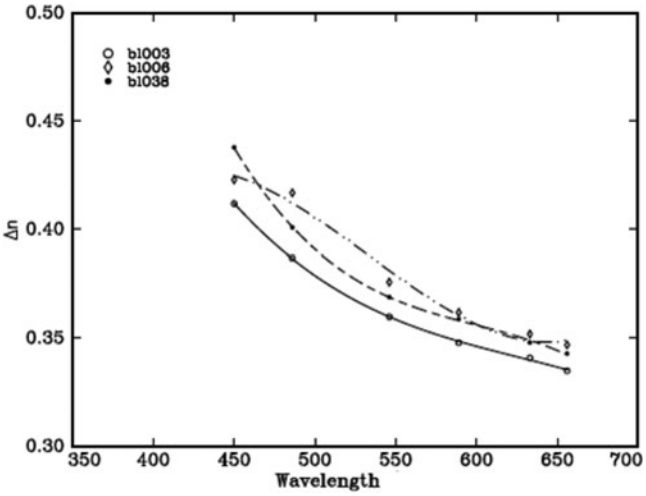

Figure 5. Variation of Δn estimated from regression analysis with the wavelength (nm) in the three mixtures.

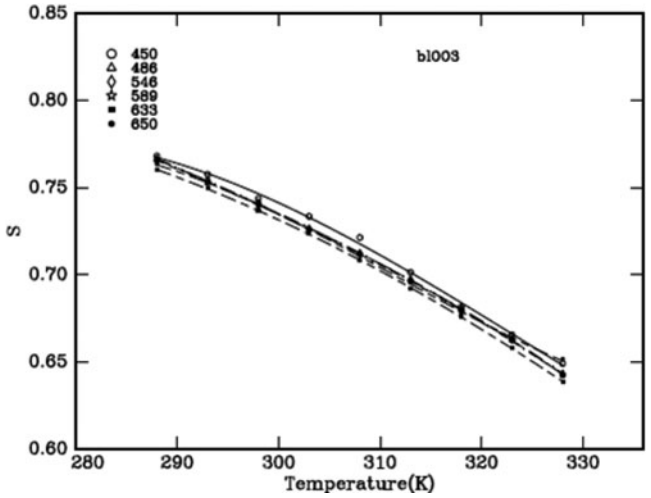

Figure 6. Variation of order parameter *S* with temperature in blOO3 compound at different wavelengths (nm)

The variation of order parameter with reduced temperature using Eq. (5) is exactly similar to that obtained by using the Eq. (4). The simplification of Eq. (5) gives rise to Eq. (4) only. Hence, no different plot is drawn using (5) for *S*. The values *C* and *D* are obtained by plotting the temperature and Square of average refractive index from above equation by linear regression. The values of *C* and *D* are given in Table 2 for the three LC mixtures at different wavelengths.

Variation of effective geometry, α_g with temperature is shown in Fig. 7 at the wavelength 589 (nm) for all the three mixtures. It is found that α_g slightly increases with temperature and approaches to unity at the clearing temperature. The next Fig. 8 shows the decreases of α_g with the increase of order parameter at the same wavelength for all the three mixtures.. When α_g reaches unity when there is no more ordering in LC and the corresponding temperature at this point ($\alpha_g = 1$) indicates the isotropic phase and it means it exhibits lower deflection of light [10]. This can be attributed to the lower orientation of the director field. Similar observations are made by Satiro et al. [4–6]. They investigated the temperature and the wavelength effect. They also studied the effect variation of the ratio on the deflection of light in some LCs. Recently, Sastry et al. [12] and Pisipati et al. [13] are also reported temperature variation of α_g.

Table 2. The vales of *C* and *D* obtained from Eq. (6).

	blOO3		blOO6		blO38	
Wavelength (nm)	*D*	*C*	*D*	*C*	*D*	*C*
450	− 0.00062	1.840	− 0.00051	1.823	− 0.00057	1.829
486	− 0.00055	1.803	− 0.00050	1.805	− 0.00055	1.809
546	− 0.00053	1.782	− 0.00048	1.779	− 0.00053	1.787
589	− 0.00052	1.771	− 0.00047	1.769	− 0.00052	1.775
633	− 0.00052	1.765	− 0.00047	1.761	− 0.00052	1.768
656	− 0.00048	1.751	− 0.00047	1.759	− 0.00051	1.764

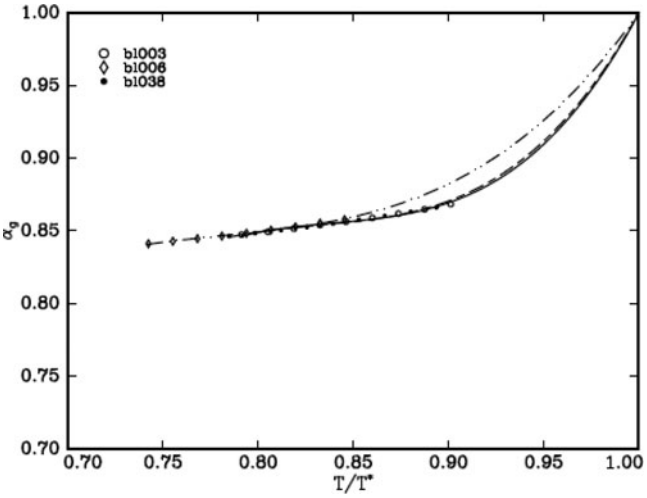

Figure 7. Variation of effective geometry parameter α_g with reduced temperature in blOO3, blOO6, and blO38 compounds.

2.3. *Crossover temperatures*

An aligned LC layer shows two refractive indices, viz., the ordinary (n_o) and extraordinary (n_e). Most of the LC compounds the temperature gradient of n_e is always negative while the temperature gradient of n_o could change from negative to positive depending on the LC material and the operating temperature. These guidelines can be utilized to prepare LC mixtures with large $\mathrm{d}n_o/\mathrm{d}T$ at room temperature. When $T \cong T^*$, $\mathrm{d}n_o/\mathrm{d}T$ jumps to a large positive value. However, in the intermediate stage there exists a cross over temperature, T_{CO}, where $\mathrm{d}n_o/\mathrm{d}T = 0$. The expression for T_{CO} is given as

$$T_{\mathrm{CO}} = T * [1 - \{3\mathrm{D}\, T * /(\beta \Delta n)\}^{1/(1-\beta)}]. \tag{7}$$

Using the Eq. (7) cross over temperatures, which is the temperature of minimum in the ordinary index for all the three mixtures for all the wavelengths are estimated and the Fig. 9

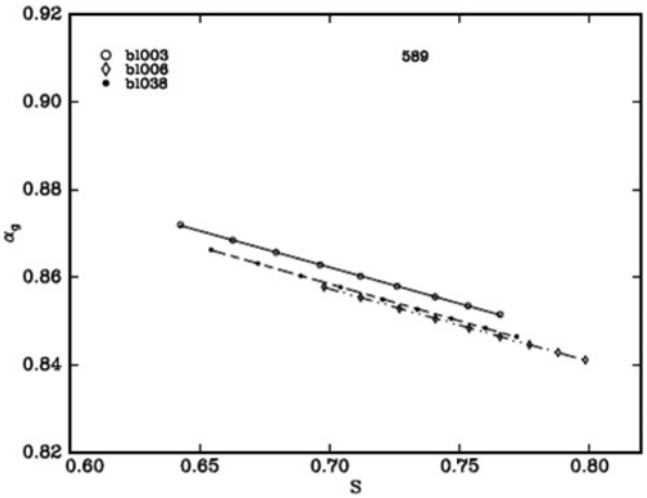

Figure 8. Variation of effective geometry parameter α_g with order parameter *S* in blOO3, blOO6, and blO38 compounds at 589 nm.

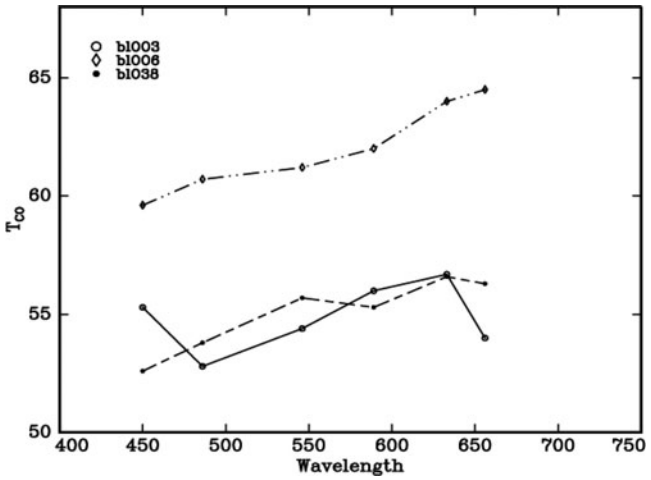

Figure 9. Variation of cross over temperature T_{CO} with different wavelengths (nm) in blOO3, blOO6, and blO38.

exhibits the variation of T_{CO} with the wavelength in all the mixtures. The figure reveals the T_{CO} shows some kind of even odd effect.

Conclusions

1. The order parameter estimated directly (without considering any field that the nematic molecule experiences) from birefringence, δn or from α_g is compared with each other. It is found that the equations used for the calculation of S either from birefringence, δn, or from the effective geometry parameter, α_g, are identically equal to one another.
2. The cross over temperature T_{CO} is found to be more in the case of blO38 than in the remaining two compounds and also the variation in this case is increasing order with the .variation of wavelength. The lower T_{CO} infers that the materials exhibit a strong light deflection.
3. Following the rule (T^* is about 1—4cK higher than the clearing temperature and the exponent β is close to 0.20) by Kuczynski et al. [9,10] the clearing temperatures in these three LC mixtures are predicted.
4. The order parameter, S is same within the experimental errors irrespective of the wavelength used.

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References

[1] Collings, P. J., & Hird, M. (1997). *Introduction to liquid crystals: Chemistry and physics*. Taylor & Francis: UK, London.
[2] Bahadur, B. (1984). *Mol. Cryst. Liq. Cryst.*, *109*, 3–93.

[3] Satiro, C., & Moraes, F. (2009). *Mol. Cryst. Liq. Cryst.*, *508*, 261–266.
[4] Satiro, C., & Moraes, F. (2005). *Mod. Phys Lett.*, *A20*, 2561–2565.
[5] Satiro, C., & Moraes, F. (2006). *Eur. Phys. J E.*, *20*, 173–178.
[6] Satiro, C., & Moraes, F. (2008). *Eur. Phys. J E.*, *25*, 425–429.
[7] Li, J., Bard, G., Lin, Y., Ren, H., & Wu, S. T. (2005). *J. SID.*, *13/12*, 1017–1026.
[8] de Gennes, P. G., & Prost, J. (1993). *The Physics of Liquid Crystals*, Oxford University Press: New York (NY).
[9] Zywucki, B. J., & Kuczynskim, W. (2001). *Dielectr Electr Insul, IEEE Trans.*, *8*, 512–515.
[10] Kuczynski, W., Zywucki, B., & Malecki, J. (2002). *Mol. Cryst. Liq. Cryst.*, *381*, 1–19.
[11] Sreehari Sastry, S., Vindhya Kumari, T., Mallika, K., Gowri Sankara Rao, B., Ha, S.-T., & Lakshminarayana, S. (2012). *Liq. Cryst.*, *39*, 295–301.
[12] Sreehari Sastry, S., Vindhya Kumari, T., Begum, S. S., & Rao, V. V. (2011). *Liq. Cryst.*, *38*, 277–285.
[13] Saraswati Devi, G., Datta Prasad, P. V., Madhavi Latha, D., & Pisipati, V. G. K. M. (2013). *Liq. Cryst.*, *40*, 1274–1281.