Jordan Journal of Physics

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Electro-Optical Parameters with Adverse Order of 10CB Liquid Crystal Molecules Studied under the Influence of an External High Electric Field: A Theoretical Approach

Shivani Chaudhary, Narinder Kumar, Pawan Singh, Khem B. Thapa and Devesh Kumar

Department of Physics, School of Physical & Decision Sciences, Babasaheb Bhimrao Ambedkar University, VidyaVihar, Raebareli Road, Lucknow (U.P.) 226025 INDIA.

<i>Doi:</i> https://doi.org/10.47011/14.1.8	
Received on: 18/02/2020;	Accepted on: 24/05/2020

Abstract: The 10CB liquid crystal (LC) at the higher electric field has a negative-order parameter. The 10CB LC has a definite order that maintains smectic phase stability. 10CB LC has supported the isotropic phase stability at an elevated external electric field and exhibited an unfavorable orientation of the order parameter. At the more upper electric field, the director angle (θ) fluctuated and contained θ less than 90°. The negative orientation of the order parameter responsible for the IR absorbance has increased instead of reduction. The 10CB liquid crystal is a member of the cyano biphenyl series; therefore, the dipolar strength is maximum contributed to by the C-H atom asymmetric stretching of the alkyl chain length. The 10CB LC has a large bandgap (3.60 eV).

Keywords: 10CB, Electric field, Electro-optical effect, Spectroscopy, Density functional theory (DFT).



Introduction

Liquid crystals are considered to lie in the mesomorphic phase. The properties of nematic liquid crystals have been widely studied by different research groups. The transitional properties of this compound depend on the length and parity of flexible spacers. It is also useful in optical communication, as it has a high value of molecular polarizability. In the fabrication of display devices, molecular polarizability plays a vital role as it reveals the

Corresponding Authors: Narinder Kumar and Devesh Kumar

action of light (EM wave) with liquid crystals [1-2]. The rod-like gold nanoparticles exhibit a negative orientation order parameter and the large absorption anisotropy enhanced the optical birefringence with a reversal of sign [3-4]. The rod-like negative ordered nematic liquid crystal exists in the parallel form with the 90° director angle [5-8]. Under the effect of the external electric field, the positive dipole liquids are perpendicular to the electric field and exhibit the maximum torque [9-10]. The order parameter of the nematic phase comes from the quenching of the director orientation at a very high electric field in the order of 10^8 V/m. The nanosecond switching under electrical modification of the order parameter affect the ultrafast electro-optic applications ranging from displays modulators, optical shutters, limiters, beam steerers and switches as the switchable optical retardance [11-12].

The structure of decyl cyano biphenyl contains a methyl group attached to the carbon chain, which gives rise to a stable smectic phase. It is used to calculate the surface temperature as different colors which are observed over a surface. This property is utilized in medical applications to detect skin cancer. After the discovery of pentyl cyano biphenyl by George William Gray, many attempts were made to synthesize similar homologous versions of this compound. Cyano group acts as a substituent in the aromatic ring and changes acidity in ground as well as excited states. Since the cyano group is an electron acceptor, the need for an aqueous solvent has also been eliminated. The homologous compound of cyano biphenyl is extensively used in electro-optical devices, as it is stable, gives the colorless intermediate phase at room temperature and has a positive value of dielectric anisotropy; one particular effect shown by these compounds is known as the odd-even effect [13]. It alters the physical properties of the compound, depending upon the number of carbon atoms. This odd-even effect is also studied with the help of molecular dynamics. Due to the peculiar nature in order and mobility at the microscopic and bulk levels, such compounds respond to stimuli very quickly [14-15].

The main keynote kept in mind while modeling these compounds is their configuration and corresponding to that particular configuration their ground-state energy. This ground-state energy helps in the interaction of these compounds with various other compounds. The relative energies are also useful in the calculation of thermodynamic properties, such as entropy, free energies, ... etc. The alkyl chain can be easily broken down or displaced, which gives rise to multi conformational changes [16-18]. The higher homologous compound shows a more planar structure as compared to the lower homologous one. This planar structure helps in the stacking of the compound, which leads to rigidity. Based on Homo Lumo analysis, 10CB liquid crystal has a higher value of bandgap, indicating that it has a low amount of conductivity. Also, it is highly complex due to the significant amount of dipole moment along the molecular axis. Based on these properties, cyano biphenyl is considered a suitable compound in the list of liquid crystals [19-21].

Computational Methodology

The 10CB molecules are optimized by the Gaussian 09 Software [22] with the help of the density functional theory (DFT) method B3LYP [23-24] by 6-31G** basis set [25]. After optimization, the electric field is applied to the 10CB liquid crystal compound along with the molecular axis (x-axis) and perpendicularth (yaxis). The range of the applied electric field is 0.000 a.u to 0.200 a.u at the interval of 0.0020 a.u., where 1 a.u=5.14 x 10^{11} V/m [26] or 1 a.u.= 6.5×10^{15} Hz. After electric field application, the molecular polarizability of the 10CB liquid crystal is calculated. The molecular polarizability along the x-axis is considered as extraordinary molecular polarizability (α_e) and along the y-axis, it is considered as ordinary molecular polarizability (α_0). The extraordinary molecular polarizability (α_e) and ordinary molecular polarizability (α_0) calculate the order parameter with the help of Equation 1. The finite-field approach framework predicts the total molecular energy under the impact of the electric field as given below:

$$E = E_o - \mu_i F_i - \frac{1}{2} \alpha_{ij} F_i F_j - \frac{1}{6} \beta_{ijk} F_i F_j F_k$$

where E_o is the total energy in the absence of the electric field and F_i , α_{ij} , μ_i and β_{ijk} are equivalent to the components of the electric field, polarizability, dipole moment, and first-order hyperpolarizability, where the respective directions are specified along with the subscripts i, j and k=x, y and z. The α , β , μ and molecular

anisotropy in polarizability ($\Delta \alpha$) can be expressed as numerical differentiation with an electric field of magnitude 0.002 a.u. The respective equations are given below [27-28]:

$$\alpha = \frac{1}{3} (\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$$

$$\beta = \left[(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{xxz} + \beta_{yyz})^2 \right]^{1/2}$$

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2}$$

$$\Delta \alpha = 2^{-1/2} \left[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 \right]^{1/2}$$

$$\Delta \widetilde{\alpha} = \alpha_{\rm e} - \alpha_{\rm o}$$

 $\Delta \widetilde{\alpha} = S \Delta \alpha$

where $\tilde{\alpha}$ is the mean isotropic polarizability.

Order parameter (S) is given as:

$$S = \frac{\alpha_e - \alpha_o}{\alpha_e + \alpha_o}.$$
 (1)

Director angle or magic angle (θ) is calculated as:

$$\theta = \cos^{-1} \left[\frac{\left(2S+1\right)}{3} \right] \tag{2}$$

Birefringence (Δn) is obtained as follows:

$$\alpha = \frac{2\alpha_0 + \alpha_e}{3}, \quad \gamma_e = \alpha + \frac{2(\alpha_e - \alpha_o)}{3S},$$

$$\begin{split} \gamma_{o} &= \alpha - \frac{(\alpha_{e} - \alpha_{o})}{3S} \\ n_{e} &= \\ & \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}} + \frac{(4\sqrt{10}/15)\pi NS(\gamma_{e} - \gamma_{o})}{1 - \frac{4\pi N\alpha}{3}} \\ n_{o} &= \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}} - \frac{(2\sqrt{10}/15)\pi NS(\gamma_{e} - \gamma_{o})}{1 - \frac{4\pi N\alpha}{3}} \\ \Delta n &= \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}} \end{split}$$
(3)

Results and Discussion

The 10CB LC expresses three phases under the influence of an electric field, as shown in Fig. 1: from 0.010 a.u. to 0.028 a.u. having the first phase of LC and the molecule is more stable in this range, from 0.034 a.u. to 0.052 a.u. 10CB LC expresses the second phase, where the molecule is less stable in comparison with the previous phase and from 0.056 a.u. to 0.072 a.u. represents the third phase, where the molecule is not stable for this range. Finally, the molecule is converted into the isotropic phase. The values 0.008 a.u., 0.032 a.u. and 0.054 a.u. reveal the phase transition field of 10CB. In the field of 0.074 a.u., the molecule finally gains the isotropic phase. The positive-order parameter of 10CB is 0.63 and the negative-order parameter is -0.40, as given in Fig. 1. In the field of 0.098 a.u. the molecule reveals a negative-order parameter. The maximum and minimum range of the order parameter for ordinary liquid crystal is from +0.8to -0.5.



FIG. 1. Order parameter of 10 CB LC under the influence of the electric field (The order parameter is calculated by the mathematical Equation 1. Molecular polarizabilities of 10CB LC are optimized with the help of DFT (B3LYP) methodology by Gaussian 09 software package).

The 10CB liquid crystal has an order parameter in the range between +0.8 and -0.5. At a higher electric field (0.098 a.u.), the molecule maintains the stability of the isotropic phase. After the field of 0.078 a.u., the molecule gains 0.00 order parameter and exhibits the isotropic phase. The C-H asymmetric stretching corresponds to IR absorbance in the benzene ring, an improvement for the odd member, and falls for the even member of the alkyl chain. The 10CB liquid crystal shows an even member of the cyano biphenyl series, where the IR absorbance has increased instead of a decrease; that is the reason for the negative-order parameter.

Liu *et al.* [29] reported that under the influence of an electric field, the bandgap of liquid crystals is controlled, which is used in tunable bandgap applications. The magic angle of liquid crystals is 54.74. The maximum value of the director angle is 75.09 and the minimum value of the director angle is 29.52, as shown in Fig. 2. The director angle (θ) is stable for the smectic A phase and with an expension of the

electric field, θ is finally stable for the isotropic phase. The director angle is related to the order parameter according to Eq. (2). Under the influence of the electric field, the bandgap decreases for the smectic A phase and the bandgap increases for the isotropic phase. For a positive-order parameter, the bandgap decreases, while the bandgap increases for a negative-order parameter.

Mitra et al. [30-31] utilized the molecular polarizability calculated by Vuks and Neugebauer's formula responsible for the order parameter, birefringence and refractive index. In the present work, we are using the modified formula of birefringence [28]. The order parameter is remarkably related to the director angle, where the director angle is easily calculated by the order parameter as given in Eq. (2). Liu et al. [3-4] reported a negative orientation order parameter and the large absorption anisotropy enhanced the optical birefringence with a reversal of sign, as shown in Fig. 3.



FIG. 2. Director angle of 10CB LC under the influence of an electric field. (The director angle is stable for the smectic and isotropic phases. The minimum director angle is 29.52 and the maximum director angle is 75.09. This means that the molecule of 10CB is not perfectly parallel to the electric field. At the angle of 90°, all the molecules are parallel to the electric field with negative order of the liquid crystal).



FIG. 3. Birefringence of 10CB LC under the effect of an electric field. (The maximum birefringence of 10CB LC is $\Delta n = 0.1197$ and the minimum birefringence is $\Delta n = -0.0960$. The birefringence is calculated with the help of Eq. (3), under the influence of an electric field).

Wood et al. [32] reported that the bandgap of nematic LC decreases under an applied electric field. Busch et al. [33] reported on inverse birefringent nematic LC used for photonic bandgap materials under the influence of an electric field. The dipole moment of 10CB liquid crystal is 6.09 Debye and the existing bandgap is 3.60eV, as shown in Fig 4. Due to the large bandgap of 10CB, the liquid crystal behaves as an insulator; therefore, insulating materials are used in the THz frequency range for better performance. The HOMO-LUMO bandgap is indicating the molecular stability of 10CB. The dipolar strength of 10CB LC is maximum contributed to by the asymmetric stretching of C-H atom of the alkyl chain length, as shown in Fig. 5.



FIG. 4. Bandgap of 10CB liquid crystal molecule calculated by DFT methodology (Red color indicates a negative charge and green color indicates a positive charge).



FIG. 5. Dipolar strength of 10CB liquid crystal measured by DFT methodology.

Conclusions

It has been found that the 10CB LC expresses a negative-order parameter with higher electric field. The C≡N atom stretching has decreased only in 10CB, which indicates the decrement of the order parameter. The HOMO 'Highest Occupied Molecular Orbital' and LUMO 'Lowest Unoccupied Molecular Orbital' gap increases for the negative-order parameter and decreases for the positive-order parameter. The director angle is related to the order parameter; if the order parameter is affected, then the director angle is also affected. The negative orientation of the order parameter with the large absorption anisotropy enhanced the optical birefringence with a reversal of sign. In 10CB LC, the IR absorbance has increased instead of a decrease, which is responsible for the negative-order parameter. The bandgap is affected under the influence of an electric field; so, liquid crystals are used in tunable bandgap applications. The 10CB liquid crystal is a member of the cyano biphenyl series; therefore, dipolar strength is maximum contributed to by the C-H atom asymmetric stretching of the alkyl chain length and 10CB LC has a large bandgap (3.60 eV). The order parameter affects the ultrafast electro-optic applications ranging from displays to modulators, optical shutters, limiters, beam steerers and switches as the switchable optical filter. The 10 CB liquid crystal is also suitable for terahertz applications, because it has negative birefringence at higher electric fields.

Acknowledgments

Narinder Kumar is thankful to the University Grants Commission (UGC) New Delhi for providing fellowship (RGNF) for this work. We are very grateful to Dr. Anoop Ayyappan (IIT KGP, WB) for delivering computational help for this work. Mr. Pawan Singh and Shivani Chaudhary are thankful to UGC for providing a non-net fellowship.

Electro-Optical Parameters with Adverse Order of 10CB Liquid Crystal Molecules Studied under the Influence of an
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Supportive	Information	f ACD	
TABLE ST	1. Molecular specti	Coscopy of 4CB	T 0 1 1 1
S. No.	Frequency (cm ⁻)	Vibrations of 4CB	Intrared absorbance
l.	567	C-H atom wagging	14.4115
2.	841	C-H atom wagging	32.7990
3.	1017	C-C symmetric scissoring in the benzene ring	10.6536
4.	1431	Stretching in C-H atom	10.6063
5.	1531	H atom rocking in both benzene rings	47.1805
6. 7	1646	H atom rocking in both benzene rings	/5.5904
/.	2266	C II atom stretching	00.03/4 40.0012
ð. 0	3029	C-H symmetric stretching in the alkyl chain	49.9012
9. 10	3098	C-H asymmetric stretching in the alkyl chain	50.5/2/ 18.0204
$\frac{10}{T \Lambda DI E ST}$	2 Molecular spects	C-H asymmetric stretching in the benzene ring	18.9294
IADLE SI	2. Wolecular speci	Vibratiana of 5CD	Infranced absorbance
5. INO.	Frequency (cm)	C Heterson Sch	Intrared absorbance
1.	269	C-H atom wagging	14.2007
2.	843	C-H atom wagging	38.8040
3. 4	101/	U store as shing in both handon sin as	11.3/04
4.	1531	H atom rocking in both benzene rings	4/./280
5.	1646	H atom rocking in both benzene rings	//.6846
6.	2266	C≡N atom stretching	66.6334
7.	3026	C-H symmetric stretching in the alkyl chain	51.4412
8.	3096	C-H asymmetric stretching in the alkyl chain	60.4378
9.	3184	C-H asymmetric stretching in the benzene ring	19.0613
TA <u>BLE ST</u>	3. Molecular spect	roscopy of 6CB	
S. No.	Frequency (cm ⁻¹)	Vibrations of 6CB	Infrared absorbance
1.	569	C-H atom wagging	14.3463
2.	845	C-H atom wagging	32.6777
3.	1017	C-C symmetric scissoring in the benzene ring	11.5199
4.	1531	H atom rocking in both benzene rings	48.4753
5.	1646	H atom rocking in both benzene rings	78.8627
6.	2266	C≡N atom stretching	66.9738
7.	3027	C-H symmetric stretching in the alkyl chain	69.0056
8.	3096	C-H asymmetric stretching in the alkyl chain	60.9689
9.	3184	C-H asymmetric stretching in the benzene ring	18.6464
TABLE ST	4. Molecular spectr	coscopy of 7CB	
S. No.	Frequency (cm ⁻¹)	Vibrations of 7CB	Infrared absorbance
1.	569	C-H atom wagging	14.4318
2.	844	C-H atom wagging	30.2113
3.	1017	C-C symmetric scissoring in the benzene ring	11.9051
4.	1531	H atom rocking in both benzene rings	48.7830
5.	1646	H atom rocking in both benzene rings	79.8968
6.	2266	C≡N atom stretching	67.2729
7.	3027	C-H symmetric stretching in the alkyl chain	52.4092
8.	3076	C-H asymmetric stretching in the alkyl chain	78.0385
9.	3184	C-H asymmetric stretching in the benzene ring	18.7277
TABLE ST	5. Molecular spectr	coscopy of 8CB	
S. No.	Frequency (cm ⁻¹)	Vibrations of 8CB	Infrared absorbance
1.	570	C-H atom wagging	14.0818
2.	844	C-H atom wagging	32.6066
3.	1017	C-C symmetric scissoring in the benzene ring	11.3718
4.	1531	H atom rocking in both benzene rings	49.1511
5.	1646	H atom rocking in both benzene rings	80.3690
6.	2266	C≡N atom stretching	67.4233
7.	3027	C-H symmetric stretching in the alkyl chain	68.0403
8.	3076	C-H asymmetric stretching in the alkyl chain	84.3813
9.	3184	C-H asymmetric stretching in the benzene ring	18.7214

TABLE ST6. Molecular spectroscopy of 9CB					
S. No.	Frequency (cm ⁻¹)	Vibrations of 9CB	Infrared absorbance		
1.	570	C-H atom wagging	14.1481		
2.	844	C-H atom wagging	32.2473		
3.	1017	C-C symmetric scissoring in the benzene ring	12.0875		
4.	1531	H atom rocking in both benzene rings	49.3004		
5.	1647	H atom rocking in both benzene rings	80.8472		
6.	2266	C≡N atom stretching	67.5816		
7.	3027	C-H symmetric stretching in the alkyl chain	103.2722		
8.	3064	C-H asymmetric stretching in the alkyl chain	107.3792		
9.	3184	C-H asymmetric stretching in the benzene ring	18.9479		
TABLE ST7	7. Molecular spectr	oscopy of 10CB			
S. No.	Frequency (cm ⁻¹)	Vibrations of 10CB	Infrared absorbance		
1.	570	C-H atom wagging	14.1221		
2.	844	C-H atom wagging	32.1331		
3.	1017	C-C symmetric scissoring in the benzene ring	11.3436		
4.	1532	H atom rocking in both benzene rings	49.3276		
5.	1646	H atom rocking in both benzene rings	80.9406		
6.	2265	C-N atom stretching	67.6449		
7.	3026	C-H symmetric stretching in the alkyl chain	72.6780		
8.	3064	C-H asymmetric stretching in the alkyl chain	135.1362		
9.	3184	C-H asymmetric stretching in the benzene ring	19.6324		
TABLE ST8	3. Molecular spectr	oscopy of 11CB			
S. No.	Frequency (cm ⁻¹)	Vibrations of 11CB	Infrared absorbance		
1.	570	C-H atom wagging	14.2334		
2.	844	C-H atom wagging	31.6043		
3.	1017	C-C symmetric scissoring in the benzene ring	9.3491		
4.	1531	H atom rocking in both benzene rings	49.5608		
5.	1646	H atom rocking in both benzene rings	81.3196		
6.	2266	C≡N atom stretching	67.7372		
7.	3027	C-H symmetric stretching in the alkyl chain	109.3245		
8.	3065	C-H asymmetric stretching in the alkyl chain	163.9189		
9.	3184	C-H asymmetric stretching in the benzene ring	19.8023		
TABLE ST9. Molecular spectroscopy of 12CB					
S. No.	Frequency (cm ⁻¹)	Vibrations of 12CB	Infrared absorbance		
1.	570	C-H atom wagging	14.2432		
2.	844	C-H atom wagging	31.5740		
3.	1017	C-C symmetric scissoring in the benzene ring	11.6812		
4.	1531	H atom rocking in both benzene rings	49.64089		
5.	1646	H atom rocking in both benzene rings	81.4398		
6.	2266	C≡N atom stretching	67.7678		
7.	3027	C-H symmetric stretching in the alkyl chain	96.2863		
8.	3065	C-H asymmetric stretching in the alkyl chain	193.9285		
9.	3184	C-H asymmetric stretching in the benzene ring	20.5369		

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