

Odd-Even Effect Observed in the Electro-Optical Properties of the Homologous Series of HnCBP Liquid Crystal Studied under the Impact of the Electric Field: A Theoretical Approach

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ABSTRACT

The liquid crystal (LC) 4-4'-disubstituted biphenyls (HnCBP) of the general line formula $\text{HO}-(\text{C}_n\text{H}_{2n+1})-\text{O}-\text{C}_6\text{H}_4-\text{C}_6\text{H}_4-\text{CN}$ ($n=1-12$) shows the odd-even effect under the applied electric field. The odd-even effects are observed in the HOMO-LUMO gap, birefringence, order parameter, and dipole moment. The odd carbon atom number of the alkyl chain shows HOMO-LUMO gap, birefringence, and order parameter in the upward direction, and even the carbon atom number of the alkyl chain shows in the downward direction; however, the dipole moment exhibits a shift of even carbon number of alkyl chain in the upward direction and odd carbon number of alkyl chain in the downward direction.

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1. INTRODUCTION

Most of the liquid crystals having a rod-like structure and contains one or more benzene rings. The dihedral angle betwixt the two benzene rings expresses the odd-even effect in LC parameters. The odd values of the carbon number of the alkyl chain show a higher perspective as compared to the even carbon number of the alkyl chain in the HnCBP Liquid Crystal [1–8]. The strong dipole-dipole interaction exhibits the crystalline phase and has higher thermal stability. The higher thermal stability of liquid crystal indicates a higher melting point and also presents the position of smectic liquid crystal. The intermolecular distance (Å) from H7CBP- H11CBP shows the odd-even effects.

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The intermolecular distance of odd (H7CBP, H9CBP, H11CBP) carbon atom number dimer is higher while the intermolecular distance between the even (H8CBP, H10CBP) carbon atom number dimer is lower. The intermolecular hydrogen bond length exhibits the odd-even effect. The odd (H7CBP, H9CBP, H11CBP) liquid crystal has a smaller bond length as a comparison with the even ((H8CBP, H10CBP) liquid crystal [9–11]. The dihedral angle betwixt the two phenyl rings changing during the alkyl chain increasing in the tail of the HnCBP liquid crystal. The entropy of the molecule increases with the alkyl chain of the HnCBP liquid crystal molecule. The strong dipolar interactions are present in H7CBP, H9CBP and H11CBP. While all the antiparallel conformation of HnCBP exhibits strong interactions, and they also exhibit higher thermal stability for the crystalline phase [9,12–15]. The transition temperature of HnCBP liquid crystals from the crystal to the Nematic phase shows the odd-even effect. The even numbers of alkyl chains exhibit a more crystalline state and require a higher temperature to reach the nematic phase from the crystalline state [11,16–18]. The odd number of alkyl chains represents the less crystal phase in comparison with the even number of alkyl chains in the HnCBP mesogen. The odd-even effects observed in the transition temperature of isotropic to the nematic phase. The H3CBP-H5CBP is crystalline, but H7CBP-H11CBP is crystalline in an isomorphic layer structure [9–11,19].

2. METHODOLOGY

All the molecules are optimized by the NWChem software package [20] with the help of the Density functional theory (DFT) method with B3LYP [21–22] and 6-31G basis set [23]. After the optimization of all the molecules, we have applied the electric field to the HnCBP liquid crystals along the molecular axis (x-axis) and perpendicular (y-axis) to it from 0.0000 (a.u.) to 0.2000 (a.u.) at an interval of 0.0020 (a.u.) where 1 a.u.=5.14 x 10¹¹ V/m [24] or 1 a.u.= 6.5 x 10¹² Hz. After the applied electric field, we have calculated the molecular polarizabilities of the HnCBP liquid crystal molecules. The x-axis is considered extraordinary molecular polarizability (α_e), and the y-axis is considered ordinary molecular polarizabilities (α_o). With the help of extraordinary molecular (α_e) and ordinary molecular polarizabilities (α_o), we have calculated the order parameter, magic angle, refractive index, and birefringence as per the equations are given below [25–27]:

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

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

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

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

$$\tilde{\alpha} = \alpha_e - \alpha_o, \Delta\tilde{\alpha} = S\Delta\alpha.$$

Order Parameter (S):

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

Birefringence (Δn):

$$\Delta n = \frac{(\alpha_e - \alpha_o)}{6.3631} \left[R^3 - \left(\frac{2\alpha_o + \alpha_e}{20.244} \right) \right]^{-1}, \quad (2)$$

where R is the radius of the liquid crystal molecule.

Magic angle (θ):

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

Refractive index (n):

$$\begin{aligned} \alpha &= \frac{2\alpha_o + \alpha_e}{3}, \gamma_e = \alpha + \frac{2(\alpha_e - \alpha_o)}{3S}, \gamma_o = \alpha - \frac{(\alpha_e - \alpha_o)}{3S}, \\ n_e &= \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}} + \frac{(4\sqrt{10}/15)\pi NS(\gamma_e - \gamma_o)}{1 - \frac{4\pi N\alpha}{3}}, \\ n_o &= \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}} - \frac{(2\sqrt{10}/15)\pi NS(\gamma_e - \gamma_o)}{1 - \frac{4\pi N\alpha}{3}}, \\ n &= \frac{7}{2\sqrt{10}} + \frac{(2\sqrt{10}/5)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}}, \end{aligned} \quad (4)$$

where N is the number of liquid crystal molecule.

3. RESULT AND DISCUSSION

The birefringence and the order parameter exhibit the odd-even effect, but the refractive index does not express any odd-even effect. The odd-even effects are observed in the crystalline to a nematic phase transition temperature and nematic to Isotropic phase transition temperature [16] shown in Figure 2. The HOMO-LUMO gap and the Dipole Moment express the odd-even effect with the alkyl chain length increased of the HnCB LC. The order parameter and the refractive index are observed to continuously grow with the alkyl chain of HnCBP liquid crystal because C-C stretching IR absorbance in the benzene ring continually increases. The birefringence and the order parameter are inversely related to each other, shown in Figure 7. The range of Director Angle and the Refractive Index has shown in Table 1 and Table 2. Figure 1 represents the optimized geometry of HnCBP LC. Director Angle represents the maximum range of the order for the H9CBP LC shown in Figure 11.

3.1 TRANSITION TEMPERATURE FROM CR-N AND N-ISO

The odd-even effect observed in the crystalline to nematic phase and nematic to isotropic phase transition temperature shown in Figure 2. Zugenmaier et al. [9] reported that LC's higher thermal stability indicates a higher melting point in the present work; even the carbon atom number of alkyl chain shows a higher melting point. The transition

temperature increases for the even carbon atom number and decreases for the odd carbon atom number due to the IR absorbance generated by C-H symmetric stretching in the tail of the alkyl chain length. The IR absorbance increases for the even carbon atom number and decreases for the odd carbon atom number; that is the reason the transition temperature increases for even carbon atom number and falls for odd carbon atom number.

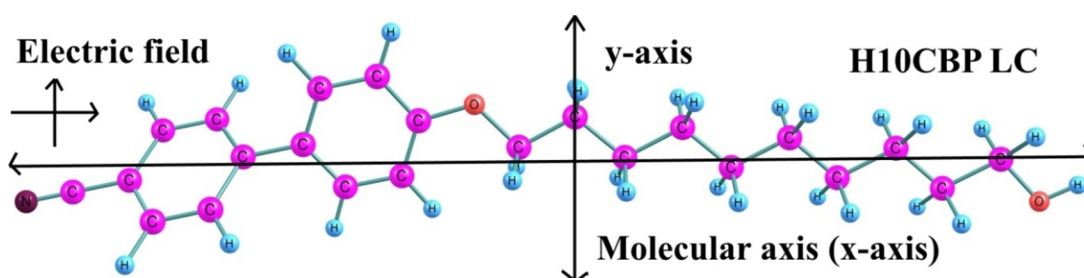


Figure 1. Optimized geometry of HnCBP LC.

3.2 REFRACTIVE INDEX

The refractive index was calculated with the help of equation 4. The refractive index increases continuously with the alkyl chain of the HnCBP LC molecule. The H6CBP expresses the even carbon atom number of the alkyl chain, while H11CBP expresses the odd carbon atom number of the alkyl chain. The refractive index decreases the H6CBP and H11CBP because C-O stretching, C-C stretching, O-H stretching, C-N stretching, and symmetric stretching of C-H atom in the tail of HnCBP LC are responsible. The C-O stretching (oxygen terminal atom- carbon atom of alkyl tail) shows high absorbance for H6CBP and H11CBP LC at the frequency of 1073 cm^{-1} , which is the reason for the decrement of refractive index. The stretching frequency continually increases with increases in the carbon atoms of alkyl chain length, but it will decrease in H11CBP. The C-O stretching (oxygen terminal atom- carbon atom of benzene) shows high absorbance for H6CBP liquid crystal at the frequency of 1298 cm^{-1} . The C-N and C-C IR absorbance continually increase with increases the carbon atoms of alkyl chain length, but it will decrease in H11CBP at the frequency of 2340 cm^{-1} and 1657 cm^{-1} . The C-C stretching frequency observed very high in H11CBP as a comparison with the complete series of HnCBP. The O-H stretching shows the higher frequency for the odd carbon atom number of an alkyl chain; however, it shows the lower frequency for even carbon atom number of the alkyl chain. The O-H stretching decrease in H11CBP at the frequency of 3828 cm^{-1} and the IR absorbance continually decreases in the HnCBP liquid crystal series. The refractive index of HnCBP ($n=1,2,3$.12) shown in Figure 3. From H1CBP to H3CBP, the

liquid crystal molecules are not stable, but H4CBP to H12CBP liquid crystal molecules are more stable. From H4CBP to H12CBP, the molecules have a nematic phase.

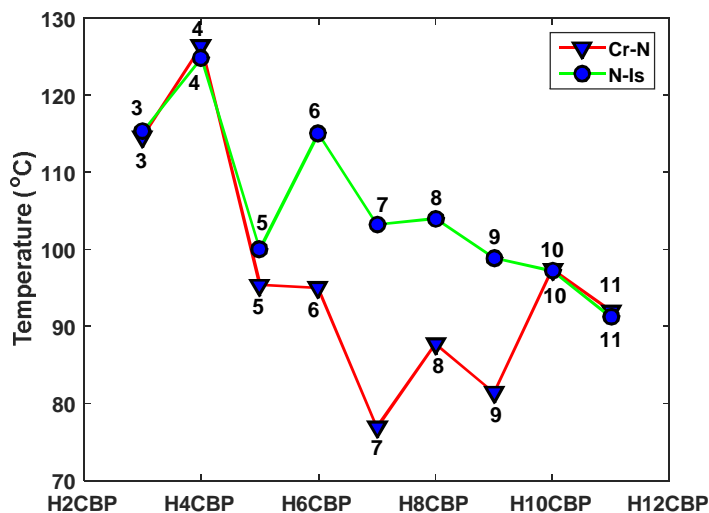


Figure 2. Transition temperature From Cr-N and N-Is HnCBP LC [16] (extension of alkyl chain length under the impact of temperature).

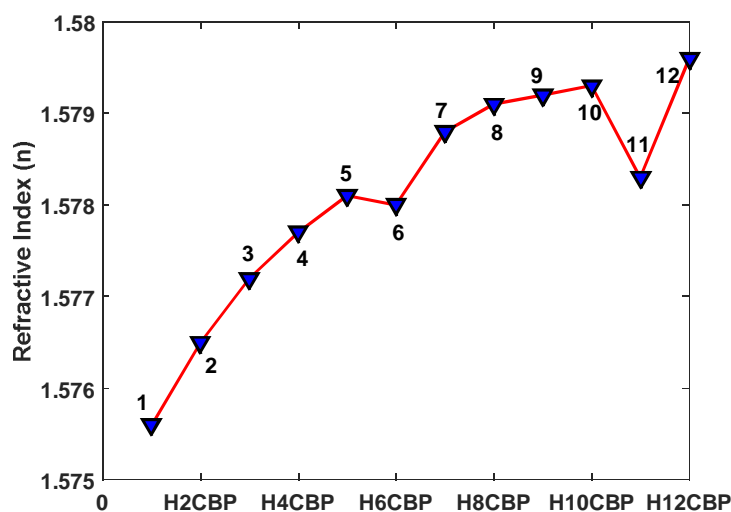


Figure 3. Refractive index of HnCBP LC (extension of alkyl chain length under the impact of electric field, calculated by DFT methodology).

3.3 ORDER PARAMETER

The order parameter was calculated with the help of equation 1. The order parameter exhibits the odd-even effect as shown in Figure 5. Lalanne et al. and Capar et al. reported

the odd carbon atom number has a higher perspective, and even carbon atom number has a lower perspective in this work; also, odd perspective is higher, and even perspective is lower [6–8]. The O-H and C-H symmetric stretching is responsible for the odd-even effect in HnCBP liquid crystal. The O-H stretching shows a higher-order parameter for odd carbon atom number; however, O-H stretching shows a lower-order parameter for even the carbon atom number of the alkyl chain. The C-H symmetric stretching shows higher IR absorbance for the even carbon atom, while C-H symmetric stretching shows lower IR absorbance for the odd carbon atom number of the alkyl chain. The odd carbon atom number of the alkyl chain expresses the higher value of the order parameter, and even the carbon atom number of the alkyl chain shows the lower value of the order parameter. The Order parameter from H1CBP to H4CBP does not indicate any odd-even effect, but after H5CBP to H12BP, the molecule perfectly shows the odd-even effect. The range of the Order parameter for the liquid crystal molecule is 0.3 to 0.8. The HnCBP also have a range of order parameter from 0.3 to 0.7 as shown in Figure 4. The H5CBP and H6CBP have approximate the same order parameter (0.60). The H7CBP and H8CBP have the same order parameter (0.64). The H9CBP and H10CBP have the same order parameter (0.69).

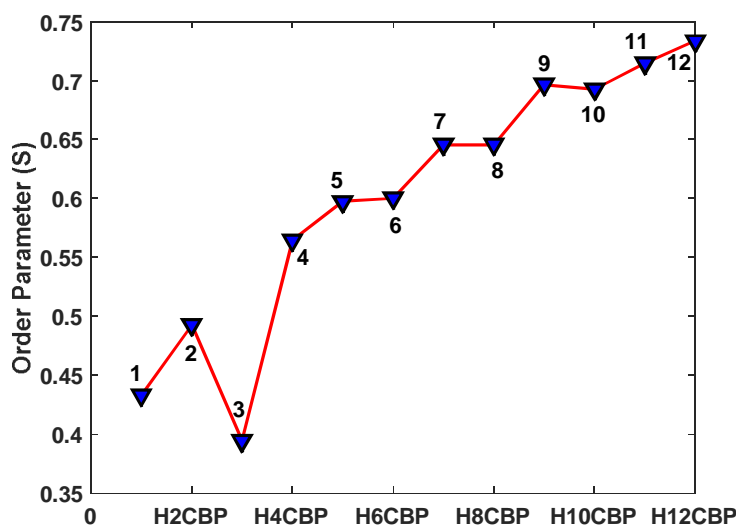


Figure 4. Order Parameter of HnCBP LC (extension of alkyl chain length under the impact of the electric field).

The birefringence was calculated with the help of equation 2. The birefringence decreases continuously with increasing alkyl chain, as shown in Figure 5. The birefringence also exhibits the odd-even effect. During the alkyl chain length increment, the molecule's viscosity increases; hence, the birefringence decreases. From H1CBP to H4CBP, molecules

do not exhibit any odd-even effect. After H5CBP, the molecules express the perfectly odd-even effect shown in Figure 5. The birefringence increases for the odd carbon atom number and decreases for the even carbon atom number because O-H stretching frequency increases for the odd carbon atom number and falls for the even carbon atom number.

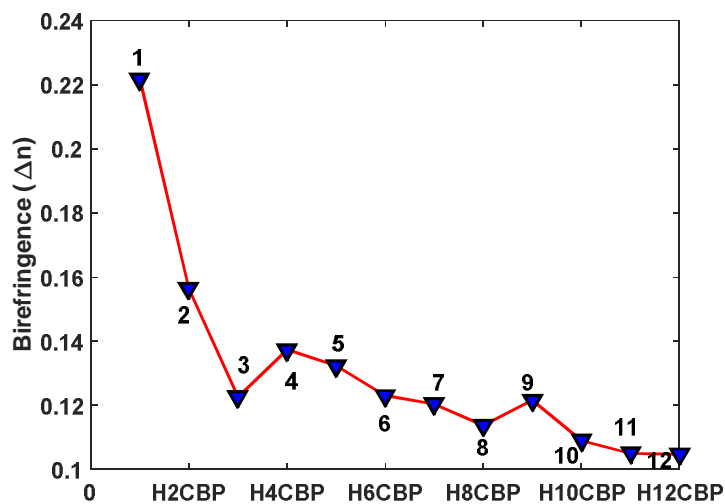


Figure 5. Birefringence of HnCBP LC (extension of alkyl chain length under the impact of electric field).

3.5 MAGIC ANGLE (θ)

The magic angle was calculated with the help of equation no. 3. The magic angle of liquid crystal molecules is 54.74° , which remains constant for the homologous series of HnCBP LC shown in Figure 6. The theoretically calculated Magic angle perfectly matched with the experimentally derived Magic angle. Table 1. represents the range of director angle (θ).

3.6 BIREFRINGENCE VERSUS ORDER PARAMETER

Birefringence and order parameters are inversely related to each other of the series of HnCBP LC molecules, as shown in Figure 7. The O-H wagging frequency in the tail of H5CBP and H6CBP continually increases, so that is the reason they are vertically aligned; the second reason is they are having the same order parameter (0.60) shown in the Figure 3. The O-H wagging frequency in the tail of H7CBP and H8CBP continually decreases, so that is the reason they are vertically aligned; the second reason is they are having the same order parameter (0.64). The O-H wagging frequency in the tail of H9CBP and H10CBP continually increases, so that is the reason they are vertically aligned; the second reason is they are having the same order parameter (0.69). The O-H atom wagging frequency decrease for H11CBP and Increase in H12CBP because they have different order

parameter, and the second reason is the refractive index decreases in H11CBP and increases in H12CBP aligned horizontally.

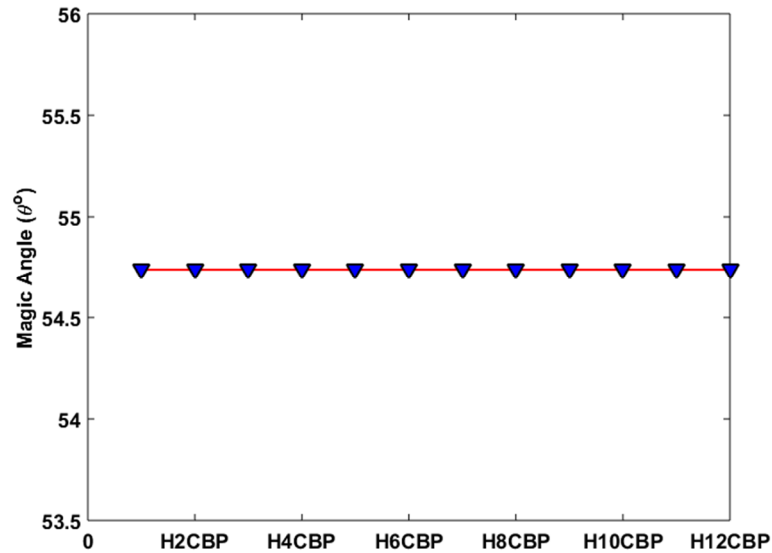


Figure 6. Birefringence of HnCBP LC (extension of alkyl chain length under the impact of electric field along the X-axis and Y-axis).

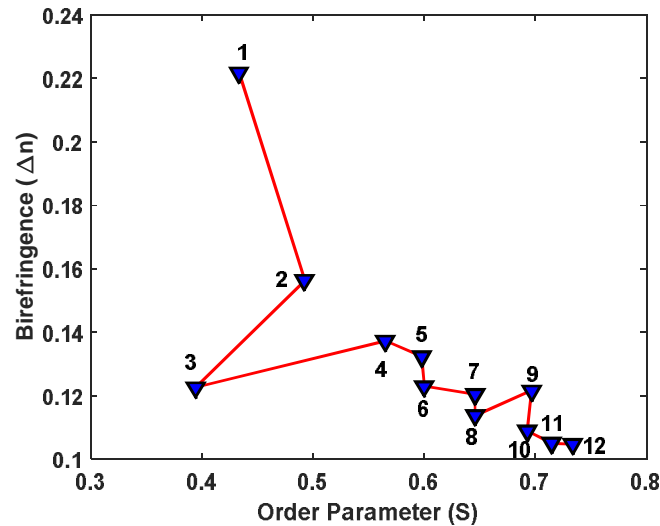


Figure 7. Birefringence versus Order Parameter of HnCBP LC (Under the impact of an electric field).

3.7 IONIZATION POTENTIAL

The ionization potential decreases continuously with an increase in the HnCBP liquid crystal molecule's alkyl chain, as shown in Figure 8. The H1CBP and H2CBP molecules

have higher ionization potential because these molecules have the mostly crystalline state. The relative reactivity of the liquid crystal increases with a decrease in ionization potential. H12CBP is more reactive as compared with H1CBP liquid crystal.

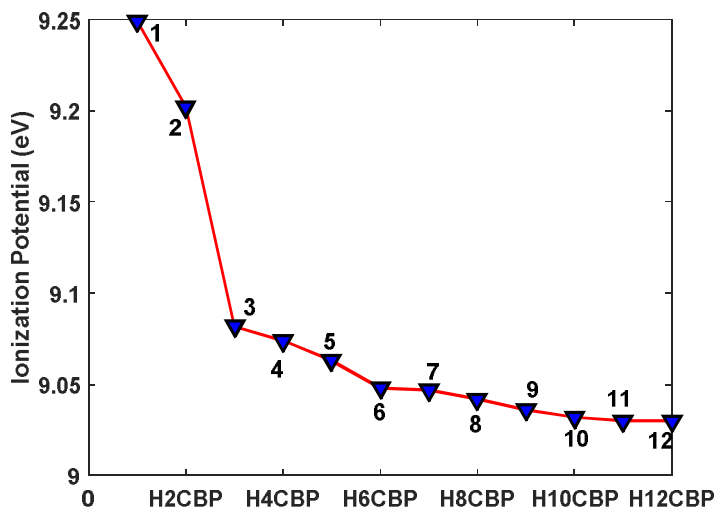


Figure 8. Ionization potential of HnCBP LC (extension of alkyl chain length optimized by DFT methodology).

3.8 DIPOLE MOMENT

The dipole moment exhibits the perfectly odd-even effect. The dipole moment presents a shift of even carbon number of alkyl chain in the upward direction and odd carbon number of alkyl chain in the downward direction because C-H symmetric stretching IR absorbance increases in the even carbon atom of alkyl chain and IR absorbance decreases in the odd carbon atom of alkyl chain length. H1CBP to H3CBP liquid crystals does not express a perfect odd-even effect, but H4CBP to H12CBP liquid crystals reveal the perfectly odd-even effect shown in Figure 9. The dipole moment values predict the shape of liquid crystal molecule; based on this result, we can predict that during the increment of the alkyl chain, the HnCBP liquid crystal molecule changes its own shape and size.

3.9 HOMO-LUMO GAP

The HOMO-LUMO gap expresses a little odd-even effect. The HOMO-LUMO bandgap decreases continuously with the alkyl chain of the HnCBP liquid crystal molecules. The H3CBP and H10CBP exhibit the lowest HOMO-LUMO Gap because C-C stretching generates the lowest frequency. The O-H wagging in the tail of H10CBP shows the highest frequency of 279.85 cm^{-1} compared to all the series of HnCBP that is the reason it will decrease. The H3CBP LC is having the second highest frequency, so that it is falling.

H1CBP to H4CBP liquid crystals does not express any odd-even effect, but H5CBP to H12CBP liquid crystals reveal a perfectly odd-even effect, as shown in Figure 10.

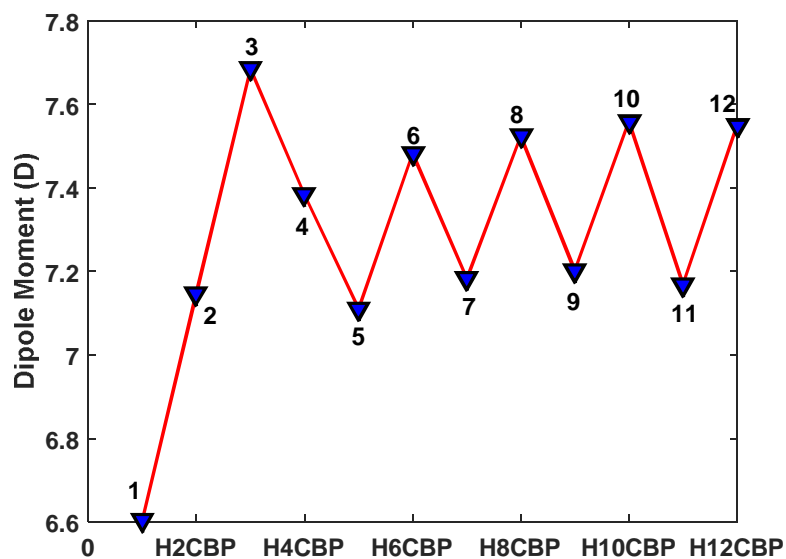


Figure 9. Dipole Moment of HnCBP LC (extension of alkyl chain length optimized by DFT methodology).

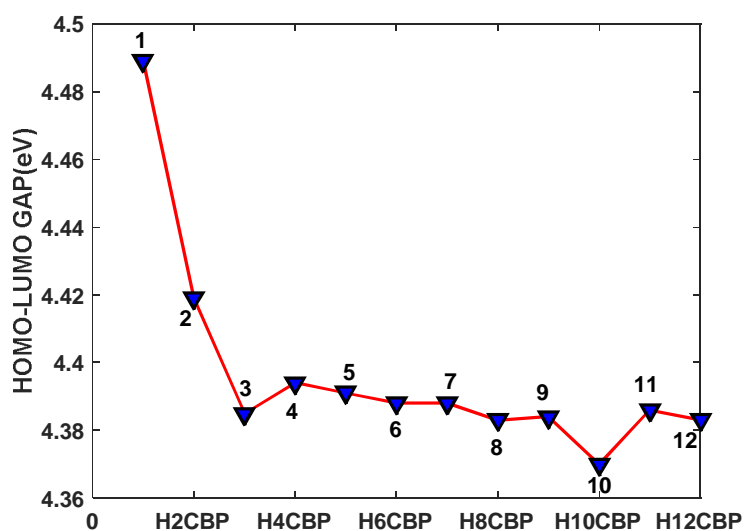


Figure 10. HOMO-LUMO gap of HnCBP LC (extension of alkyl chain length optimized by DFT methodology).

3.10 RANGE OF DIRECTOR ANGLE (θ)

The H9CBP has the most massive range of the director angle; that is the reason the birefringence and order parameter suddenly increase. The H9CBP LC is suitable for the

flexoelectric-optic application because it has a massive director angle [28]. The H7CBP and H12CBP molecules have a reasonable range of director Angle. All the other H_nCBP liquid crystals have a small director Angle range, as shown in Figure 11. The maximum range of the director angle is given in Table 1.

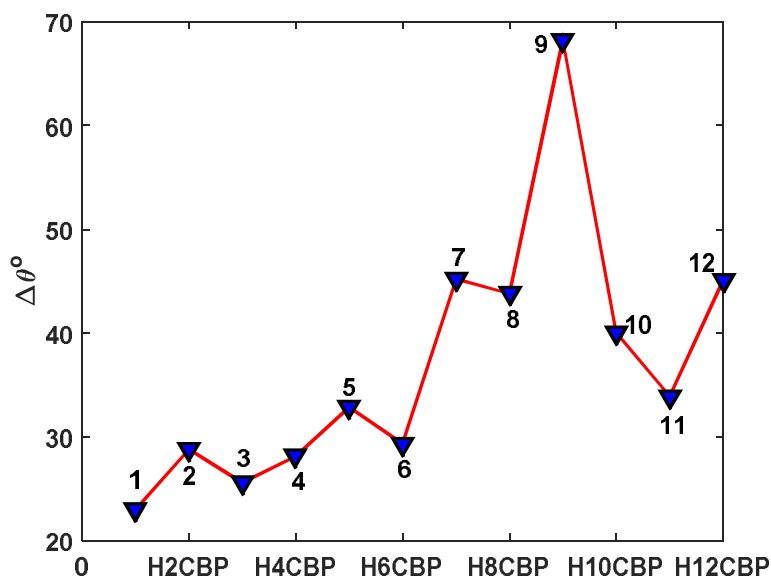


Figure 11. Variation in Director Angle of H_nCBP LC (extension of alkyl chain length under the impact of an electric field).

Table 1. Range of Director Angle.

Molecules	Minimum Director Angle	Maximum Director Angle	Difference between Director Angle
H1CBP	37.92	60.95	23.03
H2CBP	35.56	64.35	28.79
H3CBP	39.45	65.03	25.58
H4CBP	32.59	60.72	28.13
H5CBP	31.19	64.03	32.84
H6CBP	31.09	60.43	29.34
H7CBP	29.10	74.32	45.22
H8CBP	29.08	72.88	43.80
H9CBP	26.72	70.94	68.22
H10CBP	26.92	66.95	40.03
H11CBP	25.86	54.74	28.88
H12CBP	24.93	69.97	45.04

3.12 DIFFERENCE OF REFRACTIVE INDEX

The H6CBP and H11CBP liquid crystals have the smallest range of the refractive index. All the other liquid crystal decreases continually with alkyl chain length increment, as shown in Figure 12. The maximum and minimum range of the refractive index as shown in Table 2.

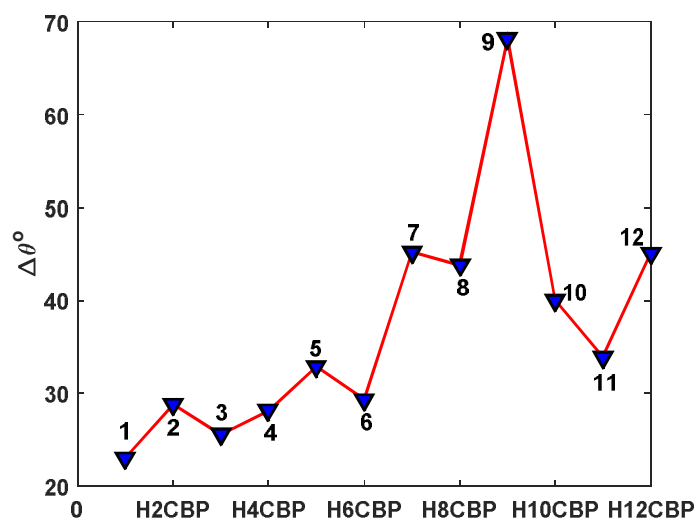


Figure 11. Refractive index of HnCBP LC (extension of alkyl chain length under the impact of an electric field).

Table 2. Range of Refractive Index.

Molecules	Minimum Refractive Index	Maximum Refractive Index	Difference between Refractive Index
H1CBP	1.5680	1.5756	0.0076
H2CBP	1.5689	1.5765	0.0075
H3CBP	1.5697	1.5772	0.0075
H4CBP	1.5704	1.5777	0.0073
H5CBP	1.5710	1.5781	0.0071
H6CBP	1.5715	1.5780	0.0065
H7CBP	1.5719	1.5788	0.0069
H8CBP	1.5723	1.5791	0.0068
H9CBP	1.5727	1.5792	0.0065
H10CBP	1.5731	1.5793	0.0062
H11CBP	1.5734	1.5783	0.0049
H12CBP	1.5737	1.5796	0.0059

4. CONCLUSIONS

In this work, it has been found the order parameter, dipole moment, and birefringence exhibit the odd-even effect, but the refractive index does not express any odd-even effect. The birefringence and order parameters are inversely related to each other. The transition temperature of crystalline to nematic phase and nematic to isotropic phase exhibit the odd-even effect. The birefringence and ionization potential decreases continuously with an increased alkyl chain of the HnCBP LC. The odd carbon number of alkyl chain shows HOMO-LUMO gap, birefringence, and order parameter in the upward direction because O-H stretching frequency increases for the odd carbon atom and even carbon number of alkyl chain shows in the downward direction because O-H stretching frequency decreases for the even carbon atom; while the dipole moment exhibits a shift of even carbon number of alkyl chain in the upward direction because of C-H symmetric stretching (alkyl chain) IR absorbance increases for the even carbon atom and odd carbon number of alkyl chain in the downward direction because C-H symmetric stretching (alkyl chain) IR absorbance decreases for the odd carbon atom. The refractive index and order parameter increases continuously with the increase in the alkyl chain length because C-C IR absorbance continually increases; but the refractive index decreases in H6CBP and H11CBP because the range of director angle is less as compared with neighboring liquid crystal however the second reason for decrement is C-O, C-N, C-H and O-H stretching frequency is responsible. The H11CBP one an only liquid crystal that is suitable for the very high THz frequency because it maintains the nematic phase stability for an extensive range of THz frequency; secondly, it is not converted into the isotropic phase; therefore, it is best for the THz applications. The H9CBP liquid crystal has the most massive range of Director angle that is the reason the birefringence suddenly increases in the H9CBP LC. The novelty of this work is the estimated equations that can predict the optical properties of liquid crystal.

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