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Electro-optical Effect of 4-*n*-alkyl-sulfanyl-4' isothiocyanate-biphenyl Liquid Crystal Homologous Series Under Terahertz Frequency: A Theoretical Approach

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Abstract

This work presented the electro-optical effect of the homologous series 4-*n*-alkyl-sulfanyl-4'-isothiocyanate-biphenyl (N1SC13H8-SH_{2n+1}C_n) under an electric field with terahertz (THz) frequency. The increase in alkyl sulfanyl chain length reduces the birefringence but increases the order parameter in THz frequency. An inverse relationship exists between the birefringence and order parameter. Meanwhile, the increase in alkyl sulfanyl chain length increases the refractive index with an even–odd effect. Birefringence, refractive index, order parameter, and director angle show an even–odd effect in the THz frequency range. The calculation is performed between 1 and 1,200 THz frequency. The isothiocyanate stretching corresponding to infrared absorbance remains unchanged for the whole series, showing potential in filtering and sensing applications.

Keywords: density functional theory, electro-optical effect, electric field (THz), liquid crystal, odd–even effect

Introduction

Liquid crystals (LCs) contain isothiocyanate (NCS) as a terminal group connected to biphenyl and alkyl sulfanyl chain (H_{2n+1}C_nS) that has a moderate viscosity, an acceptable melting point, and the highest birefringence. As terminal substitutes, chlorine, fluorine, and methyl group decrease the melting point of LCs. The cyclohexane that is connected to the phenyl ring has the lowest birefringence due to its lack of π -electrons. The biphenyl expresses the highest birefringence due to the maximum contribution of π -electron conjugation. The LC with the highest birefringence is the most suitable for application in gigahertz (GHz) and terahertz (THz) frequencies [1–3]. The π -electrons donated by the biphenyl group and the d-electrons of the sulfur atom contribute to the enhancement of extraordinary rays for optical applications. The phenyl ring and connected cyclohexane ring decrease the π -electrons that are responsible for the decrement in optical anisotropy. The alkyl sulfanyl connected to the biphenyl group has higher birefringence than the oxygen atom-based group. Nematic-to-isotropic and crystalline-to-smectic phase transitions decrease with the elongation of alkyl sulfanyl chain length and exhibit the even–odd effect; however the order parameter increases [4]. The NCS group is a highly polar terminal that can enhance the order parameter. Its derivatives have higher birefringence in

the nematic phase than the cyanobiphenyl (CN) group. The extended alkyl chain length along the molecular axis (x-axis) contributes to the extraordinary refractive index and the wide range of nematic phase [5]. In addition, the NCS group is suitable for GHz and THz frequency applications because of its higher absorption rate within extraordinary rays compared with that within ordinary rays; however, the CN group [6] and a fluorine atom show an even greater absorption rate along the ordinary axis. The NCS group enhances the π -electrons system due to the increase in birefringence [7], is less viscous than the CN group, and exists in smectic phase. The dipole moment of the CN group is higher than that of the NCS group due to its linear structure. The triple bond between C and N atoms contributes to the high molecular charge due to its extreme polarization. The CN group LC exhibits antiparallel conformation that accounts for its high viscosity; however, the NCS group is incapable of any antiparallel conformation, leading to its less viscous behavior. The less viscous behavior of the NCS group enhances the birefringence of the LC [8]. The rod-like alkylthio groups are not suitable for high birefringence because they have few melting points. The alkylthio group increases the transition temperature for the odd member of alkyl chain length but decreases the transition temperature for the even member of chain length [9]. The refractive index and birefringence have remained constant in the THz frequency region and thus are

suitable for absorbing applications [10]. Reuter *et al.* [11] reported that LCs with NCS terminal group are the best for GHz and THz frequency applications due to its low viscosity and high birefringence. The NCS group is also predominant in a wide range of nematic phase LC and has greater UV stability than the CN group due to its excellent electron delocalization [12]. In the present study, LC molecules are subjected to an electric field with a THz frequency. All the optical parameters are affected within the THz frequency, which is desirable for different applications.

Computational Methodology

The molecule of *4-n-alkyl-sulfanyl-4'-isothiocyanate-biphenyl* is optimized by the NWChem software [13] with the help of density functional theory (DFT) method B3LYP [14–15] and M062X [16] using the 6-31G** basis set [17–18]. After the optimization, we applied an

electric field to the 4-deca-alkylamino-4'-cyanobiphenyl LC along the x-axis (molecular axis) and perpendicular (y-axis) to it from 0.0000 a.u. (hartree) to 0.1500 a.u. at the interval of 0.0020 (a.u) with 1 a.u = 5.14×10^{11} V/m or 1 a.u. = 6.5×10^{15} Hz [19]. After the optimization of the applied external electric field, we calculated the molecular polarizability of *4-n-alkyl-sulfanyl-4'-isothiocyanate-biphenyl* LC molecules. Molecular polarizability along the x-axis is considered extraordinary (α_e) and that along the Y-axis is considered ordinary (α_o). Using α_e and α_o as basis, we calculated the order parameter, birefringence, director angle or magic angle, and refractive index with the formula given below, where α , μ , and β are equivalent to the components of polarizability. The letters present at the end of the equations mentioned before the "Order parameter," are: (a), dipole moment, (c) first-order hyperpolarizability, (b) average polarizability (d, e, and f) [20–21].

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

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

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

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

$$\Delta\tilde{\alpha} = \alpha_e - \alpha_o \quad (e), \text{ and}$$

$$\Delta\tilde{\alpha} = S\Delta\alpha \quad (f).$$

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 = radius of the LC molecules.

Magic angle (θ):-

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

Refractive index (n):-

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

where N , γ_e , and γ_o represent the number of LC molecules ($N = 300$) and extraordinary and ordinary internal field constants, respectively. The difference between γ_e and γ_o indicates differential molecular polarizability. n_e and n_o are the extraordinary and ordinary refractive indices, respectively.

Results and Discussion

All optical characteristics must exhibit the even-odd effect within the THz frequency range. The energy bandgap constantly narrows down as the dipole moment of the homologous series grows and the length of the alkyl sulfanyl chain extends. The lowered bandgap and the lengthening of the alkyl sulfanyl chain may be appropriate for semiconducting applications. For the whole sequence, the frequency of NCS stretching, C-C atom scissoring in the benzene ring, and H atom wagging all remain constant. Figure 1 shows the optimized molecular geometry of 4-alkyl-sulfanyl-4'-isothiocyanate-biphenyl LC. The optimized organic compound appears to work best with the B3LYP technique and is utilized as LC in this work. Owing to its ability to precisely predict molecule structures and other features, B3LYP is the most used DFT technique.

Birefringence. The birefringence of the series with the elongation of alkyl sulfanyl chain length is obtained using eq. (2). As shown in Figure 2a, birefringence is tested by placing a LC in an external electric field. The minimum birefringence represents the even-odd effect, and the maximum birefringence constantly decreases as the alkyl chain length increases. Negative birefringence is observed because the entire series has a re-entrant nematic phase [22–23]. The optimum LC for switching or filtering applications must have negative birefringence. All the odd members of the whole series exhibit noticeable negative birefringence, and all the even members exhibit less birefringence. According to Hird *et al.* [4], birefringence diminishes with the increase in alkyl sulfanyl chain length under the influence of temperature.

However, in the present investigation, an external electric field causes a decrease in birefringence. The melting point (molecular charge) rises because the alkyl sulfanyl chain length has an even number of carbon atoms. Large molecular axes and a large angle are used to generate the even members. With the large molecular axis, the odd members form few angles, which adversely enhance birefringence with re-entrant nematic phase [24].

Figure 1 shows that the molecular axis and even/odd members are producing small and large angles, respectively. Figure 2b displays a 3D image of the stability of the nematic phase under an external electric field (THz). Molecules exhibit re-entrant behavior at great electric fields, which is suitable for switching devices. The calculation is performed between 1 and 1,200 THz frequency as visualized in 3D (Figure 2b). The nematic phase is only seen in the range of 200–400 THz frequency. The minimum birefringence stands for negative birefringence, and the maximum birefringence stands for positive birefringence. The alkyl sulfanyl group is included in the compounds designed for extremely birefringent materials, such as 4-n-alkyl sulfanyl-4' isothiocyanate-biphenyl. Birefringence is a material's ability to divide light into two perpendicular polarization components, resulting in double refraction. This characteristic is useful in a variety of applications, including in LC displays and optical devices. The infrared (IR) spectra of 4-n-alkyl sulfanyl-4' isothiocyanate-biphenyl could be utilized to explore the link between the alkyl sulfanyl group and the compound's birefringent characteristics. In organic compounds, the NCS group often shows distinct absorption bands in the IR spectrum. The NCS group is frequently assigned an absorption band in the region of 2,000–2,200 cm^{-1} that corresponds to the NCS group's asymmetric vibrations. The NCS group's absorption band is generally strong or medium in intensity, frequently crisp, and well defined. On the basis of its particular absorption bands in the IR spectrum, the NCS group may be separated from other related functional groups, such as thiocyanates.

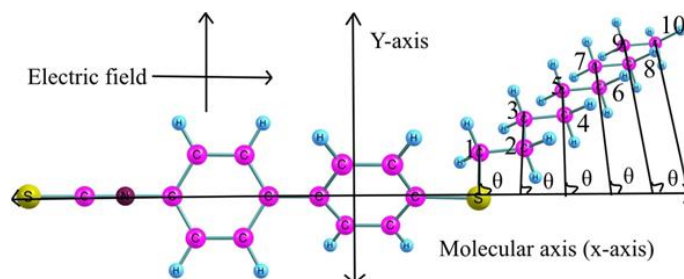


Figure 1. Optimized Molecular Geometry of 4-alkyl-sulfanyl-4'-isothiocyanate-biphenyl Liquid Crystal Molecule

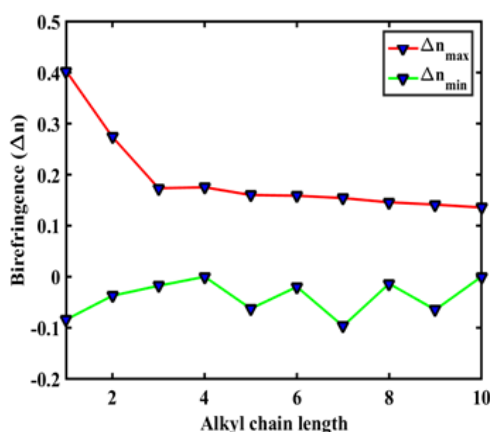


Figure 2a. Birefringence Computed with an Expansion of Alkyl Sulfanyl Chain Length Subjected to an External Electric Field (Red Line Indicates Maximum Birefringence and Green Line Shows the Minimum Birefringence of Liquid Crystal Molecules. Minimum Birefringence Represents the Even–Odd Effect, and Maximum Birefringence Constantly Decreases as Alkyl Chain Length Increases. The Even–Odd Effect in Liquid Crystals Refers to the Variation in Properties Based on the Number of Repeating Units in the Molecular Structure. This Effect has Been Observed in Various Aspects Such as Liquid Crystalline Order, Thermal Conductivity, Mass Density, and Molecular Shape)

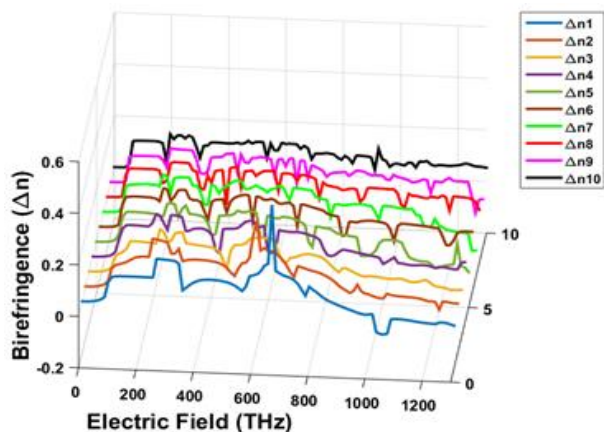


Figure 2b. 3D Birefringence Obtained by an Elongation of Alkyl Sulfanyl Chain Length Subjected to an External Electric Field (THz) (Nematic Phase Maintaining Stability with an Expansion of Sulfanyl Chain Length, with Δn_1 Representing the Birefringence with an Increment of One Carbon Atom Number of Alkyl Chain Length, Δn_2 Representing the Birefringence with an Increment of Two Carbon Atom Number of Alkyl Chain Length, Δn_3 Representing the Birefringence with an Increment of Three Carbon Atom Number of Alkyl Chain Length, Δn_4 Representing the Birefringence with an Increment of Four Carbon Atom Number of Alkyl Chain Length, Δn_5 Representing the Birefringence with an Increment of Five Carbon Atom Number of Alkyl Chain Length, Δn_6 Representing the Birefringence with an Increment of Six Carbon Atom Number of Alkyl Chain Length, Δn_7 Representing the Birefringence with an Increment of Seven Carbon Atom Number of Alkyl Chain Length, Δn_8 Representing the Birefringence with an Increment of Eight Carbon Atom Number of Alkyl Chain Length, Δn_9 Representing the Birefringence with an Increment of Nine Carbon Atom Number of Alkyl Chain Length, and Δn_{10} Representing the Birefringence with an Increment of Ten Carbon Atom Number of Alkyl Chain Length)

Order parameter. As shown in Figure 3a, the order parameter is achieved by extending the alkyl sulfanyl chain length and using eq. (1). The maximal order parameter steadily increases with the length of the alkyl sulfanyl chain exposed to the external electric field. The minimal or negative order parameter expresses the even–odd effect. Given that the odd members form fewer angles and have larger molecular axes, their order parameter decreases. Hird *et al.* [4] and Arakawa *et al.* [5] noted that the positive order parameter grows gradually as the length of the alkyl sulfanyl chain increases. The current work also suggests a similar behavior. Strong intermolecular contact between the molecules and electron conjugation are the causes of the constant increase in order parameter. As shown in 3D Figure 3b, the order parameter keeps the nematic phase stable while lengthening the sulfanyl chain. Therefore, the order parameter is the organic molecule's physical characteristic that expresses crystalline to isotropic behavior. The minimum order parameter stands for negative birefringence, and the maximum order parameter is stands for positive birefringence.

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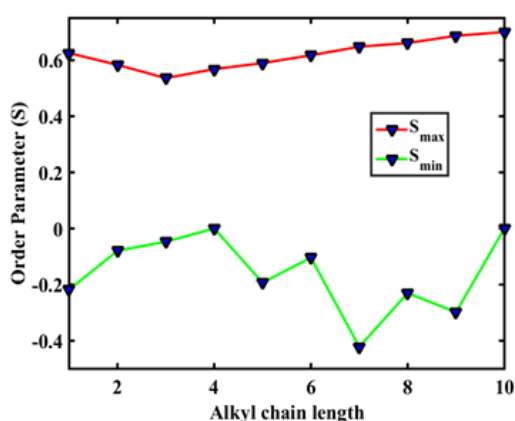


Figure 3a. Order Parameter Calculated with the Elongation of Alkyl Sulfanyl Chain Length Subjected to an External Electric Field (Red and Green Lines Indicate the Maximum and Minimum Order Parameter of Liquid Crystal Molecules, Respectively. The Even–Odd Effect in Liquid Crystals Refers to the Phenomenon where Their Properties Vary Depending on the Number of Repeating Units in the Molecular Structure)

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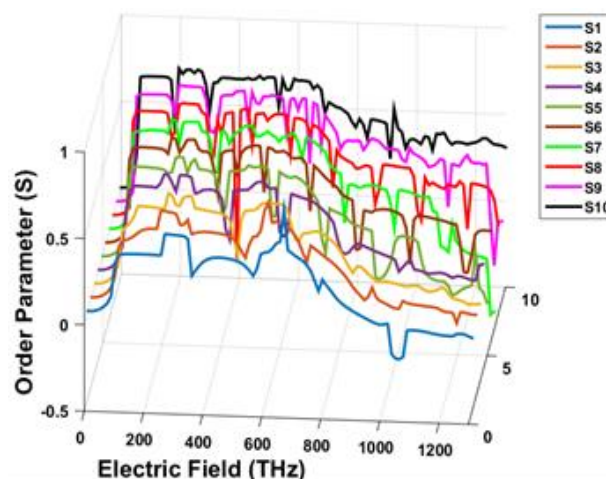


Figure 3b. 3D Order Parameter Computed During the Elongation of Alkyl Sulfanyl Chain Length Under an External Electric Field (THz) (The Nematic Phase Maintains Stability with the Elongation of Sulfanyl Chain Length. The Order Parameter Increases with Sulfanyl Chain Length, with S1 Representing the Order Parameter with an Increment of One Carbon Atom Number of Alkyl Chain Length, S2 Representing the Order Parameter with an Increment of Two Carbon Atom Number of Alkyl Chain Length, S3 Representing the Order Parameter with an Increment of Three Carbon Atom Number of Alkyl Chain Length, S4 Representing the Order Parameter with an Increment of Four Carbon Atom Number of Alkyl Chain Length, S5 Representing the Order Parameter with an Increment of Five Carbon Atom Number of Alkyl Chain Length, S6 Representing the Order Parameter with an Increment of Six Carbon Atom Number of Alkyl Chain Length, S7 Representing the Order Parameter with an Increment of Seven Carbon Atom Number of Alkyl Chain Length, S8 Representing the Order Parameter with an Increment of Eight Carbon Atom Number of Alkyl Chain Length, S9 Representing the Order Parameter with an Increment of Nine Carbon Atom Number of Alkyl Chain Length, and S10 Representing The Order Parameter with an Increment of Ten Carbon Atom Number of Alkyl Chain Length)

Refractive index. Equation (4) is used to calculate the refractive index while the alkyl sulfanyl chain length is elongated as shown in Figure 4a. The even-odd effect is visible in the highest refractive index. For even and odd members, the refractive index rises and falls accordingly. As shown in Figure 5a, this phenomenon occurs because the range of the director angle is increased for the odd members but decreased for the even members. The lowest refractive index rises steadily as the length of the alkyl sulfanyl chain extends. Meanwhile, the average refractive index falls with the eighth number as the maximum occupied molecular orbital energy is reduced. As shown in the 3D image in Figure 4b, the refractive index is unaffected by the external electric field. According to Pan *et al.* [25], a constant refractive index in the THz frequency region is ideal for regulating and managing the polarization of electromagnetic radiation. The NCS group may also display additional distinct absorption bands in other IR areas, such as vibrations involving the C-S bond. The NCS group's particular absorption bands might change depending on the product and its chemical environment. For accurate and detailed information about the characteristic absorption bands of the NCS group in this specific compound, specific studies or databases for the IR spectrum of *4-n-alkyl sulfanyl-4' isothiocyanate-biphenyl* or related compounds must be consulted. The NCS group's distinctive IR absorption bands generally fall between 2,000 and 2,200 cm^{-1} that corresponds to its asymmetric vibrations. The NCS group's absorption band is frequently crisp, well defined, and has medium to moderate intensity. In IR spectroscopy, the wavenumber range for distinctive absorption bands is generally between 600 and 4,000 cm^{-1} . By contrast, the NCS group has a smaller specific range between 2000 and 2,200 cm^{-1} .

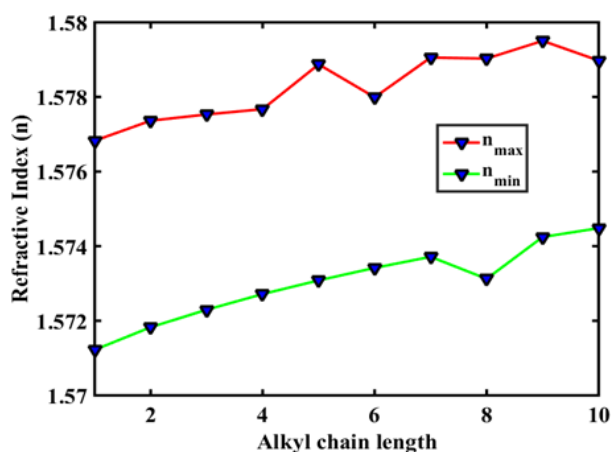


Figure 4a. Refractive Index Obtained by an Elongation in the Length of Alkyl Sulfanyl Chain Subjected to an External Electric Field (Red and Green Lines Represent the Maximum and Minimum Refractive Indices of Liquid Crystal Molecules, Respectively)

Director angle or magic angle. The director angle or magic angle is calculated using eq. (3) by increasing the alkyl sulfanyl chain length. The even-odd effect is determined by the greatest director angle range. As shown in Figure 5a, the odd members have a better range than the even members. The seventh (7) member has a maximum range of director angle that is crucial for applications involving filtering or sensing in the THz frequency band. The dipole moment caused by IR absorption from NCS stretching is enhanced by the lengthening of the alkyl sulfanyl chain. Figure 5b depicts the variation in the director angle when subjected to an external electric field. With an increase in the length of the sulfanyl chain, the nematic phase still maintains stability. The variation of the director angle is important

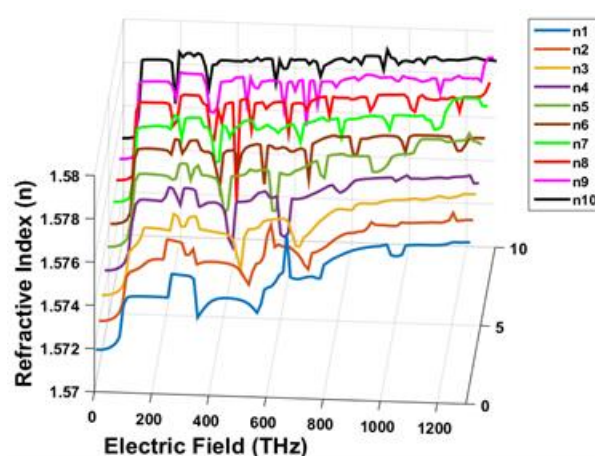


Figure 4b. 3D Refractive Index Obtained by an Elongation of Alkyl Sulfanyl Chain Length Subjected to an External Electric Field (THz) (The Refractive Index is Enhanced with the Elongation of Sulfanyl Chain Length, with n1 Representing the Refractive Index with an Increment of One Carbon Atom Number of Alkyl Chain Length, n2 Representing the Refractive Index with an Increment of Two Carbon Atom Number of Alkyl Chain Length, n3 Representing the Refractive Index with an Increment of Three Carbon Atom Number of Alkyl Chain Length, n4 Representing the Refractive Index with an Increment of Four Carbon Atom Number of Alkyl Chain Length, n5 Representing the Refractive Index with an Increment of Five Carbon Atom Number of Alkyl Chain Length, n6 Representing the Refractive Index with an Increment of Six Carbon Atom Number of Alkyl Chain Length, n7 Representing the Refractive Index with an Increment of Seven Carbon Atom Number of Alkyl Chain Length, n8 Representing the Refractive Index with an Increment of Eight Carbon Atom Number of Alkyl Chain Length, n9 Representing the Refractive Index with an Increment of Nine Carbon Atom Number of Alkyl Chain Length, and n10 Representing the Refractive Index with an Increment of Ten Carbon Atom Number of Alkyl Chain Length)

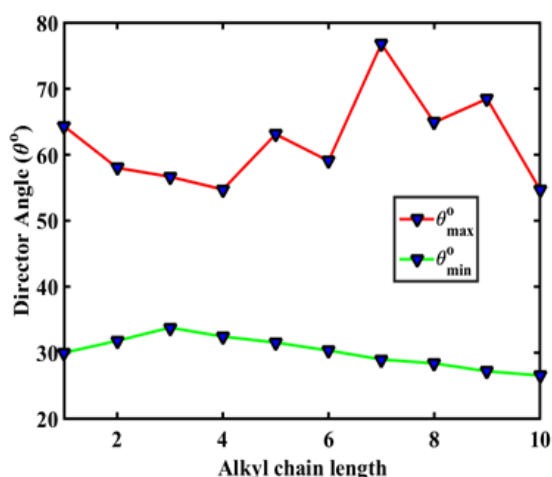


Figure 5a. Director Angle Obtained from the Elongation of Alkyl Sulfanyl Chain Length Subjected to an External Electric Field (Red Line Indicates the Maximum Director Angle and Green Line Indicates the Minimum Director Angle of Liquid Crystal Molecules. The Director Angle in Liquid Crystals Refers to the Angle Between the Preferred Orientation of The Molecules and a Reference Axis. The Director is a Dimensionless Unit Vector that Represents the Direction of Preferred Orientation of Molecules in the Neighborhood of Any Point. In the Absence of an External Field, the Director of a Liquid Crystal is Free to Point in Any Direction. The Director Angle can be Measured using Various Techniques, Such as Determining the Velocity Change of Shear Horizontal Wave. The Director Angle can Vary Depending on the Modes and Applied Voltage. The Director Angle can be Less Than 75° under Sufficient Applied Voltage and can be Numerically Analyzed Between Asymmetric Anchoring Surfaces. Chiral Nematic Liquid Crystals Exhibit a Twisted Structure, where the Director Rotates about an Axis While Moving Through the Material)

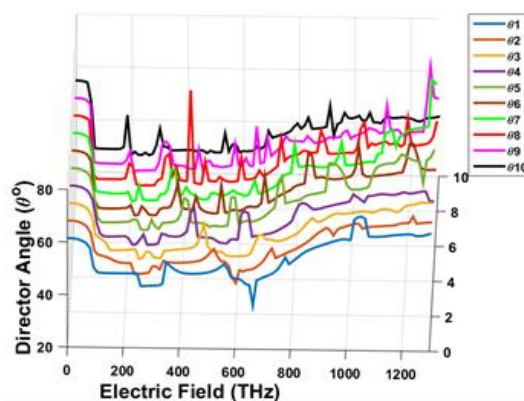


Figure 5b. 3D Director Angle Computed During the Elongation of Alkyl Sulfanyl Chain Length Subjected to an External Electric Field (THz) (The Director Angle Also Express Nematic Phase Stability with an Expansion of Sulfanyl Chain Length, with θ_1 Representing the Director Angle with an Increment of One Carbon Atom Number of Alkyl Chain Length, θ_2 Representing the Director Angle with an Increment of Two Carbon Atom Number of Alkyl Chain Length, θ_3 Representing the Director Angle with an Increment of Three Carbon Atom Number of Alkyl Chain Length, θ_4 Representing the Director Angle with an Increment of Four Carbon Atom Number of Alkyl Chain Length, θ_5 Representing the Director Angle with an Increment of Five Carbon Atom Number of Alkyl Chain Length, θ_6 Representing the Director Angle with an Increment of Six Carbon Atom Number of Alkyl Chain Length, θ_7 Representing the Director Angle with an Increment of Seven Carbon Atom Number of Alkyl Chain Length, θ_8 Representing the Director Angle with an Increment of Eight Carbon Atom Number of Alkyl Chain Length, θ_9 Representing the Director Angle with an Increment of Nine Carbon Atom Number of Alkyl Chain Length, and θ_{10} Representing the Director Angle with an Increment of Ten Carbon Atom Number of Alkyl Chain Length)

Table1. Molecular Geometry of 4-alkyl-sulfanyl-4'-isothiocyanate-biphenyl Molecules

S.No	Dipole Moment (debye)	Bandgap (eV)	HOMO Gap (eV)	LUMO Gap (eV)	Polarizability (a.u)	Hyperpolarizability (a.u)	TotalEnergy (Hartree)
N1	3.89	4.42	6.18	1.75	220.17	932.25	-1391.05
N2	4.23	4.42	6.16	1.73	234.52	648.35	-1430.35
N3	4.36	4.42	6.15	1.73	246.97	522.14	-1469.66
N4	4.43	4.42	6.15	1.72	259.32	384.97	-1508.96
N5	4.49	4.42	6.15	1.72	271.02	331.95	-1548.26
N6	4.51	4.42	6.15	1.72	282.66	293.26	-1587.57
N7	4.54	4.42	6.15	1.72	294.02	296.81	-1626.87
N8	4.54	4.42	6.15	1.72	305.38	287.84	-1666.18
N9	4.56	4.42	6.15	1.72	316.59	297.81	-1705.48
N10	4.56	4.42	6.15	1.72	327.82	293.47	-1744.79

for applications in sensing and filtering. The molecular geometry of *4-n-alkyl-sulfanyl-4'-isothiocyanate-biphenyl* molecules is given in Table 1. With the increase in alkyl chain length, the dipole moment, polarizability, and total energy of the molecule continuously increase but the hyperpolarizability continuously decreases. The HOMO, LUMO, and bandgap remain constant for the whole series of *4-n-alkyl-sulfanyl-4'-isothiocyanate-biphenyl* molecules. In addition, the *4-n-alkyl-sulfanyl-4'-isothiocyanate-biphenyl* molecular series has a constant bandgap, making it suitable for insulated application devices. In Table 1, N1 to N10 represent the number of the alkyl chain length of the whole series.

Conclusion

This study's key findings reveal that all optical properties deflect in the THz frequency range that is suitable for various optical devices. The experimental outcomes and theoretical prediction are also satisfactorily correlated. The NCS stretching frequency virtually remains constant across the whole series that is preferable for applications such as sensing and filtering. The unidentified LC molecules ideal for the THz frequency range are also recognized through theoretical prediction. Strong intermolecular contact between the molecules and electron conjugation are the causes of the constant increase in the order parameter. The lowest refractive index rises steadily as the length of the alkyl sulfanyl chain grows. The even-odd effect is determined by the greatest director angle range. We conclude that our results are similar, different, and consistent with the experimental evidence.

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