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INVESTIGATION OF PHYSICAL, OPTO-ELECTRONICS AND INSULATING PROPERTIES OF PPPCC LIQUID CRYSTAL MOLECULE BY DENSITY FUNCTIONAL THEORY (DFT) METHOD: A THEORETICAL APPROACH

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In this paper, we have studied the physical, electro-optical and thermal properties of PPPCC liquid crystal molecule. Density functional theory (DFT) with the B3LYP functional and the 6-31G(d,p) basis set is employed for the optimization and analysis of the p-Propoxyphenyl trans-4-pentylcyclohexanecarboxylate (PPPCC) LC molecule. Various physical properties, such as HOMO-LUMO energy levels, electro-optical properties, and global parameters, are computed and analysed for the PPPCC liquid crystal. We have reported the birefringence of p-Propoxyphenyl trans-4-pentylcyclohexanecarboxylate (PPPCC) liquid crystal under the effect of an external electric field. The UV-Visible analysis leaves a strong peak at 252 nm due to π-π* transitions. HOMO-LUMO band gap found to be 5.1 eV. The maximum stretching was observed at 1000 cm^{-1} due to the C-O stretching caused by the Ether in the PPPCC liquid crystal. The C-C stretching around 1600 cm^{-1} is found due to phenyl group present in PPPCC. The temperature-sensitive birefringence value of PPPCC makes it a suitable choice for modern optical technology applications. The refractive index remains unchanged at large applied electric fields, making it a suitable choice for opto-electronic devices in THz applications. Due to the large band gap, this molecule could be a suitable choice for insulating applications.
Keywords: *PPPCC; Electric field (THz); HOMO-LUMO; UV-Visible; IR; DFT*
PACS: 61.30.-b, 61.30.Dk, 61.30.Jf, 61.30.Gd, 78.30.-j

1. INTRODUCTION

Liquid crystals (LCs) have properties of both solids and liquids. In recent years, LCs have gained the interest of researchers due to their potential applications in display technology. LCs possess a mesomorphic phase due to the molecular arrangement in the compound. Further study of the mesomorphic phase of LCs has led to the development of new materials for optoelectronic applications. Also, understanding the various properties of LCs leads to modifying existing ones. LCs have the property of changing their alignment under an external electric field. This property of LCs is helpful for researchers to develop high-performance display devices [1].

To investigate the various properties of LCs, it is important to understand the structural and chemical properties of the material. Also, it is important to understand the correlation of mesogenic phase of LCs with temperature and chemicals. In general, the shape and size of the molecule influence the property and phase transition behaviour of LC substances [2]. Intra and inter molecular interactions alter the molecular property of the molecule during the LC phase. As a result, vibrational spectroscopy has a high potential for understanding the compound's molecular dynamics. IR spectroscopy is an important tool to reveal the molecular dynamics in the LC molecule [3-6]. Also, molecular polarizability plays an important role to define the opto-electronic properties of LC molecule. Modifying the shape, size and arrangement of atoms in the molecule, researchers can create the new LC molecule with desired opto-electronic properties which is useful for making modern opto-electronic devices such as LCDs [7-10].

In recent years, computational techniques have been modified a lot. Researchers have tested various computational techniques over the past years to investigate properties of LC molecules. Density functional theory (DFT) combined with the B3LYP functional gives good results for LC molecules [11]. This paper reports the molecular conformation, atomic orbital composition, electronic density, HOMO, LUMO, and relative energy gap of the PPPCC LC molecule. This LC molecule is known for its applications in liquid crystal technology applications.

The p-Propoxyphenyl trans-4-pentylcyclohexanecarboxylate (CAS No. 67589-54-2) is an organic compound. This compound has a molecular formula $C_{21}H_{32}O_3$ and a molecular weight of 332.48 g/mol. This compound consists of two groups; propoxyphenyl group and pentyl chain. These groups present in PPPCC LC molecule enhance the thermal stability of the material, makes it suitable for advanced material used in display devices. This compound has a density of 0.996 g/cm^3 and relatively high boiling point, which makes it suitable for high-temperature applications [12]. Further research on this compound continues to explore the tailored properties for advanced opto-electronic devices.

Also, the thermal stability and optical clarity of this compound make it suitable candidate for research in material science, particularly in synthesis of new LC compound with tailored properties. Understanding the various properties of this compound can lead to the advancement in theoretical and applied chemistry [13].

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2. COMPUTATIONAL METHODOLOGY

Density functional theory (DFT) techniques using the NWChem Software optimises every molecule with basis set 6-31G** [14]. We are applying the electric field (a.u.) to the liquid crystal compound along the molecular axis (x-axis) and perpendicular axis (y-axis). At the intervals of 0.0020 (a.u.), the applied electric field ranges from 0.0000 (a.u.) to 0.1000 (a.u.), where 1 a.u. = 5.14 x 10^{11} V/m and 1 a.u. = 6.5 x 10^{12} Hz [15]. We have determined the molecular polarizability of the molecule upon the application of an electric field. Extraordinary molecular polarizability (α_e) is measured along the x-axis, whereas ordinary molecular polarizability (α_o) is measured along the y-axis. According to the following equations, we have determined the birefringence, order parameter, refractive index, and magic angle using α_e and α_o. where α, μ, and β stand for the first-order hyper-polarizability, dipole moment, and polarizability components, respectively [16].

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

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

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

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

$$\Delta\tilde{\alpha} = \alpha_e - \alpha_o$$

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

Order Parameter (S):

$$S = \frac{\alpha_e - \alpha_o}{\alpha_e + \alpha_o} \tag{1}$$

Birefringence (Δn):

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

Where, R is the radius of the liquid crystal molecule.

Magic angle (θ):

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

Refractive index (n):

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

$$n_o = \frac{7}{2\sqrt{10}} + \frac{\left(2\sqrt{10}/5\right)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}} - \frac{\left(2\sqrt{10}/15\right)\pi NS(\gamma_e - \gamma_o)}{1 - \frac{4\pi N\alpha}{3}}$$

$$n = \frac{7}{2\sqrt{10}} + \frac{\left(2\sqrt{10}/5\right)\pi N\alpha}{1 - \frac{4\pi N\alpha}{3}} \tag{4}$$

Where, N is the number of liquid crystal molecules and γ_e, γ_o is representing the extraordinary and ordinary internal field constant. The difference of γ_e-γ_o is to serve the differential molecular polarizability. The n_e and n_o is representing the extraordinary and ordinary refractive index.

Radius of the PPPCC molecule=10.69

Electronegativity (χ):

$$X = \frac{I+A}{2}$$

Hardness (η):

$$\eta = \frac{I-A}{2}$$

Chemical Softness (S):

$$S = \frac{1}{\eta}$$

Chemical Potential (μ):

$$\mu = -X$$

Electrophilicity Index (ω):

$$\omega = \frac{\mu 2}{2\eta}$$

3. RESULTS AND DISCUSSIONS

The optimized structure of PPPCC liquid crystal was obtained by using density functional theory (DFT) through NWChem software are shown in the Figure 1.

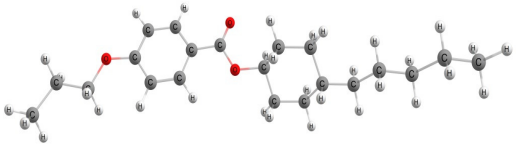

Figure 1. Optimised geometry of PPPCC liquid crystal molecule

3.1 Director angle

The director angle in important parameter of a liquid crystal molecule to understand the various optical parameters. It is the inclination of the long molecular axis over the reference direction of the molecule. The maximum value of director angle of the PPPCC liquid crystal was found to be 58.58^0 whereas the minimum value was found to be 27.47^0. Like other liquid crystal molecules, PPPCC liquid crystal shows magic angle value 54.73^0 as shown in the Figure 2.

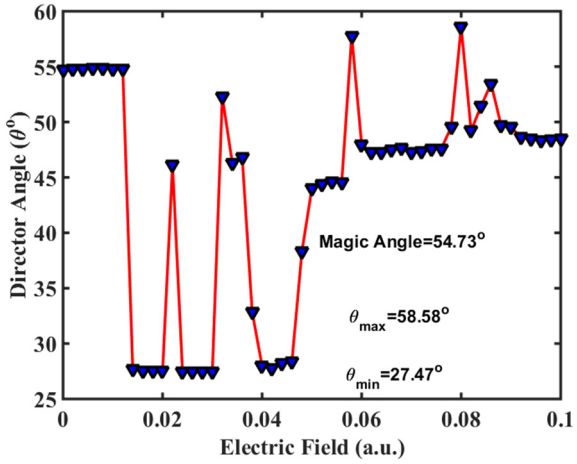

Figure 2. Director Angle of PPPCC liquid crystal molecule

3.2 Refractive index

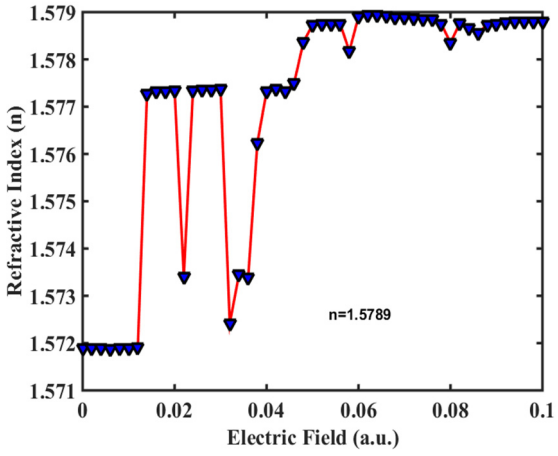

Figure 3. Refractive Index of PPPCC liquid crystal molecule

Liquid crystals are generally anisotropic in nature. This anisotropic nature of liquid crystals is an important feature used in light manipulation applications. Light manipulation is widely used in light moderator applications. This anisotropic nature of liquid crystals provides two refractive indices namely; extra-ordinary refractive index and ordinary refractive index. Refractive index is temperature-dependent property. As the temperature increases, extra-ordinary refractive index decreases whereas ordinary refractive index can either increase or decrease depending on the specific liquid crystal and its phase transitions. Other than temperature, electric field and impurities can also affect the molecular structure of the liquid crystal and hence change the optical parameters [17]. Refractive index of the PPPCC liquid crystal molecule was measured under the effect of external electric field. The average value of

the refractive index of PPPCC is found to be 1.5789. The variation in refractive index as a function of applied electric field is shown in the Figure 3. The nematic phase stability was observed at low THz frequency range in the refractive index characteristics. The refractive index remains constant at the higher frequency, which is suitable for the THz applications.

3.3 Birefringence

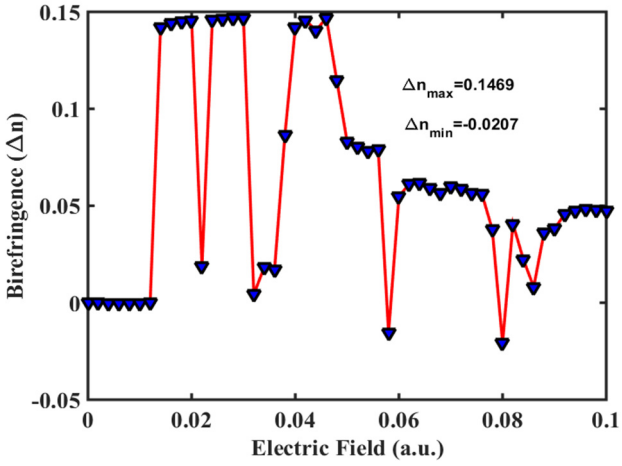

Figure 4. Birefringence of PPPCC liquid crystal molecule

Birefringence is the optical property of a material where the refractive index varies depending on the polarization and propagation direction of light. This anisotropy property of the material is important for display and optical applications. Polarisation Optical Microscope (POM) can be used to analyse the birefringence of the PPPCC liquid crystal molecule. This anisotropic property changes as a function of temperature or electric field. As temperature increases, birefringence decreases. In our study, we found the change in the birefringence of the PPPCC liquid crystal molecule as the external electric field varied as shown on the Figure.4. The maximum and minimum value of the birefringence of the PPPCC molecule were found to be 0.1469 and -0.0207 respectively. Negative value of birefringence is important for opt-electronic applications. This birefringence value makes it suitable for various optical applications. The birefringence of liquid crystals is temperature-dependent, generally exhibiting higher values near their nematic phase transition temperature (T*) [18]. As the temperature increases towards the clearing point, the order parameter decreases, leading to reduced birefringence. The birefringent properties of this compound make it suitable for use in liquid crystal displays (LCDs), tuneable lenses, and other optical devices where precise control over light propagation is necessary. High birefringence enhances contrast and brightness in displays, making it a desirable characteristic.

3.4 Order Parameter

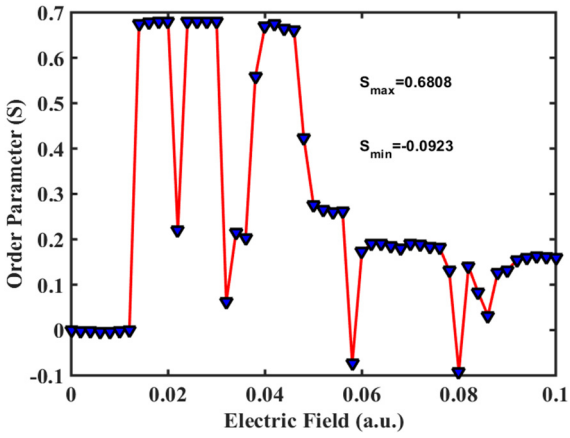

Figure 5. Order Parameter of PPPCC liquid crystal molecule

Order parameter is the angle between the molecular axis and the local director. For completely disordered isotropic liquid, order parameter is S=0 whereas for perfectly ordered liquid crystal, order parameter is S=1. Typical values for liquid crystals range from 0.3 to 0.8 [19]. The value of order parameter varies depending on the temperature or external electric field. In our study, we found the change in the birefringence of the PPPCC liquid crystal molecule as the external electric field varied as shown on the Figure 5.

The maximum and minimum values of the order parameter of PPPCC were found to be 0.6808 and -0.0923 respectively. The value of order parameter varies depending on the temperature and molecular interactions. Generally by increasing the temperature, liquid crystal loss its orientation order and hence order parameter decreases. As temperature increases p-propoxyphenyl trans-4-pentylcyclohexane carboxylate (PPPCC) undergoes phase transitions (e.g., from solid to nematic to isotropic liquid), the order parameter will exhibit distinct changes, providing insight into its molecular alignment and behavior under different conditions. Experimental techniques such as NMR and Raman Scattering can insight the molecular alignment and interactions with the liquid crystal phase.

3.5 IR Analysis

The IR analysis of PPPCC can provide valuable information about its molecular structure and functional group presents in the molecule. The presence of the aromatic ring will show C-H stretching vibrations, typically observed in the range 3000-3100 cm^{-1}. The pentyl chain contributes to C-H stretching vibrations in the region of 2850-2950 cm^{-1}. The carbonyl group from the carboxylic acid derivative will exhibit a strong absorption band in the region of 1700-1750 cm^{-1}. Aromatic C-C stretching vibrations will appear in the range of 1500-1600 cm^{-1}, indicating the presence of the phenyl group. The C-O stretching vibrations in the range of 1000-1300 cm^{-1} is due to the propoxy substitution in the ether

functional group. Also, the vibrations in the range of 675-900 cm^{-1} reveals the bending modes in the aromatic ring. In PPPCC liquid crystal molecule, Out of plane wagging of the hydrogen atom in Benzene found at 823 cm^{-1}, H-atom Rocking in the alkyl chain 972 cm^{-1}, C-O Stretching in either group at 1000 cm^{-1}, C-H wagging at 1246 cm^{-1}, C-H rocking at 1386 cm^{-1}, C-C stretching in benzene ring at 1524 cm^{-1} and C-H stretching in benzene ring at 3027 cm^{-1} as shown in the Figure 6. The obtained vibrational modes of PPPCC liquid crystal matches well with the literature. Various vibrational modes are given in the Table.1.

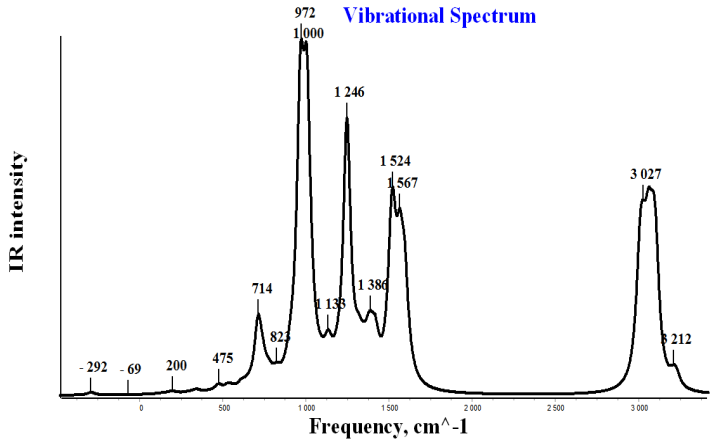

Figure 6. IR Spectrum of PPPCC liquid crystal molecule

Table 1. Vibrational Modes of PPPCC liquid Crystal

S. No.	Frequency (cm^{-1})	Modes of Vibration
1.	823	Out of plane wagging of the hydrogen atom in Benzene
2.	972	H-atom Rocking in the alkyl chain
3.	1000	C-O Stretching
4.	1246	C-H wagging
5.	1386	C-H Rocking
6.	1524	C-C stretching in benzene ring
7.	3027	C-H stretching in benzene ring

3.6 Raman Analysis

The structural and chemical properties of a molecule can be assessed through the vibrational modes present in it. Raman spectroscopy being a non-destructive technique is an important tool to identify the vibrational modes in the molecule. This technique is very useful for the studying the properties of sensitive compounds or those requiring further analysis [20]. For compound PPPCC, Raman spectroscopy can be particularly useful in identifying the functional groups, molecular conformation and interaction within the molecule. In our study, for PPPCC molecule, pentyl group of aromatic ring contributes to the C-H stretching and bending. C=O stretching is due to the carboxylate group. Cyclohexane contribute to the C=O stretching. 3023 cm^{-1} and 3232 cm^{-1} indicates asymmetric stretching of C-H. 1510 cm^{-1} indicates symmetric stretching in C-H. 1182 cm^{-1} indicates the C-C stretching in C-C as shown in the Figure 7. The higher frequency at 3023 cm^{-1} clearly indicates a change in the bonding or molecular interactions of the PPPCC.

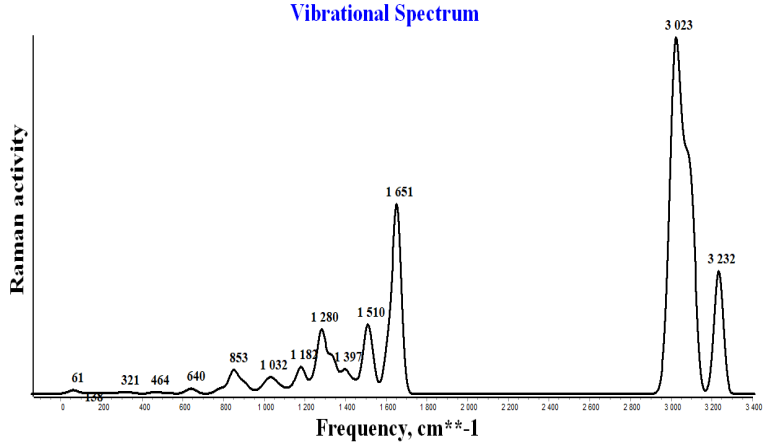

Figure 7. Raman Spectrum of PPPCC liquid crystal molecule

3.7 UV-Visible Analysis

UV-Visible spectroscopy is an efficient technique for determining the conjugated system and functional groups present in the sample. The presence of conjugated double bonds in the molecule will lead to π-π* transitions, which are responsible for light absorption in the UV-Vis range. Whereas the presence of functional groups will lead to n-π* transitions. The π-π* transitions occur at lower wavelengths (nearly 250 nm), whereas n-π* transitions occur at longer wavelengths (nearly 300-400 nm). The ultraviolet-visible (UV-Vis) absorption spectrum of p-propoxyphenyl trans-4-pentylcyclohexanecarboxylate depicts a strong peak at 252 nm, which clearly indicates the π-π* transitions due to the presence of conjugated double bonds in the molecule, as shown in Figure 8. This strong absorption in the UV at 252 nm yields an optical band gap of 4.9 eV.

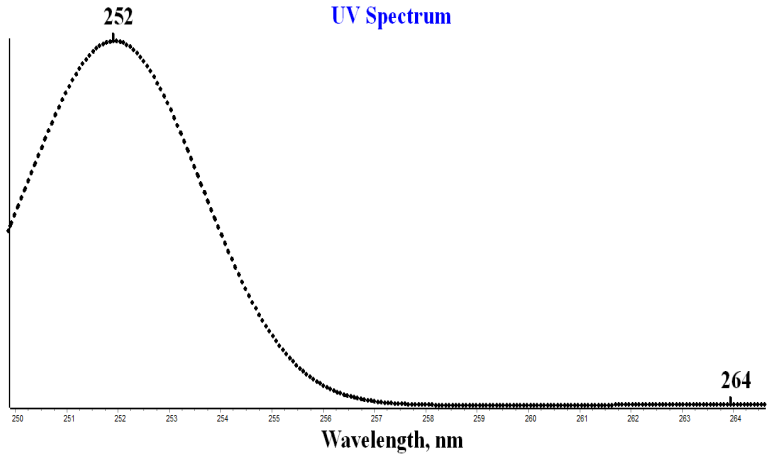

Figure 8. UV-Visible Spectrum of PPPCC liquid crystal molecule

3.8 Frontier Molecular Orbitals (FMO) and Density of States (DOS)

FMO's give insights into the electronic states of the molecule. HOMO-LUMO provides important information about the thermal properties of the molecule [21]. Frontier Molecular Orbitals (FMO) and Density of States (DOS) of the PPPCC molecule are shown in Figure 9. HOMO has a higher density of states (DOS), whereas the LUMO has a lower density of states (DOS). The band gap between HOMO and LUMO is found to be 5.1 eV. High value of the energy band gap leads to the insulating behaviour of the PPPCC molecule.

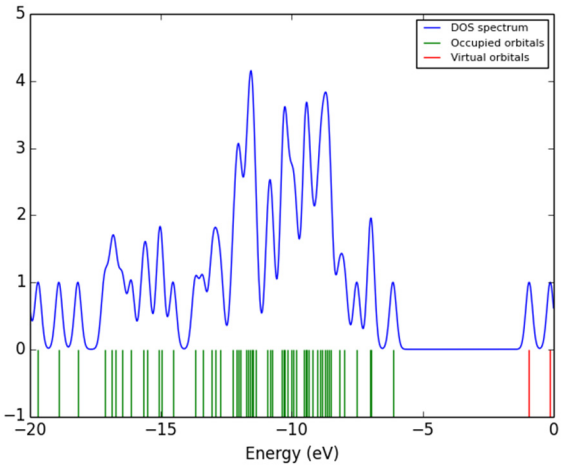

Figure 9. Frontier Molecular Orbitals (FMO's) and Density of States (DOS) of PPPCC liquid crystal molecule

3.9 Global Parameters

The Table 2 presents key electronic parameters that describe an atom or molecule's chemical behavior. The ionization potential (6.13 eV) is the energy needed to remove an electron, while electron affinity (0.93 eV) is the energy change upon gaining an electron. Electronegativity (3.53 eV) indicates the tendency to attract electrons in a bond. Hardness (2.60 eV) measures resistance to changes in electron distribution, with chemical softness (0.38 eV) being its inverse, reflecting how easily the electron cloud can be distorted. Chemical potential (-3.53 eV) shows the tendency of electrons to escape the system; its negative value suggests stability. Lastly, the electrophilicity index (2.39 eV) integrates electronegativity and hardness to quantify the ability to accept electrons. Together, these values provide a concise picture of the species' reactivity and stability in chemical processes.

Table 2. Global parameters of the PPPCC liquid crystal calculated by DFT methodology

Name of the parameter	Value in eV
Ionization Potential (I)	6.13
Electron Affinity (A)	0.93
Electronegativity Index (χ)	3.53
Hardness (η)	2.60
Chemical Softness (S)	0.38
Chemical Potential (μ)	-3.53
Electrophilicity Index (ω)	2.39

CONCLUSIONS

In summary, p-propoxyphenyl trans-4-pentylcyclohexane carboxylate exhibits significant orientational order characterized by its order parameter (S). This parameter varies with temperature and reflects the material's transition between different phases, providing essential insights into its liquid crystal properties and potential applications in display technologies and other optoelectronic devices. The molecular structure of p-propoxyphenyl trans-4-pentylcyclohexanecarboxylate plays a crucial role in determining its physical properties, including thermal stability, optical behaviour, and dielectric characteristics. These properties make it a valuable compound in the field of liquid crystals, particularly for applications in electronic displays where precise control over light manipulation and thermal behavior is required. Understanding these structural influences enables researchers and manufacturers to optimize formulations for enhanced performance in practical applications. In summary, p-propoxyphenyl trans-4-pentylcyclohexane carboxylate likely possesses high birefringence values that are temperature-sensitive, making it valuable for applications in advanced optical technologies. In our study, we found the change in the birefringence of p-Propoxyphenyl trans-4-pentylcyclohexanecarboxylate (PPPCC) liquid crystal under the effect of external electric field. At higher electric field PPPCC possess, negative birefringence, which is suitable for opt-electronic applications. π-π* transitions contribute to a significant peak at 252 nm in UV-Visible region. IR analysis confirms the presence of propoxy and pentyl present in PPPCC liquid crystal. 1000 cm^{-1} due to the C-O stretching caused by Ether in PPPCC liquid crystal. The C-C stretching around 1600 cm^{-1} is found due to phenyl group present in PPPCC. The refractive index remains unchanged for the large value of applied electric field which makes it suitable choice for opto-electronic devices in THz applications. FMO and DOS study depict a large value of energy band gap of 5.1 eV. Due to the high value of band gap this molecule could be a suitable choice for the insulating applications.

The molecular structure impacts the thermal stability and phase transition temperatures. The bulky groups (propoxy and pentyl) present in PPPCC can lower the melting point, facilitating a liquid crystalline state at room temperature. This is crucial for applications in displays that require a stable liquid crystal phase. Also, the arrangement of the propoxyphenyl and pentyl groups within the PPPCC contributes to the high value of birefringence of the material. Birefringence is vital for liquid crystals used in display technologies, as it affects how light is manipulated within the device. The dielectric anisotropy, influenced by the orientation of polar groups within the PPPCC molecule, is essential for liquid crystal applications. The propoxy group introduces polar characteristics that can enhance or reduce dielectric anisotropy depending on its orientation in the liquid crystal matrix. This property is significant for controlling switching speeds in display technologies. The presence of both hydrophobic (pentyl) and hydrophilic (propoxy) components improves solubility across various solvents, enhancing compatibility with other liquid crystal materials. This versatility is essential for formulating liquid crystal mixtures that require specific solubility characteristics. Dipole moment and electrochemical thermal analysis contribute to developing a new, unique optical-based liquid crystalline material. This study helps generate new optoelectronic devices and advanced liquid-crystalline materials.

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ДОСЛІДЖЕННЯ ФІЗИЧНИХ, ОПТОЕЛЕКТРОННИХ ТА ІЗОЛЯЦІЙНИХ ВЛАСТИВОСТЕЙ РІДКОКРИСТАЛІЧНОЇ МОЛЕКУЛИ PPPCC МЕТОДОМ ТЕОРІЇ ФУНКЦІОНАЛА ГУСТИНИ (DFT): ТЕОРЕТИЧНИЙ ПІДХІД

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У цій статті ми досліджували фізичні, електрооптичні та теплові властивості рідкокристалічної молекули PPPCC. Теорія функціоналу густини (DFT) з функціоналом B3LYP та базисним набором 6-31G(d,p) використовується для оптимізації та аналізу рідкокристалічної молекули р-пропоксифеніл транс-4-пентилциклогексанкарбоксилату (PPPCC). Для рідкокристалічної молекули PPPCC обчислюються та аналізуються різні фізичні властивості, такі як енергетичні рівні HOMO-LUMO, електрооптичні властивості та глобальні параметри. Ми повідомили про двопроменезаломлення рідкокристалічного р-пропоксифеніл транс-4-пентилциклогексанкарбоксилату (PPPCC) під впливом зовнішнього електричного поля. УФ-видимий аналіз залишає сильний пік при 252 нм через π-π* переходи. Ширина забороненої зони HOMO-LUMO становила 5,1 еВ. Максимальне розтягнення спостерігалося при 1000 см-1 через розтягнення C-O, спричинене ефіром у рідкокристалі PPPCC. Розтягнення C-C близько 1600 см-1 виявлено завдяки фенільній групі, присутній у PPPCC. Температурно-чутливе значення двопроменезаломлення PPPCC робить його придатним вибором для сучасних застосувань в оптичних технологіях. Показник заломлення залишається незмінним у великих прикладених електричних полях, що робить його придатним вибором для оптоелектронних пристроїв у терагерцовому діапазоні. Завдяки великій ширині забороненої зони ця молекула може бути придатним вибором для ізоляційних застосувань.

Ключові слова: *PPPCC; Електричне поле (ТГц); HOMO-LUMO; УФ-видимий діапазон; ІЧ; DFT*