

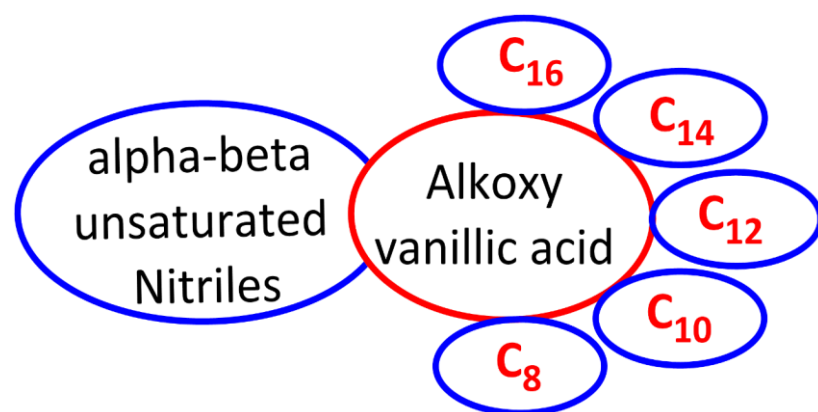
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Synthesis and Characterization of Liquid Crystalline Derivatives Derived from Alkoxy Vanillic Acid and α , β -Unsaturated Nitriles

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Liquid crystals (LCs) are unique materials that combine the fluidity of liquids with the molecular ordering of crystals, making them valuable in optoelectronic and advanced material applications. In this work, new liquid crystalline compounds were synthesized from (Z)-3-(4-butoxyphenyl)-2-(4-hydroxyphenyl) acrylonitrile and alkoxy-substituted vanillic acid derivatives. These structural modifications were introduced to enhance mesophase stability and tailor thermal and optical properties for potential technological applications. The synthesis was achieved via esterification or condensation reactions under controlled conditions. Structures were confirmed using Nuclear Magnetic Resonance (NMR) and Infrared (IR) spectroscopy. Differential Scanning Calorimetry (DSC) was employed to determine phase transition temperatures, while Polarized Optical Microscopy (POM) was used to observe mesophase textures. The findings reveal that alkoxy vanillic acid units significantly influence mesophase behavior, yielding compounds with stable mesophases and tunable transition points. This study highlights the relationship between molecular structure and mesomorphic properties, providing a foundation for designing advanced liquid crystal materials for optoelectronic devices.

Graphical abstract



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1. Introduction

Nitrile and alkoxy vanillic acid derivatives play a crucial role in the development of liquid crystal (LC) materials by enhancing thermal stability, dipolar interactions, and mesomorphic characteristics. The polar nitrile group ($-\text{CN}$) in

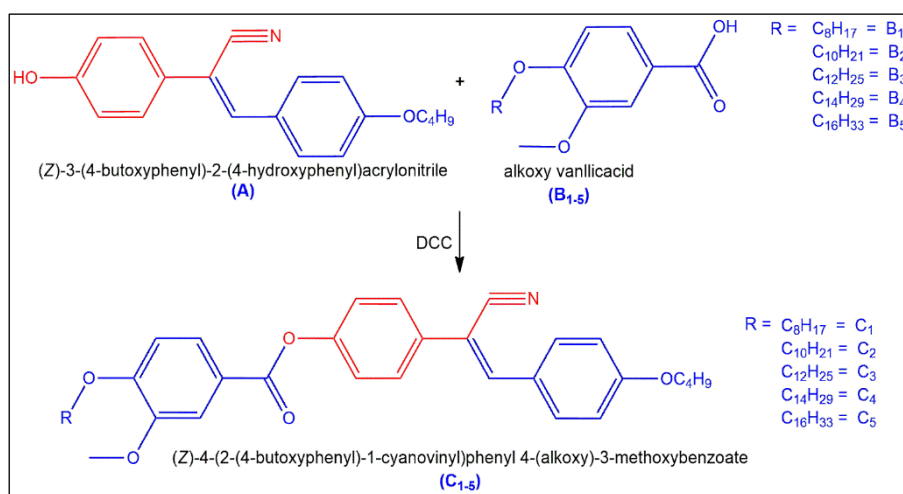
acrylonitrile significantly contributes to dielectric anisotropy, while alkoxy vanillic acid moieties promote self-assembly through hydrogen bonding. When combined, these functional groups produce liquid crystalline materials that exhibit broad

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temperature ranges, enhanced phase stability and tunable optical properties. As a result, they are widely applied in display technologies, sensors and other optical devices. Current research focuses on refining molecular structures to further improve the performance of LCs in advanced systems [1–2]. α,β -Unsaturated nitriles, characterized by a nitrile group conjugated with a carbon–carbon double bond, are highly reactive intermediates in organic synthesis which serves as a rigid, conjugated, and polar unit that enhances intermolecular interactions and facilitates mesophase formation. This reactivity enables the construction of a wide variety of derivatives, many of which can be engineered to exhibit liquid crystalline properties. When compounds of this type are combined with an ester-based core, such as vanillic acid derivatives, the resulting systems exhibit significant structural anisotropy and tunable mesomorphic properties, attributes governed by the length of the terminal alkyl chains owing to the integration of the conjugated nitrile system with the flexible and functionalized vanillic acid moiety, which together form mesogenic units responsible for liquid crystalline behavior with specific mesophases and thermal characteristics [3–12]. Investigations into alkoxy vanillic acid derivatives explore how different alkoxy chain lengths and positions affect mesophase formation, thermal transitions, and molecular self-organization. Such studies provide valuable insights into tailoring material properties for optoelectronic and multifunctional applications [13–15].

Despite extensive research in related systems, the specific reaction between alkoxy vanillic acids and α,β -unsaturated nitriles has not been extensively explored. Motivated by this gap, we undertook a study to synthesize and characterize new LC materials. We began by synthesizing (Z)-3-(4-butoxyphenyl)-2-(4-hydroxyphenyl)acrylonitrile (A), a molecule that incorporates features favorable for liquid crystalline behavior. Its structure includes a conjugated acrylonitrile core, a butoxy-substituted aromatic ring providing flexibility and solubility, and a hydroxyl-functionalized phenyl ring that facilitates hydrogen bonding interaction known to influence phase transitions and mesophase stability. Subsequent reactions with alkoxy vanillic acid derivatives (B_1 – B_5) introduce additional flexible alkyl chains and polar groups, which can further modulate thermal stability and phase behavior. This study outlines the synthesis of these novel derivatives in three main steps as mentioned in the Scheme 1: (1) Synthesis of Compound A through a condensation reaction, forming an α,β -unsaturated nitrile (2) Preparation of alkoxy vanillic acid derivatives (B_1 – B_5) (3) Esterification or condensation of Compound A with Compounds B_1 – B_5 . The resulting products were characterized using spectroscopic techniques. Polarized Optical Microscopy (POM) was used to examine mesophase textures, while Differential Scanning Calorimetry (DSC) was employed to analyze thermal transitions. Electronic features and intermolecular interactions within these liquid crystalline compounds can be effectively explored through Density Functional Theory (DFT). DFT allows for the computation of optimized geometries, HOMO–LUMO energy levels, and dipole moments, which are crucial in understanding molecular alignment and phase behavior. Further, Molecular Electrostatic Potential (MEP) mapping provides insight into the electron density distribution, indicating potential sites for non-covalent interactions and aiding in the interpretation of self-assembly patterns observed in mesophases. Scheme 1 summarizes the synthetic approach and the various phases of this work.



Scheme 1. Synthesis of aryl acrylonitrile and compounds C_1 – C_5 .

2. Material and Methods

2.1. Materials and measurements

4-Butoxybenzaldehyde (CAS No. 5736-88-9, >98% purity), 4-hydroxybenzaldehyde, n -alkyl bromides ($\geq 99\%$ purity), and solvents including acetone, ethanol, and dichloromethane (DCM) were procured from S. D. Fine-Chem. Ltd., Mumbai, India. All chemicals were of analytical grade. Solvents were dried and distilled following standard procedures prior to use. Special reagents such as 4-dimethylaminopyridine (DMAP) and N,N' -dicyclohexylcarbodiimide (DCC) were also obtained from the same source. Proton nuclear magnetic resonance (1H NMR) and Carbon nuclear magnetic resonance (^{13}C NMR)

spectra were obtained using a Bruker Avance III™ HD 400 MHz spectrometer (Bruker Corporation, USA), with $CDCl_3$ as the solvent and tetramethylsilane (TMS) as the internal standard. Fourier-transform infrared (FT-IR) spectra were recorded using the ATR method over the range of 400–4000 cm^{-1} on a Nicolet-760 FT-IR spectrophotometer (Canada). Elemental (CHN) analysis was performed using a Thermofing Flash 1101EA analyzer (Italy). Differential Scanning Calorimetry (DSC) measurements were carried out using a DSC 4000 Thermal Analyzer (PerkinElmer Inc., CA, USA). Polarizing optical microscopy (POM) was employed to study surface textures in the heating stage under finite temperature conditions using a Nikon Eclipse LV-100POL microscope equipped with a CFI60 infinity optical system (Nikon

Instruments Inc., NY, USA).

2.2. Synthesis of (Z)-3-(4-butoxyphenyl)-2-(4-hydroxyphenyl)acrylonitrile (A)

4-butoxy benzaldehyde (5.0 g, 17.0 mmol), 2-(4-hydroxyphenyl)acetonitrile (2.7 g, 20.0 mmol) and NaOH (1.7 g, 43.0 mmol) were added into a 250 mL round bottom flask, and 150 mL ethanol was added as a solvent. The mixtures were reacted at 80 °C for 12 hrs. When the reaction completed, the mixtures were cooled to room temperature and then poured into acidic ice water, and the pH of the solution was adjusted using HCl (aq) to pH = 2–5. Then the yellow precipitates were collected and washed with deionized water until pH = 7. Subsequently, methanol was used as the solvent to recrystallized and purify the crude product. Finally, 5.0 g of yellow crystalline solid was obtained after drying [16].

(Z)-3-(4-butoxyphenyl)-2-(4-hydroxyphenyl)acrylonitrile (A): M.F.: $C_{19}H_{19}NO_2$, M. Wt.: 293.36 g/mol, Yellow to light brown crystalline solid, 1H NMR (400 MHz, $CDCl_3$) (δ ppm): 9.81 (s, 1H, -OH) 7.92 (d, 2H, Ar-H), 7.69 (d, 1H -CH=CH-), 7.32 (d, 2H, Ar-H), 7.02–7.10 (d, 2H, Ar-H), 6.92 (d, 1H, Ar-H), 6.85 (d, 2H, Ar-H), 4.00 (t, 2H, -O-CH₂), 1.82 (m, 2H, -CH₂-), 1.50 (m, 2H, -CH₂-), 1.32 (t, 3H, -CH₃). ^{13}C -NMR (δ ppm): 160.2 (C=O, Ar-OH), 158.4 (C=O, Ar-O-R), 140.6, 132.5 (C=C), 130.2 (Ar-C acrylonitrile), 128.4 (Ar C-O-Bu), 122.6 (-C≡N), 115.8, 114.2 (Ar C-OH), 69.4 (O-CH₂), 32.8, 29.5 (-CH₂-), 19.2 (-CH₂- of CH₃), 13.7 (-CH₃). FT-IR (v cm⁻¹): 3312 cm⁻¹ (-OH, phenol), 3060 cm⁻¹ (C-H aromatic), 2902 cm⁻¹ (-OCH₂-group), 2225 cm⁻¹ (C≡N), 1620 cm⁻¹ (C=C acrylonitrile), 1575 cm⁻¹ (C=C), 1220 cm⁻¹ (C-O ether), 790 cm⁻¹ (C-H bending). CHN analysis, calculated % (found %): C = 77.79 (77.71); H = 6.53 (6.50); N = 4.77 (4.72); O = 10.91 (10.83).

2.3. Synthesis of Alkoxy vanillic acid (B₁–B₅)

Alkoxy vanillic acid derivatives (B₁–B₅) were synthesized following a previously reported method [17–18] as shown in the Scheme 1.

2.4. Synthesis of (Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(alkoxy)-3-methoxy benzoate (C₁–C₅)

Each of the synthesized 4-n-alkoxy-3-methoxybenzoic acid derivatives (B₁–B₅) was dissolved in dichloromethane (DCM), followed by the addition of DCC/EDC as a coupling agent. The reaction mixture was stirred at 0 °C for 15 minutes. Subsequently, (Z)-3-(4-butoxyphenyl)-2-(4-hydroxyphenyl)acrylonitrile (A) was added to the solution of alkoxy vanillic acid and the mixture was stirred at room temperature for 24 hours. After completion, the resulting byproduct, dicyclohexylurea (DCU), was removed by filtration. The solvent was then evaporated under reduced pressure to obtain the crude product. Purification was achieved through column chromatography using a mixture of ethyl acetate and hexane as the eluent. The final products were further recrystallized from ethanol to enhance purity. In total, five liquid crystalline derivatives, labeled as C₁–C₅, were successfully synthesized following this procedure.

(Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 3-methoxy-4-(octyloxy)benzoate (C₁): M.F.: $C_{35}H_{41}NO_5$, M. Wt.: 555.70 g/mol, 1H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, J = 16.0 Hz, 1H, CH=CH-CN), 7.70–6.99 (m, 8H, Ar-H), 4.11 (t, J = 6.6 Hz, 2H, -OCH₂-C₄H₉), 4.01 (t, J = 6.5 Hz, 2H, Ar-OCH₂-), 3.80 (s, 3H, -OCH₃), 1.81–1.67 (m, 4H, -CH₂-), 1.40–1.25 (m, 6H, -CH₂-), 0.82 (t, J = 7.0 Hz, 3H, -CH₃). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.7 (C=O), 160.5, 153.2, 151.8 (Ar-C-O), 142.1, 132.8,

131.2, 128.5, 124.3, 122.9, 120.0, 118.2 (Ar-C, CH=CH-CN), 113.8 (C≡N), 68.9 (Ar-OCH₂-), 65.5 (-OCH₂-), 56.1 (-OCH₃), 31.9, 29.3, 26.2 (-CH₂-), 13.9 (-CH₃). FTIR (KBr, cm⁻¹): ν 3059–3020 (Ar-C-H), 2960, 2931, 2859 (aliphatic C-H), 2228 (C≡N, nitrile), 1739 (C=O, ester), 1601, 1579, 1508 (Ar-C=C), 1459, 1362 (C-H bending), 1283, 1244 (C-O-C stretch, ester and alkoxy), 1185, 1044 (Ar-O-CH₂), 830, 758 (C-H out-of-plane bending). CHN analysis, calculated % (found %): C = 75.65 (75.52); H = 7.44 (7.38); N = 2.52 (2.49); O = 14.40 (14.33).

(Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(decyloxy)-3-methoxybenzoate (C₂): M.F.: $C_{37}H_{45}NO_5$, M. Wt.: 583.76 g/mol, 1H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, J = 16.0 Hz, 1H, CH=CH-CN), 7.70–6.83 (m, 8H, Ar-H), 4.07 (t, J = 6.6 Hz, 2H, -OCH₂-C₄H₉), 4.07 (t, J = 6.5 Hz, 2H, Ar-OCH₂-), 3.85 (s, 3H, -OCH₃), 1.89–1.62 (m, 4H, -CH₂-), 1.48–1.20 (m, 6H, -CH₂-), 0.86 (t, J = 7.0 Hz, 3H, -CH₃). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0 (C=O), 160.1, 153.9, 151.0 (Ar-C-O), 142.8, 132.0, 131.9, 128.3, 124.7, 122.7, 120.8, 118.8 (Ar-C, CH=CH-CN), 113.0 (C≡N), 68.0 (Ar-OCH₂-), 65.9 (-OCH₂-), 56.8 (-OCH₃), 32.3, 29.9, 25.8 (-CH₂-), 14.2 (-CH₃). FTIR (KBr, cm⁻¹): ν 3050–3000 (Ar-C-H), 2954, 2927, 2854 (aliphatic C-H), 2223 (C≡N, nitrile), 1732 (C=O, ester), 1604, 1572, 1511 (Ar-C=C), 1456, 1354 (C-H bending), 1278, 1239 (C-O-C stretch, ester and alkoxy), 1178, 1036 (Ar-O-CH₂), 837, 753 (C-H out-of-plane bending). CHN analysis, calculated % (found %): C = 76.13 (75.93); H = 7.77 (7.63); N = 2.40 (2.38); O = 13.70 (13.59).

(Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(dodecyloxy)-3-methoxybenzoate (C₃): M.F.: $C_{39}H_{49}NO_5$, M. Wt.: 611.81 g/mol, 1H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J = 16.0 Hz, 1H, CH=CH-CN), 7.80–7.15 (m, 10H, Ar-H), 6.91 (d, 1H, Ar-H), 4.04 (t, J = 6.6 Hz, 2H, -OCH₂-C₄H₉), 3.98 (t, J = 6.5 Hz, 2H, Ar-OCH₂-), 3.88 (s, 3H, -OCH₃), 1.82–1.42 (m, 4H, -CH₂-), 1.41–1.22 (m, 6H, -CH₂-), 0.92 (t, J = 7.0 Hz, 3H, -CH₃). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0 (C=O), 161.5, 154.2, 152.0 (Ar-C-O), 143.1, 133.0, 131.9, 128.5, 124.8, 122.0, 120.5, 118.9 (Ar-C, CH=CH-CN), 113.1 (C≡N), 68.0 (Ar-OCH₂-), 65.9 (-OCH₂-), 56.7 (-OCH₃), 31.2, 29.8, 26.7 (-CH₂-), 13.0 (-CH₃). FTIR (KBr, cm⁻¹): ν 3066–3073 (Ar-C-H), 2960, 2933, 2864 (aliphatic C-H), 2229 (C≡N, nitrile), 1730 (C=O, ester), 1610, 1580, 1502 (Ar-C=C), 1462, 1363 (C-H bending), 1270, 1242 (C-O-C stretch, ester and alkoxy), 1170, 1039 (Ar-O-CH₂), 830, 750 (C-H out-of-plane bending). CHN analysis, calculated % (found %): C = 76.56 (76.42); H = 8.07 (8.01); N = 2.29 (2.22); O = 13.08 (12.89).

(Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 3-methoxy-4-(tetradecyloxy)benzoate (C₄): M.F.: $C_{41}H_{53}NO_5$, M. Wt.: 639.86 g/mol, 1H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, J = 16.0 Hz, 1H, CH=CH-CN), 7.68–6.69 (m, 8H, Ar-H), 4.06 (t, J = 6.6 Hz, 2H, -OCH₂-C₄H₉), 4.08 (t, J = 6.5 Hz, 2H, Ar-OCH₂-), 3.78 (s, 3H, -OCH₃), 1.83–1.60 (m, 4H, -CH₂-), 1.49–1.29 (m, 6H, -CH₂-), 0.83 (t, J = 7.0 Hz, 3H, -CH₃). ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2 (C=O), 161.7, 154.4, 151.0 (Ar-C-O), 143.7, 133.8, 133.2, 127.5, 125.3, 123.1, 121.2, 119.7 (Ar-C, CH=CH-CN), 114.7 (C≡N), 69.7 (Ar-OCH₂-), 65.9 (-OCH₂-), 56.8 (-OCH₃), 31.3, 29.0, 26.7 (-CH₂-), 13.1 (-CH₃). FTIR (KBr, cm⁻¹): ν 3060–3050 (Ar-C-H), 2966, 2930, 2861 (aliphatic C-H), 2225 (C≡N, nitrile), 1730 (C=O, ester), 1611, 1579, 1520 (Ar-C=C), 1461, 1350 (C-H bending), 1270, 1247 (C-O-C stretch, ester and alkoxy), 1170, 1042 (Ar-O-CH₂), 831, 751 (C-H out-of-plane bending). CHN analysis, calculated % (found %): C = 76.96 (76.75); H = 8.35 (8.28); N = 2.19 (2.04); O = 12.50 (12.37).

(Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(hexadecyloxy)-3-methoxybenzoate (C₅): M.F.: $C_{43}H_{57}NO_5$, M.

Wt.: 667.92 g/mol, ^1H NMR (400 MHz, CDCl_3): δ 7.85 (d, J = 16.0 Hz, 1H, $\text{CH}=\text{CH}-\text{CN}$), 7.69–6.66 (m, 8H, Ar-H), 4.10 (t, J = 6.6 Hz, 2H, $-\text{OCH}_2-\text{C}_4\text{H}_9$), 4.02 (t, J = 6.5 Hz, 2H, Ar- OCH_2-), 3.85 (s, 3H, $-\text{OCH}_3$), 1.83–1.60 (m, 4H, $-\text{CH}_2-$), 1.44–1.32 (m, 6H, $-\text{CH}_2-$), 0.89 (t, J = 7.0 Hz, 3H, $-\text{CH}_3$). ^{13}C NMR (100 MHz, CDCl_3): δ 164.0 (C=O), 161.9, 153.7, 152.7 (Ar-C-O), 143.7, 133.3, 132.2, 129.5, 125.9, 123.3, 121.0, 119.2 (Ar-C, $\text{CH}=\text{CH}-\text{CN}$), 114.0 ($\text{C}\equiv\text{N}$), 69.4 (Ar- OCH_2-), 66.7 ($-\text{OCH}_2-$), 57.1 ($-\text{OCH}_3$), 32.4, 29.9, 26.9 ($-\text{CH}_2-$), 14.7 ($-\text{CH}_3$). FTIR (KBr, cm^{-1}): ν 3059–3007 (Ar-C-H), 2950, 2921, 2859 (aliphatic C-H), 2220 ($\text{C}\equiv\text{N}$, nitrile), 1737 (C=O, ester), 1608, 1578, 1517 (Ar-C=C), 1450, 1358 (C-H bending), 1271, 1233 (C-O-C stretch, ester and alkoxy), 1172, 1033 (Ar-O- CH_2), 837, 750 (C-H out-of-plane bending). CHN analysis, calculated % (found %): C = 77.32 (77.02); H = 8.60 (8.43); N = 2.10 (2.07); O = 11.98 (11.78).

2.5. Texture analysis by Polarized Optical Microscopy (POM)

Polarizing optical microscopy (POM) was used to examine the surface textures and mesomorphic properties of the synthesized liquid crystalline samples. Clean, dry glass slides were prepared, and uniform molecular alignment was achieved by gently rubbing the slide in one direction using a cotton swab. The sample was placed on the slide, heated to its isotropic phase to ensure complete melting, then rapidly cooled to room temperature and sealed with a cover slip to stabilize the mesophase. The resulting textures were observed and recorded using POM, and mesophases were identified based on their characteristic optical appearances. The liquid crystal cell thickness was maintained between 5 and 20 μm .

2.6. Thermal Analysis by Differential Scanning Calorimetry (DSC)

The mesomorphic behavior of the synthesized liquid crystalline derivatives was analyzed using differential scanning calorimetry (DSC). Approximately 3–5 mg of each sample was sealed in aluminum pans and analyzed under a nitrogen atmosphere. Thermal scans were performed from room temperature to 410 $^{\circ}\text{C}$ at a heating rate of 10 $^{\circ}\text{C}/\text{min}$. The heat flow curves were used to determine phase transition temperatures and enthalpy changes (ΔH), providing insight into melting and transitions to the isotropic phase, characteristic of α,β -unsaturated nitrile systems.

2.7. Density Functional Theory (DFT) analysis

Density Functional Theory (DFT) is a robust quantum mechanical method employed to analyze the electronic properties, molecular geometry, and frontier molecular orbitals (FMOs) of Schiff base-derived liquid crystalline compounds. The energy levels of the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) play a crucial role in determining the electronic characteristics of these materials.

3. Results and Discussion

A series of compounds (Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(alkoxy)-3-methoxybenzoates (C_1-C_5), was successfully synthesized as illustrated in Scheme 1 and their structures were confirmed through comprehensive characterization techniques.

3.1. Structural elucidation

3.1.1. α,β -unsaturated nitrile (Z)-3-(4-butoxyphenyl)-2-(4-hydroxyphenyl)acrylonitrile (A)

The ^1H NMR spectrum of Compound A confirms its structure. A deshielded singlet at δ 7.69 ppm, corresponding to the vinylic proton ($\text{CH}=\text{}$) of the α,β -unsaturated nitrile. Aromatic protons appear as multiplets in the region of δ 6.85–7.92 ppm, attributable to the two para-substituted phenyl rings. The phenolic $-\text{OH}$ proton usually resonates as a broad singlet at δ 9.81 ppm [19], possibly exchangeable. The butoxy ($-\text{OCH}_2-$) group appears at 4.0 ppm, while aliphatic $-\text{CH}_2-$ and $-\text{CH}_3$ signals are found at 1.50–1.82 ppm and 1.32 ppm, respectively. The ^{13}C NMR spectrum supports the structural framework. The nitrile carbon ($\text{C}\equiv\text{N}$) typically appears around δ 130 ppm in the spectrum [20]. The vinylic carbons ($\text{C}=\text{C}$) resonate between δ 130–140 ppm, with the more deshielded carbon adjacent to the nitrile group ($\text{C}-\text{CN}$) appearing closer to δ 122 ppm. The aromatic ring carbons are observed in the range of δ 128–130 ppm, with the phenolic carbon ($\text{C}-\text{OH}$) and the ether-linked aromatic carbon ($\text{C}-\text{OCH}_2$) appearing more downfield due to deshielding effects. The OCH_2 group of the butoxy side chain resonates at δ 69 ppm, while the remaining aliphatic carbons in the butyl chain ($-\text{CH}_2-$ and $-\text{CH}_3$) appear in the δ 13.7–32.8 ppm region. The FT-IR spectrum confirms the presence of key functional groups. A broad absorption band observed in the 3312 cm^{-1} region corresponds to the phenolic ($-\text{OH}$) stretching, indicating hydrogen bonding [21]. A sharp and intense peak at 2225 cm^{-1} confirms the presence of the nitrile ($-\text{C}\equiv\text{N}$) functional group [22]. The $\text{C}=\text{C}$ stretching vibrations of the aromatic rings and conjugated vinyl ($-\text{CH}=\text{}$) system appear in the 1620 cm^{-1} region. The aromatic C-H stretching is observed between 3060–2902 cm^{-1} , while the aliphatic C-H stretching from the butoxy ($-\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$) group is detected in the 2800–2950 cm^{-1} region. The C-O stretching of the ether ($-\text{OCH}_2-$) group appears in the 1050–1250 cm^{-1} range, confirming the butoxy substitution. Additionally, the C-H out-of-plane bending vibrations in the 790 cm^{-1} regions support the para-substituted benzene system. These spectral features collectively validate the structural composition of the compound.

3.1.2. (Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(alkoxy)-3-methoxybenzoate (C_1-C_5)

The structures of (Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(alkoxy)-3-methoxybenzoates (C_1-C_5) were confirmed by various spectroscopic techniques. In the FTIR spectra, all compounds exhibit a strong and sharp nitrile ($\text{C}\equiv\text{N}$) stretching vibration in the range $\sim$ 2230 cm^{-1} , indicative of the acrylonitrile moiety. A prominent ester carbonyl ($\text{C}=\text{O}$) stretching band is observed at $\sim$ 1730 cm^{-1} , confirming the benzoate ester functionality. The C-O-C stretching vibrations of the alkoxy and methoxy substituents are seen between 1240–1280 cm^{-1} [21], while the aromatic $\text{C}=\text{C}$ stretching bands appear near $\sim$ 1600–1500 cm^{-1} . Aliphatic C-H stretching vibrations corresponding to the butyl and alkyl chains occur in the 3000–3050 cm^{-1} regions, and their intensities increase with longer alkyl chain lengths. The ^1H -NMR spectra of all derivatives show a characteristic vinylic proton signal as a doublet at δ $\sim$ 7.8 ppm, with a large coupling constant, indicative of the (Z)-configuration across the $\text{C}=\text{C}$ bond [23]. Aromatic protons appear as multiplets between δ $\sim$ 6.7–8.0 ppm, consistent with the substituted phenyl systems. The methoxy protons on the benzoate ring give a singlet at δ $\sim$ 3.8 ppm, while the OCH_2 protons of both the butyl and varying alkoxy chains resonate as triplets in the δ $\sim$ 3.8–4.1 ppm range. Methylene groups appear as multiplets at δ

~1.3–1.7 ppm, and the terminal methyl protons resonate as triplets around δ ~0.80–0.90 ppm, with expected signal broadening as chain length increases. In the ^{13}C -NMR spectra, the nitrile carbon ($\text{C}\equiv\text{N}$) is detected at δ ~117–120 ppm, while the vinylic carbons appear in the δ ~125–145 ppm range [20]. The ester carbonyl carbon ($\text{C}=\text{O}$) is observed downfield at δ ~165 ppm, confirming the benzoate ester linkage [24]. Aromatic carbons are distributed between δ ~114–160 ppm, including deshielded carbons bonded to oxygen ($\text{C}-\text{O}$ and $\text{C}=\text{O}$). The methoxy carbon resonates at δ ~55 ppm, and the OCH_2 carbons from the alkoxy chains appear around δ ~65 ppm. Aliphatic methylene and methyl carbons resonate in the δ ~13–35 ppm region, with the number and intensity of peaks increasing systematically from C_5 to C_{16} due to longer chain lengths.

The structural differences between Compound A and the series C_1 – C_5 are distinctly reflected in their spectroscopic characteristics, confirming the successful transformation from the hydroxy precursor to the corresponding ester derivatives. In the FTIR spectra, both Compound A and C_1 – C_5 exhibit a prominent absorption band around $\sim 2230\text{ cm}^{-1}$, characteristic of the nitrile ($-\text{C}\equiv\text{N}$) functional group, indicating that this moiety remains unaffected during the reaction. However, Compound A shows a broad and intense $\text{O}-\text{H}$ stretching band around $\sim 3312\text{ cm}^{-1}$, which is completely absent in the spectra of C_1 – C_5 , confirming the consumption of the phenolic hydroxyl group during esterification. Instead, the ester derivatives display a strong carbonyl ($\text{C}=\text{O}$) stretching band near $\sim 1735\text{ cm}^{-1}$ along with $\text{C}-\text{O}-\text{C}$ stretching vibrations in the range of ~ 1240 – 1280 cm^{-1} , providing clear evidence for the formation of the ester linkage [21]. Further support for this structural transformation is obtained from the ^1H NMR spectra. In all compounds, the aromatic protons resonate in the δ 6.7–8.0 ppm region, while the (Z)-configured vinylic proton appears as a characteristic doublet around δ ~7.8 ppm. In Compound A, a distinct phenolic $-\text{OH}$ proton signal is observed in the δ ~5.5–6.0 ppm range, which disappears completely in the spectra of C_1 – C_5 , confirming its involvement in ester formation. This is accompanied by the appearance of a methoxy proton singlet around δ ~3.8 ppm in the ester derivatives. Additionally, the alkyl chain protons in C_1 – C_5 give rise to characteristic signals in the upfield region, further supporting the successful incorporation of varying alkoxy chains. Overall, these spectroscopic changes clearly demonstrate the conversion of the hydroxy precursor into the corresponding ester-based

liquid crystalline derivatives. The OCH_2 protons of the chains appear at δ ~4.0 ppm, while terminal methyl protons resonate at δ ~0.88 ppm. ^{13}C -NMR confirms nitrile (δ ~118 ppm), vinylic (δ 125–145 ppm), ester carbonyl (δ ~165 ppm), and methoxy/ OCH_2 carbons (δ ~55–72 ppm) [20]. Aliphatic chain signals increase in intensity with longer chains, while core signals remain consistent, validating structural integrity across the series.

3.2. Polarized Optical Microscopy (POM) Observation

The mesophase textures of the synthesized liquid crystalline compounds (C_1 – C_5) were examined using polarized optical microscopy (POM) during controlled heating. The POM images in Figure 1 reveal distinct textural changes that are indicative of mesophase formation and type, which correlate strongly with alkyl chain length and the dipolar character predicted by DFT analysis. C_1 exhibited a relatively isotropic dark texture, suggesting poor mesophase formation or a very narrow nematic range close to the melting or clearing point. This behavior is consistent with its lower dipole moment and higher optimization energy (least negative), indicating weak intermolecular interactions insufficient to promote mesophase stability. The absence of clear birefringent textures supports the assignment of a short-range or unstable nematic phase. C_2 & C_3 compounds showed typical thread-like and schlieren textures, characteristic of enantiotropic nematic phases. The birefringence and formation of tactoids (elongated thread patterns) suggest better molecular alignment and dipolar interactions compared to C_1 . This trend aligns with increasing chain length and dipole moment (up to $\sim 9.90\text{ D}$), which enhances intermolecular attractions and promotes more stable mesophase formation. The textures observed are dynamic and well-defined, indicating stable nematic ranges over a wider temperature span. For the longer-chain homologues C_4 & C_5 , POM images displayed highly birefringent, fan-shaped and mosaic textures, typical of smectic A or smectic C phases. These textures suggest the presence of a lamellar structure with layered molecular organization, supported by the greater thermodynamic stability (more negative optimization energy) and highest dipole moments ($\sim 9.91\text{ D}$). The increase in molecular length facilitates efficient packing, while the enhanced polarity supports stronger lateral and longitudinal interactions, favoring smectic phase formation over simple nematic alignment.

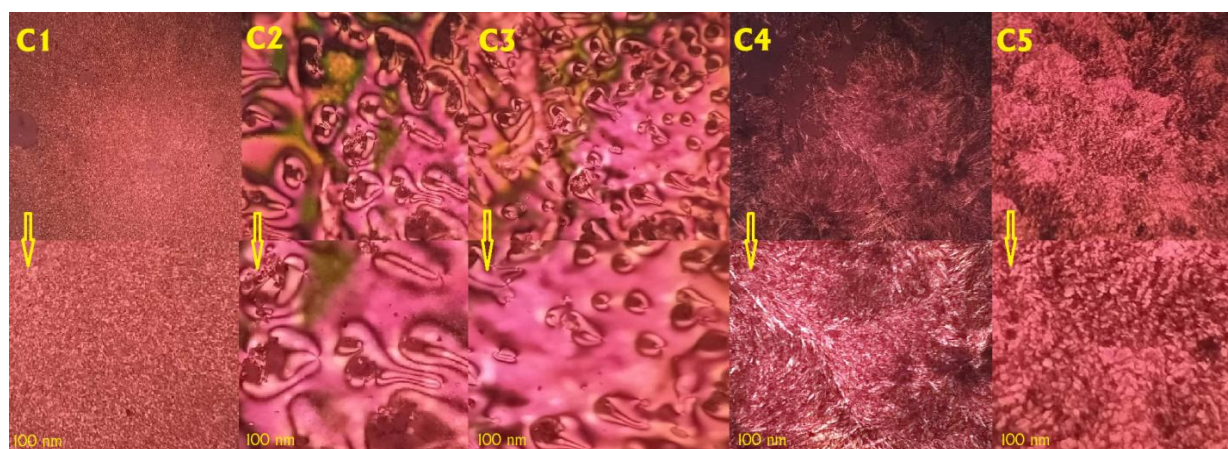


Fig. 1. POM images of C_1 – C_5 .

Structure–Mesophase Relationship: The evolution of mesophase texture from isotropic/nematic (C_1) to well-

ordered smectic (C_4 , C_5) is clearly driven by two factors: (1) Increasing alkyl chain length, which enhances flexibility and

van der Waals packing (2) Higher dipole moments, which stabilize intermolecular alignment and increase order [25–28]. The polarizing optical microscopy (POM) analysis data presented in Table 1 reveals the liquid crystalline phase behavior of a homologous series of compounds (C_1 to C_5) bearing varying alkyl chain lengths ranging from carbon 8 to carbon 16.

Table 1. POM Analysis, Transition Phase(s) & Transition Temperature ($^{\circ}\text{C}$).

Sample	Carbon Chain	Cr–Sm ($^{\circ}\text{C}$)	Sm–N ($^{\circ}\text{C}$)	N–Iso ($^{\circ}\text{C}$)
C_1	C8	---	70	78
C_2	C10	---	57	75
C_3	C12	49	66	81
C_4	C14	45	60	70
C_5	C16	50	56	65

Note: Cr = Crystalline; N = Nematic; Sm = Smectic, Iso = isotropic; -- = not performed, - = not obtained

The observed mesophase transitions, specifically Cr–Sm, Sm–N, and N–Iso, offer insightful correlations between molecular structure and thermal mesophase stability. Compounds C_1 (carbon 8) and C_2 (carbon 10) exhibit a direct transition from the crystalline phase to the nematic (N) phase, bypassing the smectic (Sm) phase entirely. This absence of the Sm phase in shorter-chain derivatives suggests insufficient molecular length or packing interactions to stabilize the layered smectic arrangement. From compound C_3 (carbon 12) onward, the Sm phase becomes evident, with Cr–Sm transition temperatures observed at 49°C , 45°C and 50°C for C_3 , C_4 , and C_5 , respectively. This emergence of the smectic phase upon increasing chain length indicates that extended alkyl chains enhance van der Waals interactions and promote the formation of ordered lamellar structures typical of smectic mesophases. The Sm–N transitions for C_3 to C_5 range between 56°C and 66°C , with the highest temperature noted for C_3 , suggesting optimal chain length and mesogenic balance in this compound. Interestingly, the nematic-to-isotropic (N–Iso) transition temperatures show a decreasing trend with increasing chain length: 78°C for C_1 , gradually dropping to 65°C for C_5 . This trend implies that while longer chains favor smectic organization, they also introduce flexibility and disorder that reduce the thermal stability of the nematic phase. Among all, C_3 (carbon 12) demonstrates the most stable and extended mesophase region, undergoing all three transitions (Cr–Sm–N–Iso), indicating an ideal balance between rigidity and flexibility in the molecular architecture. Overall, the study highlights how systematic variation in terminal alkyl chain length modulates mesophase formation and thermal behavior, a key factor in designing efficient liquid crystalline materials.

3.3. Thermal Analysis by Differential Scanning Calorimetry (DSC)

To validate the phase transitions observed under polarized optical microscopy (POM), DSC analysis was performed for compound C_3 (C_{12}). The DSC thermogram (Figure 2) exhibits three well-defined endothermic transitions that are in good agreement with the Cr–Sm–N–Iso phase sequence, thereby confirming and supporting the mesophase assignments derived from POM observations.

An initial weak endothermic transition is observed at around 25°C , which is attributed to a solid–solid (crystal–crystal) phase transition. Such low-enthalpy transitions are

commonly associated with molecular rearrangements within the crystalline lattice, particularly due to conformational changes of the flexible alkyl chains or minor reorganization of the aromatic core. This transition suggests the onset of reduced crystalline order prior to mesophase formation. A second distinct endothermic peak appears at approximately 54°C , corresponding to the crystalline-to-liquid crystalline (Cr $\rightarrow$ LC) phase transition. The moderate enthalpy change associated with this transition indicates partial loss of positional order while preserving long-range orientational order, which is characteristic of the formation of a liquid crystalline mesophase. This transition confirms the mesogenic nature of the compound. Upon further heating, a prominent endothermic transition is detected in the temperature range of 77 – 80°C , which is assigned to the clearing transition (LC $\rightarrow$ Iso). This transition represents the transformation from the ordered liquid crystalline phase to the isotropic liquid state and is accompanied by a relatively high enthalpy change, reflecting the complete loss of orientational order. The sharp and well-defined nature of this transition indicates a thermally stable mesophase over a reasonably wide temperature range. Overall, the DSC thermogram suggests the following phase sequence on heating: Crystalline $\rightarrow$ Crystal–Crystal $\rightarrow$ Liquid Crystal $\rightarrow$ Isotropic. The presence of a stable mesophase window between approximately 54°C and 77°C highlights the effective balance between molecular rigidity imparted by the Schiff base linkage and flexibility provided by the terminal alkoxy chains. This balance plays a crucial role in stabilizing the liquid crystalline phase. The observed thermal behavior is in good agreement with typical thermotropic liquid crystalline Schiff base systems and supports the structure–property relationship proposed for the present compound.

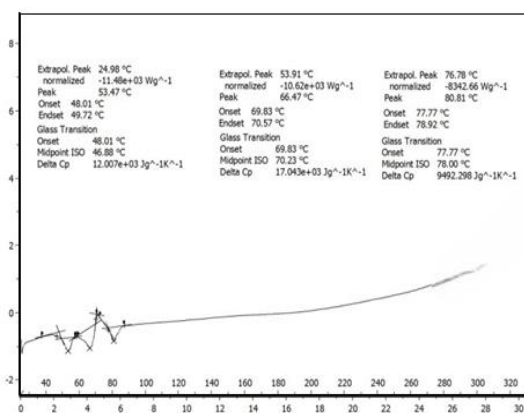


Fig. 2. DSC analysis of compound C_3 .

3.4. Frontier molecular orbitals (FMOs) and Reactivity Parameters

3.4.1. Density Functional Theory (DFT) analysis

To understand the structure–property relationships of the synthesized liquid crystalline compounds (C_1 – C_5), density functional theory (DFT) calculations were performed. The theoretical calculations and computations were performed using the Gaussian 16W software suite [29], and the frontier molecular orbitals (FMOs) of these molecules were obtained using the Gauss View 6.1 program [30]. The HOMO–LUMO energies, energy gap (Eg), ionization potential (IP), electron affinity (EA), optimization energy, and dipole moment were evaluated at the optimized geometries. The results are summarized in Table 2.

Table 2. POM Analysis Transition Phase(s) & Transition Temperature (°C).

Comp- ound	Carbon Chain	E _{HOMO} (eV)	E _{LUMO} (eV)	$\Delta E_{\text{gap}} / E_g$ (energy gap) (eV)	η = $\Delta E_g / 2$ (eV)	S = 1/ ΔE_g = 1/2 η (eV ⁻¹)	Ioniza- tion Potential (I)	Electron affinity (EA)	Optimi- zation energy (eV)	Dipole moment (Debye)
C1	C8	-8.6682	-0.828	7.8404	3.9202	0.12754	8.6682	0.8278	-5.5461	9.874527
C2	C10	-8.6685	-0.829	7.8399	3.91995	0.12755	8.6685	0.8286	-5.9779	9.889944
C3	C12	-8.6685	-0.829	7.8396	3.9198	0.12756	8.6685	0.8289	-6.41	9.899667
C4	C14	-8.6687	-0.829	7.8393	3.91965	0.12756	8.6687	0.8294	-6.8423	9.905194
C5	C16	-8.6687	-0.83	7.8391	3.91955	0.12757	8.6687	0.8297	-7.2745	9.909477

Note: ΔE_{gap} (Energy Gap) = (E_{HOMO} – E_{LUMO}); η = Chemical hardness = $\Delta E_g / 2$; S = Chemical softness; I = Ionization Potential, EA = Electron Affinity.

Frontier Molecular Orbitals (HOMO–LUMO) and Energy Gap: All compounds displayed HOMO energies around –8.668 eV and LUMO energies near –0.828 eV. As the terminal alkyl chain length increased from C₁ to C₅, both the HOMO and LUMO levels became marginally more negative, indicating a slight stabilization of frontier orbitals. The HOMO–LUMO energy gap (E_g) showed a subtle decrease from 7.8404 eV (C₁) to 7.8391 eV (C₅). This negligible variation suggests that the terminal alkyl chains, being electronically inert, do not significantly alter the π -conjugated core responsible for electronic transitions. Such narrow fluctuations in E_g indicate that electronic excitation energies remain relatively constant across the series, implying that optical and electronic properties onsets and dielectric responses will be largely governed by the core structure, rather than by the alkyl chain length.

Ionization Potential and Electron Affinity: The ionization potentials closely mirrored the HOMO values, remaining stable across the series (~8.668 eV). This further supports the notion that the electronic donating capacity of the molecules is governed by the rigid π -system. Electron affinity values exhibited a slight increase, from 0.8278 eV (C₁) to 0.8297 eV (C₅), indicating a marginal enhancement in electron-accepting ability with increasing chain length. While small, this could contribute to enhanced dipolar interactions in the bulk state, promoting better LC alignment [31].

Optimization Energy and Thermodynamic Stability: A significant trend was observed in the optimization energy, which became progressively more negative with increasing chain length: –5.5461 eV (C₁) → –7.2745 eV (C₅). This trend reflects improved thermodynamic stability in longer-chain derivatives. The increased van der Waals interactions from extended alkyl chains likely stabilize the overall molecular conformation, which may also facilitate better molecular packing and enhanced mesophase stability [32].

Dipole Moment and Polar Interactions: Dipole moments showed a consistent increase with chain elongation, ranging from 9.8745 D (C₁) to 9.9095 D (C₅). This increase is attributed to the cumulative vector contribution of the electron-withdrawing nitrile and ester groups and the growing asymmetry induced by longer flexible alkyl chains. High dipole moments are beneficial for liquid crystalline behavior as they promote strong intermolecular dipole–dipole interactions, facilitating better molecular alignment and phase ordering. These effects are particularly important in thermotropic mesophases where polar interactions drive the formation and stabilization of nematic or smectic phases.

3.4.2. Molecular Electrostatic Potential (MEP) Analysis

To further understand the intramolecular charge distribution and potential sites for intermolecular interactions, Molecular Electrostatic Potential (MEP) surface maps were

generated for compounds C₁–C₅ at their optimized geometries using DFT calculations. The MEP provides valuable insights into the electron-rich (nucleophilic) and electron-deficient (electrophilic) regions across the molecular surface, which are essential in predicting non-covalent interactions, such as dipole–dipole alignment, hydrogen bonding, and π – π stacking critical factors for liquid crystalline self-assembly [33]. The Frontier Molecular Orbital (FMO) images for all compounds are presented in Figure 3.

Charge Distribution and Reactive Sites: The MEP surfaces clearly reveal that the most negative electrostatic potential (deep red region) is localized around the nitrile (–CN) group, confirming its strong electron-withdrawing nature. This region is the primary site for dipolar interactions and may act as a hydrogen bond acceptor. The carbonyl oxygen atoms of the ester linkage also exhibit moderately negative potential, contributing to additional sites for intermolecular interactions. In contrast, positive electrostatic potential regions are observed near the hydrogen atoms of the aromatic rings and terminal alkyl chains, especially around the methylene hydrogen adjacent to the ether oxygen. These partial positive regions can participate in weak C–H...O hydrogen bonding or van der Waals interactions in the mesophase.

Effect of Alkyl Chain Length on MEP: While the core electrostatic features remain consistent across the C₁–C₅ series (as the π -conjugated mesogenic core is unchanged), minor differences arise in the overall shape and spread of the potential with increasing alkyl chain length: Longer alkyl chains slightly increase the molecular volume and influence the distribution of potential, leading to asymmetrical MEP surfaces that favor molecular ordering in specific directions. These subtle asymmetries may enhance cooperative interactions, which contribute to phase stability and textural uniformity in liquid crystalline phases [34].

Dipolar Orientation and Mesophase Stability: The combination of a highly negative nitrile terminus, moderately polar ester moieties, and increasing dipole moment with chain length (as shown in Table 2) supports strong head-to-tail dipole alignment. This orientation is particularly favorable in nematic and smectic mesophases, where dipolar interactions govern long-range order and texture formation. Furthermore, the clear charge separation indicated by the MEP surface aligns with the experimentally observed high dipole moments (9.9 D) and supports the hypothesis that polar interactions play a dominant role in mesophase formation and stability across this homologous series [35].

The MEP study complements the electronic and dipolar data by visually and quantitatively confirming that: (1) Nitrile and carbonyl groups serve as dominant polar interaction sites, (2) Alkyl chain extension modulates potential distribution without disrupting core reactivity, and (3) These features collectively facilitate anisotropic alignment, essential for

thermotropic liquid crystalline behavior [36–37].

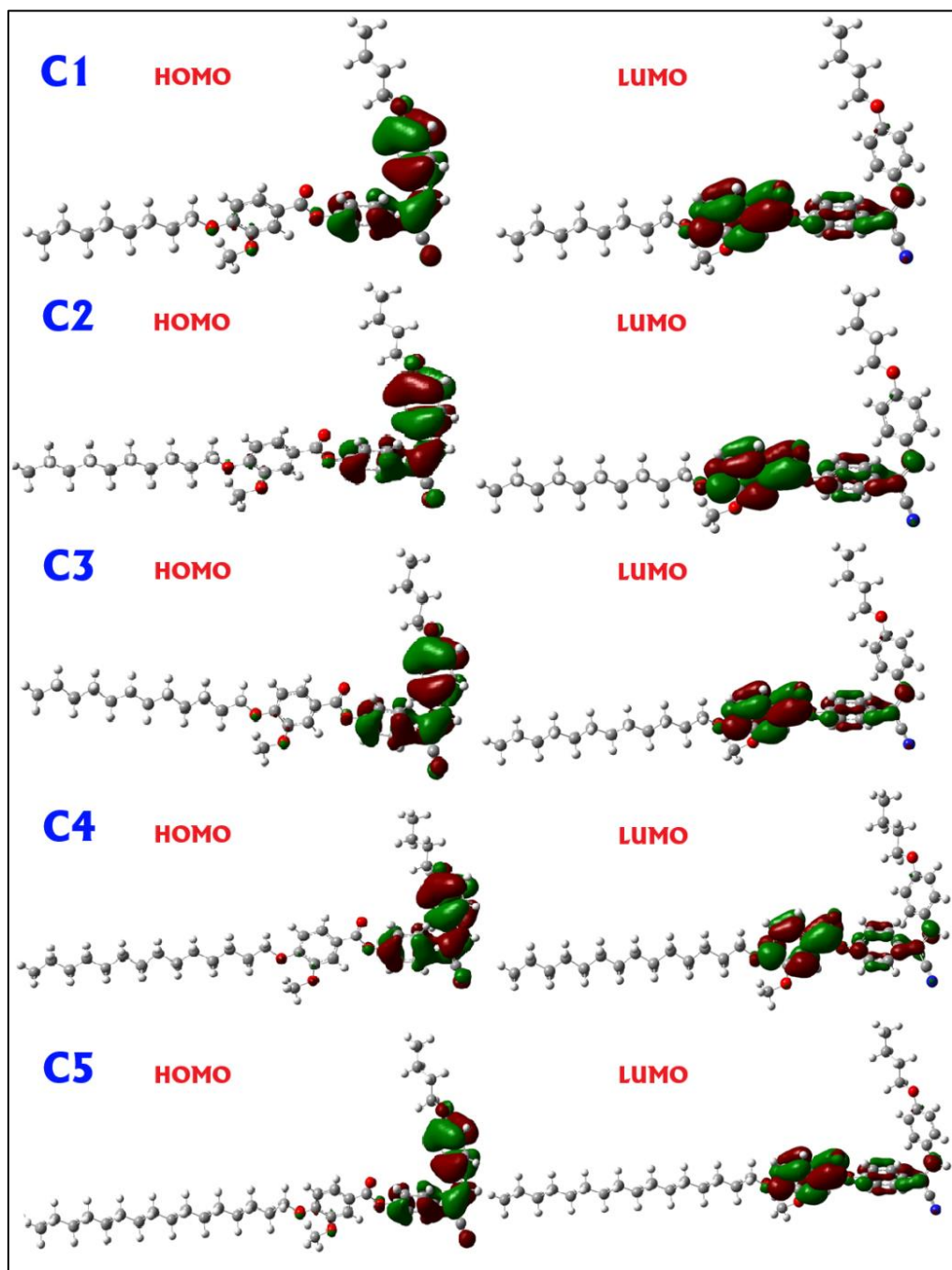


Fig. 3. FMOs images for samples C₁-C₅.

4. Conclusions

A homologous series of (Z)-4-(2-(4-butoxyphenyl)-1-cyanovinyl)phenyl 4-(alkoxy)-3-methoxybenzoates (C₁–C₅) was successfully synthesized and structurally characterized. Spectroscopic techniques confirmed the proposed molecular structures, while computational studies, including DFT calculations, provided further insight into the molecular geometry, electronic distribution, and reactivity patterns. The combination of experimental and theoretical approaches not only validated the structural integrity of the synthesized compounds but also highlighted the influence of alkoxy chain length on molecular behavior offering valuable information for the design of future liquid crystalline materials.

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Author Contributions

Ami Y. Patel, the research scholar, conducted the experimental work, developed the methodology, performed data analysis, and drafted the manuscript. Mukeshkumar L. Chauhan, the research supervisor, provided continuous

guidance throughout the research process, contributed to the conceptual framework, and reviewed and edited the final manuscript for intellectual content.

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