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New Schiff's base liquid crystals with biphenyl/benzoylphenyl tail substitutes: synthesis, characterisation, mesomorphic behaviour and DFT calculation

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ABSTRACT

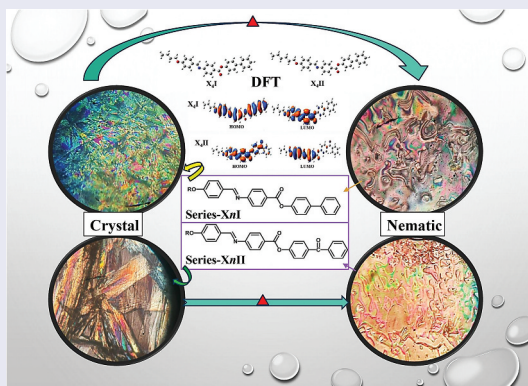
A novel series of nematic liquid crystals with rod-like structures, derived from [1,1'-biphenyl]-4-yl(E)-4-((4-*n*-alkoxybenzylidene) amino) benzoate (**X_{nI}**) and 4-benzoylphenyl (E)-4-((4-*n*-alkoxy) benzylidene) amino) benzoate (**X_{nII}**) have been successfully synthesised, where *n* ranges from 4, 6, 8 & 10. Proton magnetic resonance, mass and infrared spectroscopy were used to analyse and characterised. Differential scanning calorimetry (DSC) and polarising optical microscopy (POM) were used to examine the liquid crystal behaviour of all produced substances. All homologous series **X_{nI}** and **X_{nII}** compounds displayed a nematic mesophase. The impact of molecular flexibility, the range of transition temperatures and the comparative research were all systematically investigated. The **X_{4I}**–**X_{10I}** homologues exhibit an enantiotropic nematic mesophase within the temperature range of 177–148°C, while the **X_{4II}**–**X_{10II}** homologues show a nematic mesophase at temperatures between 169 and 122°C. **X_{nI}** & **X_{nII}** compounds studied using Gauss View 6 software and were subjected to geometry optimisation using the Density Functional Theory (DFT) calculations at the B3LYP/6-31+G(d,p) level of theory as implemented in Gaussian 16 quantum chemistry package. The band gap values, calculated by the difference of the energy values of HOMO and LUMO, were higher for the **X_{nI}** series as compared to the **X_{nII}** compounds.

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Liquid crystal; mesogenic; nematic; benzophenone



1. Introduction

Mesomorphic behaviour and mesophase stability are influenced by molecular geometry and species design [1]. A notable shift in their mesomorphic properties is provided by the modification in molecular geometry [2–4]. The inclusion of various flexible groups, terminal groups and mesogenic components can cause thermotropic liquid crystals (LCs) to differ, which in turn impacts the thermal characteristics, dipole moment and

polarisability [5–7]. The presence of azomethine group in the rigid core as a linking group helps in maintaining the linearity [8]. Stronger π – π interactions among molecules with various functionalities promote the formation of mesophases such as nematic phases. Notably, enhanced interactions ultimately result in distinctive molecular arrangements and different structural modifications [9,10]. Alamro *et al.* have investigated a biphenyl-based homologues series and examined the broad

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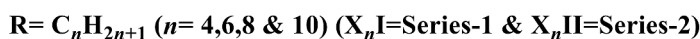
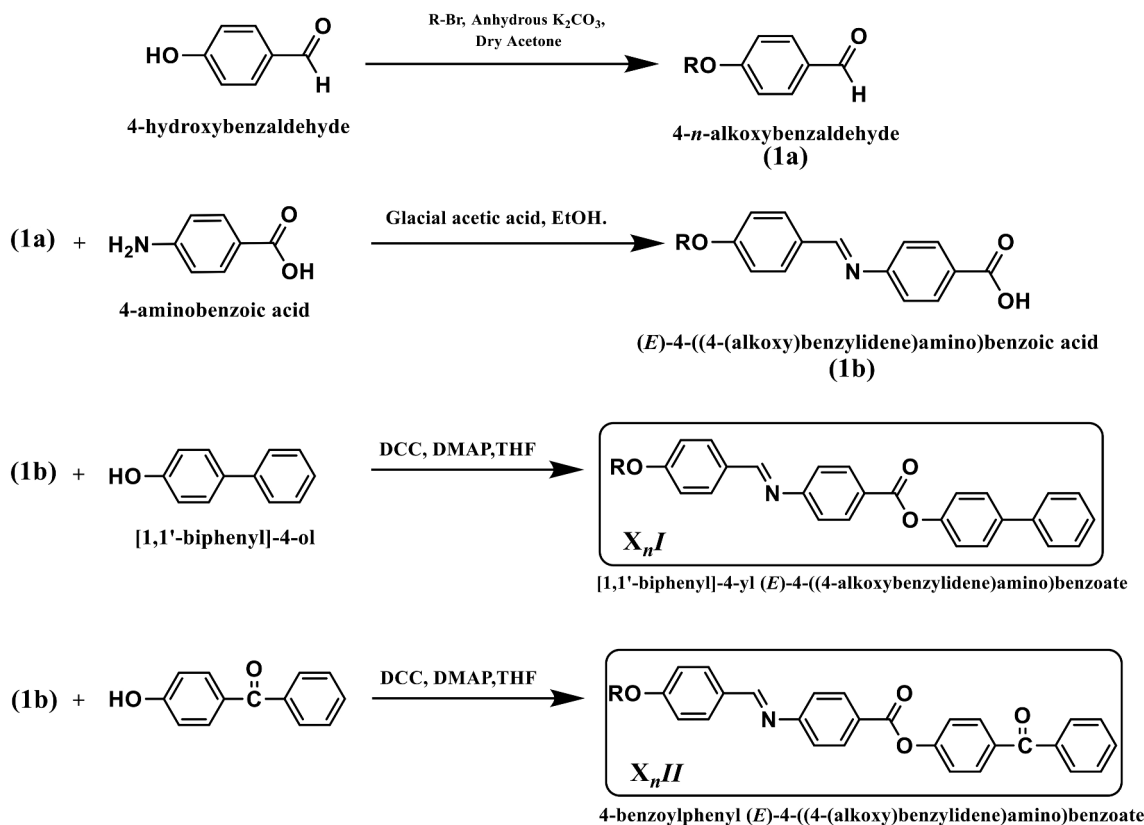
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nematogenic temperature ranges. The correlating computational studies demonstrated the increase in polarisability is due to the increased chain length. The stability of the possible geometries is highly affected by the biphenyl moiety [11]. They demonstrated the electrophysiological behaviour of nematic droplets in *Chara corallina* cells' cytoplasmic streaming, drug delivery methods and cytoplasmic streaming by applying the nematic emulsions [12]. To evaluate the effects of spacer length and chalcogen linkage on twist-bend nematic phase formation, this study predicted the characteristics of liquid crystal dimers and analysed their phase behaviour. Two novel homologous series of nonsymmetric cyanobiphenyl-based dimers were synthesised using an alkyl spacer chain, linked by ether, thioether and selenium ether [13]. The researchers investigated liquid crystal dimers in super-cooled nematic phases. Crystallisation was not detected during cooling cycles. The molecules exhibited unique fluorescence properties and were deemed to be suitable for developing photo-responsive optical sensors [14]. Two distinct series of symmetric liquid crystal dimers, 1F and 3F, have been formed by different length of the flexible odd spacer. Compared to the 1F series, which only displays the nematic phase, the 3F series exhibits both the smectic A and nematic phases, as well as greater melting temperature and clear points [15]. The presence of Schiff base makes the molecule more stable with stepped mesophase [16–19]. The Schiff's base family and ester-based moiety with crystalline phases were examined by Panchal *et al.* and further evaluated using Gauss View 6 software. As a result, the molecules were optimised using DFT calculations, and the complex permittivity data were determined [20]. A.K. Prajapati and Hemant N Patel *et al.* have investigated that Schiff bases generate a core molecular architecture that features a stepped arrangement. This structural configuration preserves the molecule's overall linearity [21–26]. Robust designing of the novel molecules helps in developing better mesophase by the use of heteroatoms like nitrogen, oxygen and sulphur [27–29]. Researchers are currently focusing on biphenyl moieties because they are less expensive, have mesogenic cores and have greater π – π interactions and structural rigidity [30,31]. Biphenyl ester-aromatic imine derivatives have been produced by Iskandar *et al.* All target compounds exhibit enantiotropic nematic phase in exposure of polarised light.

The magnetic interaction of compounds containing non-metal and non-radical moieties are mostly diamagnetic. The presence of this matter may be explained by the orientation of LC materials, which are further controlled by a weak electric or magnetic field because of the anisotropy of the electrical and magnetic characteristics [32]. V.K. Joshi *et al.* synthesised homologous series of

biphenyl-based esters and investigated comparative analysis of the mesomorphic characteristics of the novel biphenyl bis-ester liquid crystals ABAE was conducted with structurally similar compounds to understand the impact of different mesogenic components within the molecular structure [33]. Using TD-DFT computing to record the interaction energy and HOMO–LUMO orbital energy gap, two new homologous series containing cinnamates, ester central linkage and naphthalene group at the terminal position were synthesised and their impact on mesomorphism assessed [34]. They explored aspect ratio, polarisabilities, molecular electrostatic potentials and Frontier molecular orbitals via DFT calculations [35–38]. Further, the introduction of azomethine and the ester groups as central attachment guide in identifying twist-bend smectic phases [39,40]. Lateral and longitudinal arrangement alters a dipole moment, polarity, dielectric constants and geometrical array [41,42]. The researchers have investigated the application of 5CB liquid crystal (LC) based on its orientational ordering and viscosity properties. Using the Lifshitz–Slyozov–Wagner (LSW) theory, they attempted to enhance the 5CB molecule's planar ordering while adhering to the underlying mechanism [43]. The study team has developed two new photosensitive chiral-based chemicals, which are basically derivatives of cinnamic acid produced in (R) and (S) enantiomer forms. While their racemates have been shown to have nematic and smectic phases, the enantiomers have been found to have cholesteric and TGB phases [44].

Along with studying the thiadiazol heterocycle, the group created new Janus-type compounds based on biphenyl units within two hemisphere structures. The photoluminescent properties of the recently synthesised materials were examined in solution [45]. Researchers examined how the electro-optical and thermodynamic properties of the nematic liquid crystal 5CB were affected by the doping agents 4-octyloxybenzoic acid and 4-octyloxy-3-fluoro benzoic acid. The findings presented here indicate that 8OBA dopant may be utilised to create a nematic liquid crystal phase with a low threshold, good thermal stability and fast reaction times [46]. Our current research work focused on the mesophase behaviour of biphenyl liquid crystalline derivatives with core linkages of biphenyl/benzoylphenyl (shown Scheme 1) to evaluate the structure–property relationship. Our main focus was to derivatise the new designed liquid crystalline series with biphenyl group provides free rotation to the molecular skeleton also help increasing the flexibility. We hypothesise that both Series X_nI and X_nII derivatives exhibit nematogenic properties at different temperatures.



Scheme 1. Synthetic route for series X_nI & X_nII .

2. Experimental

2.1. Materials and method

4-Hydroxybenzaldehyde, potassium carbonate (K_2CO_3), dry acetone, *n*-alkyl bromide, 4-amino benzoic acid, glacial acetic acid, ethyl alcohol, *N,N'*-dicyclohexylcarbodiimide, 4-dimethylaminopyridine, tetrahydrofuran, 4-phenylphenol and 4-hydroxybenzophenone were used. Thin layer chromatography (TLC) was conducted using pre-coated Merck Kiesel 60F254 plates. Infrared spectra (IR) were measured by Shimadzu IR-408 spectrophotometer, utilising potassium bromide (KBr) pellets as the medium. Proton nuclear magnetic resonance ($^1\text{H-NMR}$) spectra at 400 MHz spectra were obtained using a Bruker Advance Neo spectrometer with deuterated chloroform as the solvent. Mass spectra was recorded using Waters Single quadrupole mass detection (80–1500 ES^- , centroid, $\text{cv} = 30$). The examination of phase manifestation and transitions was conducted utilising thermal polarising optical microscopy (POM) through a polarising optical microscope equipped with a heating stage. The Leica DM 2500P polarising optical microscope, in

conjunction with a Linksys temperature control unit, was integrated with a Leica DFC295 camera to facilitate image acquisition. For sample preparation, a thin film of the powdered sample was secured between a glass slide and a coverslip. The enthalpies corresponding to phase transitions, expressed in kilojoules per mole, were measured employing a DSC 6000 instrument (PerkinElmer), which is classified as a differential scanning calorimeter (DSC), operating at a scan rate of 10°C per minute. The electronic structures of the experimentally investigated compounds (X_4I , X_6I , X_8I , X_{10}I & X_4II , X_6II , X_8II , X_{10}II) were studied using quantum mechanical calculations. Each compound was constructed using GaussView 6 software [47] and was subjected to geometry optimisation using the Density Functional Theory (DFT) calculations at the B3LYP/6–31+G(d,p) level of theory [48,49] as implemented in Gaussian 16 quantum chemistry package [50]. Further, the nature and energy values of the lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) were characterised using Frontier Molecular Orbital Analysis using Gauss View 6.

2.2. Synthesis

2.2.1. Synthesis of 4-*n*-alkoxybenzaldehydes

4-*n*-Alkoxybenzaldehydes were prepared using the method of Vyas and Shah *et al.* [51]. A mixture of 0.1 mole of 4-hydroxybenzaldehyde, 0.15 mole of anhydrous K_2CO_3 and 0.15 mole of corresponding 1-bromoalkane were added to 60 ml dry acetone. The mixture was refluxed on water bath for 6–8 hours. In the case of higher member, the refluxing period was extended up to 10–12 hours. The whole mass was added to cold water and the separated product was extracted with ether. The ether extract was subsequently subjected to treatment with a 5% NaOH solution (25 ml $\times$ 3), followed by washing with water (25 ml $\times$ 3) and finally brine, before being dried over anhydrous Na_2SO_4 . The resultant compound was purified via column chromatography using silica (100–200 mesh size) and 10% ethyl acetate-hexane as eluent furnished the product. The completion of the reaction was monitored and confirmed using thin layer chromatography (TLC) employing a solvent system of 70% ethyl acetate and hexane. Yield: 59–64%.

2.2.2. Synthesis of (E)-4-((4-*n*-alkoxybenzylidene) amino) benzoic acid

An amount of 0.01 mole of 4-*n*-alkoxybenzaldehydes for Series (X_nI and X_nII) were dissolved in dry ethanol. The solution was added drop-wise to the RBF (round bottom flask) containing 0.01 mole of 4-aminobenzoic acid (I), which was previously dissolved in dry ethyl alcohol [52] and few drops of glacial acetic acid and mixed homogeneously. The content of the flask was then heated under reflux for 4–6 hours. The reaction mixture was then filtered in the hot condition, and the product was allowed to precipitate. The precipitated crude product was repeatedly recrystallised from the ethyl alcohol. All the compounds of the present series were synthesised with the same method. Yield, in general, was 90–96%.

2.2.3. (X_nI and X_nII) Synthesis of [1,1'-biphenyl]-4-yl (E)-4-((4-alkoxybenzylidene) amino) benzoate & 4-benzoylphenyl (E)-4-((4-alkoxybenzylidene) amino) benzoate

A mixture of 0.10 mole (E)-4-((4-*n*-alkoxybenzylidene) amino) benzoic acid, 0.15 mole [1,1'-biphenyl]-4-ol (X_nI) and (4-hydroxyphenyl)(phenyl) methanone (X_nII), 0.1 mole DCC (*N,N'*-dicyclohexylcarbodiimide) [53] and 0.01 mole DMAP (4-dimethylaminopyridine) were dissolved in dry THF (tetrahydrofuran) and kept overnight with the help of mechanical stirring. The insoluble solid of

1,3-dicyclohexyl urea was removed by filtration. Now, residue was washed with a very small amount of THF. Solvent from the filtrate was separated out using rotary evaporator, solid material was recrystallised repetitively from methyl alcohol.

3. Characterisation

3.1. [1,1'-biphenyl]-4-yl (E)-4-((4-butoxybenzylidene) amino) benzoate

IR Spectrum (KBr) ν_{max}/cm^{-1} : 2927, 2857 (aliphatic C – H stretching), 1724 (C = O stretching, ester), 1638 (–CH = N–), 1520 (–C = C– stretching), 1275 (C – O stretching, ester), 1162 (C – O stretching, ether), 845 (C – H bending). 1H -NMR Spectrum (400 MHz, $CDCl_3$) δ in ppm: 8.41 (s, 1 H, –CH = N–), 8.25 (d, J = 7.5 Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.88 (d, 2 H, ArH), 7.63–7.28 (d, 8 H, ArH), 7.19–6.99 (t, 3 H, ArH), 4.06 (t, 2 H, Ar-O-CH₂–), 1.84–1.22 (m, 4 H, 2 X CH₂), 0.93 (t, J = 6.6 Hz, 3 H, CH₃).

3.2. [1,1'-biphenyl]-4-yl (E)-4-((4-(hexyloxy) benzylidene) amino) benzoate

IR Spectrum (KBr) ν_{max}/cm^{-1} : 2931, 2856 (aliphatic C – H stretching), 1724 (C = O stretching, ester), 1641 (–CH = N–), 1524 (–C = C– stretching), 1260 (C – O stretching, ester), 1167 (C – O stretching, ether), 851 (C – H bending). 1H -NMR Spectrum (400 MHz, $CDCl_3$) δ in ppm: 8.41 (s, 1 H, –CH = N–), 8.25 (d, J = 7.5 Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.88 (d, 2 H, ArH), 7.63–7.28 (d, 8 H, ArH), 7.19–6.99 (t, 3 H, ArH), 4.06 (t, 2 H, Ar-O-CH₂–), 1.84 (m, 2 H, CH₂–C-O–), 1.81–1.22 (m, 6 H, 3 X CH₂–), 0.94 (t, J = 6.6 Hz, 3 H, CH₃).

3.3. [1,1'-biphenyl]-4-yl (E)-4-((4-(octyloxy) benzylidene) amino) benzoate

IR Spectrum (KBr) ν_{max}/cm^{-1} : 2931, 2856 (aliphatic C – H stretching), 1724 (C = O stretching, ester), 1643 (–CH = N–), 1514 (–C = C– stretching), 1248 (C – O stretching, ester), 1167 (C – O stretching, ether), 849 (C – H bending). 1H -NMR Spectrum (400 MHz, $CDCl_3$) δ in ppm: 8.41 (s, 1 H, –CH = N–), 8.25 (d, J = 7.5 Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.88 (d, 2 H, ArH), 7.63–7.28 (d, 8 H, ArH), 7.03–6.99 (t, 3 H, ArH), 4.05 (t, 2 H, Ar-O-CH₂–), 1.84 (m, 2 H, CH₂–C-O–), 1.81–1.22 (m, 10 H, 5 X CH₂–), 0.96 (t, J = 6.7 Hz, 3 H, CH₃). Mass Spectrum (ESI-MS negative ion mode): m/z 504.46 ($[M-H]^-$, 100%); calculated mass for $C_{34}H_{35}NO_3$ = 505.

3.4. [1,1'-biphenyl]-4-yl (E)-4-((4-(decyloxy)benzylidene) amino) benzoate

IR Spectrum (KBr) $\nu_{\max}/\text{cm}^{-1}$: 2925, 2850 (aliphatic C – H stretching), 1726 (–C = O stretching, ester), 1628 (–CH = N–), 1507 (–C = C– stretching), 1247 (C – O stretching, ester), 1154 (C – O stretching, ether), 831 (C – H bending). $^1\text{H-NMR}$ Spectrum (400 MHz, CDCl_3) δ in ppm: 8.41 (s, 1 H, –CH=N–), 8.25 (d, $J = 7.5$ Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.82 (d, 2 H, ArH), 7.60–7.28 (d, 8 H, ArH), 7.16–6.91 (t, 3 H, ArH), 4.06 (t, 2 H, Ar–O–CH₂–), 2.11–1.22 (m, 16 H, 8 X CH₂–), 0.96 (t, $J = 6.6$ Hz, 3 H, CH₃). Mass Spectrum (ESI-MS negative ion mode): m/z 532.61 ($[\text{M-H}]^-$, 100%); calculated mass for $\text{C}_{36}\text{H}_{39}\text{NO}_3 = 533$.

3.5. 4-benzoylphenyl (E)-4-((4-butoxybenzylidene) amino) benzoate

IR Spectrum (KBr) $\nu_{\max}/\text{cm}^{-1}$: 2925, 2850 (aliphatic C – H stretching), 1728 (–C = O stretching, ester), 1669 (ketone), 1640 (–CH = N–), 1513 (–C = C– stretching), 1250 (C – O stretching, ester), 1165 (C – O stretching, ether), 843 (C – H bending). $^1\text{H-NMR}$ Spectrum (400 MHz, CDCl_3) δ in ppm: 8.41 (s, 1 H, –CH = N–), 8.25 (d, $J = 7.5$ Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.82 (d, 2 H, ArH), 7.60–7.28 (d, 8 H, ArH), 7.16–6.98 (t, 3 H, ArH), 4.03 (t, 2 H, Ar–O–CH₂–), 1.81–1.22 (m, 4 H, 2 X CH₂), 0.96 (t, $J = 6.6$ Hz, 3 H, CH₃).

3.6. 4-benzoylphenyl (E)-4-((4-(hexyloxy)benzylidene) amino) benzoate

IR Spectrum (KBr) $\nu_{\max}/\text{cm}^{-1}$: 2937, 2856 (aliphatic C – H stretching), 1730 (–C = O stretching, ester), 1666 (ketone), 1643 (–CH = N–), 1514 (–C = C– stretching), 1259 (C – O stretching, ester), 1164 (C – O stretching, ether), 851 (C – H bending). $^1\text{H-NMR}$ Spectrum (400 MHz, CDCl_3) δ in ppm: 8.41 (s, 1 H, –CH=N–), 8.25 (d, $J = 7.5$ Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.82 (d, 2 H, ArH), 7.60–7.28 (d, 8 H, ArH), 7.16–6.91 (t, 3 H, ArH), 4.07 (t, 2 H, Ar–O–CH₂–), 1.84 (m, 2 H, CH₂–C–O–), 1.82–1.22 (m, 6 H, 3 X CH₂–), 0.95 (t, $J = 6.6$ Hz, 3 H, CH₃). Mass Spectrum (ESI-MS negative ion mode): m/z 504.54 ($[\text{M-H}]^-$, 100%); calculated mass for $\text{C}_{33}\text{H}_{31}\text{NO}_4 = 505$.

3.7. 4-benzoylphenyl (E)-4-((4-(octyloxy)benzylidene) amino) benzoate

IR Spectrum (KBr) $\nu_{\max}/\text{cm}^{-1}$: 2924, 2850 (aliphatic C – H stretching), 1729 (–C = O stretching, ester), 1673 (ketone), 1649 (–CH = N–), 1511 (–C = C– stretching),

1251 (C – O stretching, ester), 1160 (C – O stretching, ether), 852 (C – H bending). $^1\text{H-NMR}$ Spectrum (400 MHz, CDCl_3) δ in ppm: 8.41 (s, 1 H, –CH=N–), 8.25 (d, $J = 7.5$ Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.82 (d, 2 H, ArH), 7.60–7.28 (d, 8 H, ArH), 7.16–6.91 (t, 3 H, ArH), 4.06 (t, 2 H, Ar–O–CH₂–), 1.84 (m, 2 H, CH₂–C–O–), 1.81–1.22 (m, 10 H, 5 X CH₂–), 0.96 (t, $J = 6.6$ Hz, 3 H, CH₃). Mass Spectrum (ESI-MS negative ion mode): m/z 532.62 ($[\text{M-H}]^-$, 100%); calculated mass for $\text{C}_{35}\text{H}_{35}\text{NO}_4 = 533$.

3.8. 4-benzoylphenyl (E)-4-((4-(decyloxy)benzylidene) amino) benzoate

IR Spectrum (KBr) $\nu_{\max}/\text{cm}^{-1}$: 2925, 2850 (aliphatic C – H stretching), 1730 (–C = O stretching, ester), 1671 (ketone), 1651 (–CH = N–), 1512 (–C = C– stretching), 1257 (C – O stretching, ester), 1160 (C – O stretching, ether), 853 (C – H bending). $^1\text{H-NMR}$ Spectrum (400 MHz, CDCl_3) δ in ppm: 8.41 (s, 1 H, –CH=N–), 8.25 (d, $J = 7.5$ Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.82 (d, 2 H, ArH), 7.60–7.28 (d, 8 H, ArH), 7.16–6.91 (t, 3 H, ArH), 4.06 (t, 2 H, Ar–O–CH₂–), 2.11–1.22 (m, 16 H, 8 X CH₂–), 0.96 (t, $J = 6.6$ Hz, 3 H, CH₃). Mass Spectrum (ESI-MS negative ion mode): m/z 560.60 ($[\text{M-H}]^-$, 100%); calculated mass for $\text{C}_{37}\text{H}_{39}\text{NO}_4 = 561$.

4. Results and discussion

4.1. Spectral analysis

Upon analysis of the $^1\text{H-NMR}$ spectrum, it was observed that a solitary proton from the imine group exhibited a singlet peak within the range of 8.41 (s, H, –CH = N–). A total of seventeen aromatic protons demonstrated themselves in the form of doublet and triplet peaks spanning the regions of 8.25 (d, $J = 7.5$ Hz, 2 H, ArH), 7.95 (d, 2 H, ArH), 7.82 (d, 2 H, ArH), 7.63–7.28 (d, 8 H, ArH), 7.19–6.99 (t, 3 H, ArH), for Series **X_nI** and **X_nII**. Conversely, a three aromatic proton was detected as a triplet peak in the region of 7.19–6.99 (t, 1 H, ArH) for the series **X_nI** and **X_nII**. The ether (–CH₂–O–Ar) protons of the alkoxy chain showcased resonance signals within the range of 4.07–4.03 ($J = 6.4$ –5.9 Hz), appearing as a triplet. The methylene protons belonging to the alkoxy chain resonated between 2.11 and 1.22 displaying a multiplet pattern. Lastly, the methyl group of the alkoxy chain resonated at 0.96–0.93 ($J = 6.6$ –6.9 Hz) in the form of a triplet.

The infrared spectrum ($\nu_{\max}/\text{cm}^{-1}$) exhibits absorption bands of moderate intensity in the range of 2937–2850 cm^{-1} attributed to aliphatic C – H (Sp^3 hybridised) functional groups. The stretching related to

carbonyl (-C=O) in the vicinity of $1730\text{--}1724\text{ cm}^{-1}$ was detected in the context of Series X_nI and X_nII . Within the range of $1651\text{--}1628\text{ cm}^{-1}$, there was observed a moderate intensity stretching associated with the bond of imine (-C=N-). The C=C stretching frequency observed at $1524\text{--}1507\text{ cm}^{-1}$, notably $1275\text{--}1154\text{ cm}^{-1}$ is associated with the stretching vibrations of C-O bonds in ester and ether groups, respectively. The band at $853\text{--}831\text{ cm}^{-1}$ serves as a marker for the bending vibrations associated with aromatic C-H bonds.

4.2. Mesomorphic behaviour

To comprehend the impact of various substituted tails on the mesomorphic properties of a liquid crystalline compound, two novel homologous series of compounds denoted as X_nI and X_nII , which were synthesised and subjected to mesomorphic analysis using POM and DSC. The X_nI series (X_4I to X_{10}I) and (X_4II to X_{10}II) derivatives displayed exclusively an enantiotropic nematic mesophase. Transition temperature data are documented in Table 1. The phase behaviour, including the melting and clearing points upon heating of homologues X_nI with the n -alkoxy terminus, is graphed against the number of carbon atoms (n) in Figure 1. As illustrated in the diagram, the transitions from meso-phase to isotropic phase display a gradual decline starting from the X_4I point, followed by a minimal increase up to X_{10}I , and subsequently experiencing a slight decrease until the final homologues synthesis. The molecular shape and intermolecular interactions between the mesogenic units are significantly affected by an increase in tail length. The clearing temperature increases with one result and decreases with the other [54,55]. On the contrary, the series X_nII compound demonstrates a nematic phase ranging from X_4II to X_{10}II derivatives. The transition temperatures data are documented in Table 1. The melting and clearing points upon heating for homologues X_nII are likewise graphed in relation to the carbon atoms number (n) and

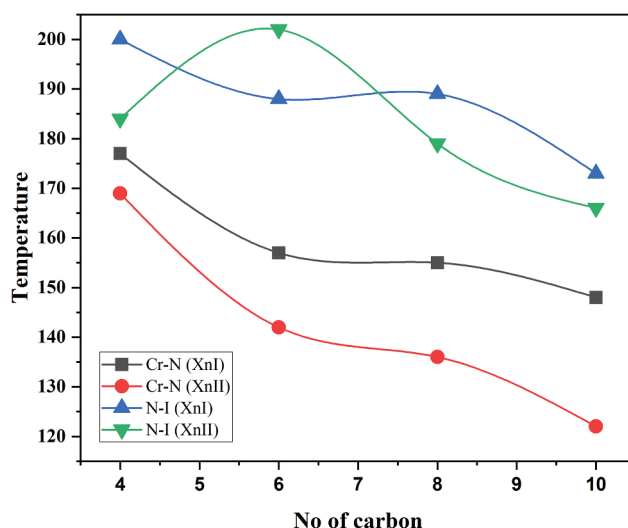


Figure 1. LCs phase behaviour of series X_nI & X_nII . Cr = crystal line solid; N = nematic phase; I = isotropic liquid phase ($n = 4, 6, 8$ & 10).

presented in Figure 1. Possible factors for separations include the mesogenic core's interaction with the mesogenic tail, influencing alkyl chain solubility. Conversely, longer chain length of X_6I and X_6II enhance tail and alkoxy chain interactions, facilitating intercalated structure development as well as it is displayed temperature variation. The phase transition data in Table 1 and Figure 1 show that increasing the alkoxy chain length significantly influences the mesomorphic behaviour of X_nI and X_nII . For both series, the Cr – N transition temperature decreases systematically with increasing carbon number. In the X_nI series, the Cr – N transition drops from 177°C (X_4I) to 148°C (X_{10}I), while in the X_nII series it decreases from 169°C (X_4II) to 122°C (X_{10}II). This downward trend is clearly reflected in the Cr – N curves of Figure 1.

4.3. Polarising optical microscope study

The analysis of the mesomorphic characteristics of the derivatives synthesised from Series X_nI and X_nII was performed using POM integrated with a thermal platform. During the experimental process, a thin layer of the samples was carefully prepared by positioning the derivatives between a glass slide and a coverslip, creating a 'sandwich' arrangement. This approach allowed for an in-depth examination of the mesogenic properties. The results indicated that both Series X_nI and X_nII derivatives exhibit mesogenic properties. Notably, the X_4I – X_{10}I homologues displayed an enantiotropic nematic mesophase across a temperature range of 177°C to 148°C , with an isotropic temperature range from 200°C to 173°C . Conversely, the X_4II – X_{10}II

Table 1. Phase transition temperatures ($^\circ\text{C}$) of series X_nI & X_nII compounds.

Compound.	$\text{R} = \text{-C}_n\text{H}_{2n+1}$ $n =$	Cr-N	N-I
X_4I	4	177	200
X_6I	6	157	188
X_8I	8	155	189
X_{10}I	10	148	173
X_4II	4	169	184
X_6II	6	142	202
X_8II	8	136	179
X_{10}II	10	122	166

*Cr = crystalline solid; phase; N = nematic phase; I = isotropic liquid phase. ($n = 4, 6, 8$ & 10).

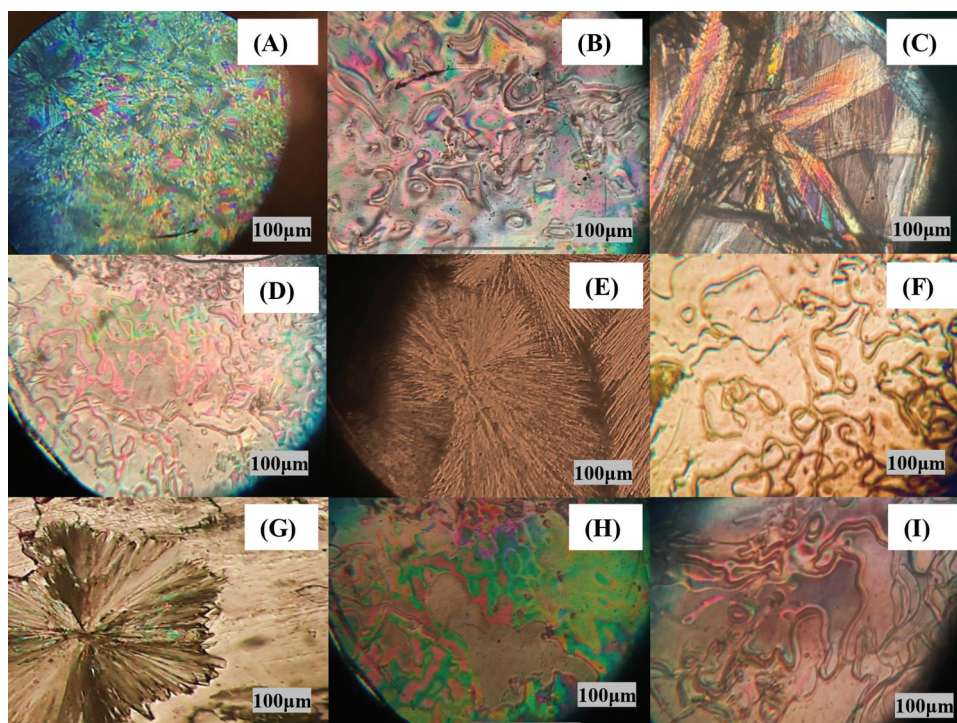


Figure 2. (Colour online) Optical micrographs of X_nI and X_nII showing crystal and nematic phases at indicated temperatures: (A) X_4I (crystal, RT); (B) X_4I (nematic, 177°C); (C) X_4II (crystal, RT); (D) X_4II (nematic, 169°C); (E) X_6I (crystal, RT); (F) X_6I (nematic, 157°C); (G) X_6II (crystal, RT); (H) X_6II (nematic, 142°C); (I) X_8I (nematic, 155°C).

homologues showed a nematic mesophase between 169°C and 122°C, while the X_nII series had an isotropic temperature range of 202°C to 166°C. Derivatives X_4I and X_4II demonstrated a schlieren nematic phase at 177°C and 169°C, respectively, along with isotropic temperature ranges of 200°C and 184°C (as illustrated in Figure 2(A-I)). In particular, the nematic phase of compound X_6I was observed at 157°C and for X_6II at 142°C, corresponding to isotropic temperature ranges of 188°C and 202°C with heating. These data support

the significant mesomorphic behaviour exhibited by the synthesised derivatives across the specified temperature ranges.

4.4. Differential Scanning Calorimetry (DSC)

DSC is used to detect phase shifts and comprehend the properties of various phases during transitions. In our study, DSC was used to analyse the heat enthalpies of substances in two series (Table 2 X_4I , X_4II , X_6I , X_6II).

Table 2. Phase transition temperatures (°C), enthalpy change, entropy change and normalised entropy of the series X_nI and X_nII (X_4I , X_6I , X_8I , $X_{10}I$, X_4II , X_6II , X_8II , $X_{10}II$) by DSC and POM measurement.

Compound	Transition	Peak temp./°C	$\Delta H/\text{kJmol}^{-1}$	$\Delta S/\text{kJmol}^{-1} \text{K}^{-1}$
X_4I	Cr-N	177	37.3562	0.08301
	N-I	200	1.15930	0.00246
X_6I	Cr-N	157	37.4607	0.08712
	N-I	188	2.56220	0.00556
X_8I	Cr-N	155	27.7752	0.06489
	N-I	189	0.99752	0.00216
$X_{10}I$	Cr-N	148	36.9807	0.08784
	N-I	173	2.15638	0.00483
X_4II	Cr-N	169	29.9574	0.06778
	N-I	184	7.35570	0.01609
X_6II	Cr-N	142	36.7588	0.08857
	N-I	202	7.45880	0.01570
X_8II	Cr-N	136	32.1041	0.07849
	N-I	179	6.69237	0.01481
$X_{10}II$	Cr-N	122	31.7473	0.08037
	N-I	166	1.96910	0.00448

DSC was employed for the determination of the enthalpies pertaining to the derivatives within both the X_nI and X_nII series, utilising the DSC 6000 instrument (PerkinElmer). The examination of phase transition phenomena was conducted through a scanning process starting from room temperature up to 250°C, with a heating rate of 10°C per minute, followed by a cooling phase from 250°C to 50°C at an equivalent rate of 10°C per minute.

Compound X_4I demonstrates two endothermic peaks at temperature of 177°C and 200°C during the heating cycle, which are associated with the transitions from crystal to nematic (Cr-N) and from nematic to isotropic (N-I), respectively. The enthalpy changes for these transitions are measured at 37.3562 kJ/mol and 1.1593 kJ/mol. In a similar manner, compound X_4II shows two endothermic peaks at 169°C and 184°C, corresponding to the Cr-N and N-I transitions, with enthalpy change values of 29.9574 kJ/mol and 7.3557 kJ/mol, respectively. Notably, compounds X_6I and X_6II undergo the Cr-N transition at 157°C and 142°C during the heating process, exhibiting enthalpy changes of 37.4607 kJ/mol and 36.7588 kJ/mol. Furthermore, X_6I and X_6II transition from the nematic state to the isotropic state (N-I) at temperatures of 188°C and 202°C, with associated enthalpy changes of 2.5622 kJ/mol and 7.4588 kJ/mol, respectively. Compound X_8I exhibits Cr – N and N – I transitions at 155°C and 189°C with enthalpy changes of 27.7752 and 0.99752 kJ/mol, respectively. Similarly, X_8II shows these transitions at 136°C and 179°C with enthalpy values of 32.1041 and 6.69237 kJ/mol. Compounds $X_{10}I$ and $X_{10}II$ undergo Cr – N transitions at 148°C and 122°C, with enthalpy changes of 36.98071 and 31.7473 kJ/mol, followed by N – I transitions at 173°C and 166°C with enthalpies of 2.15638 and 1.96910 kJ/mol. The normalised entropy changes, ΔS , of the homologues X_nI & X_nII are tabulated in Table 2. As shown in Table 2, independent of the alkoxy chain length (n), the entropy of Cr-N transitions is higher than N-I transitions. The high values observed in ΔS_{Cr-N} and ΔS_{N-I} could be attributed to the decrease in the biaxiality of the mesomeric part which lead to an increment in the conformational entropy [56].

The DSC thermograms exhibited an endothermic peak during the heating scan, representing the transition from a crystalline to an isotropic phase in Figure 3 (X_4I , X_6I , X_8I , $X_{10}I$, X_4II , X_6II , X_8II , $X_{10}II$). Conversely, during the cooling phase an exothermic peak indicated the transitions from an isotropic to a nematic mesophase, as well as from a nematic to a crystallisation phase, for the

compounds in both series. The calorimetric values at the isotropic temperature surpass significantly compared to those observed during transitions from isotropic to crystal phase changes. Validation of the DSC thermogram result was achieved by comparing them with transition temperature, determined using POM. DSC thermogram distinctly displays the transition temperatures for all compounds under investigation.

4.5. DFT calculations

All compounds (X_4I , X_6I , X_8I , $X_{10}I$, X_4II , X_6II , X_8II , $X_{10}II$) were optimised using the DFT methods at the B3LYP/6–31+G (d,p) level of theory. The optimised geometries are shown in Figure 4, and the various electronic properties are presented in Table 3. For each molecule, we calculated the energy gap ($E_{HOMO} - E_{LUMO}$), which is an important parameter to assess the thermal stability and the chemical reactivity of a molecule. The E_{HOMO} and E_{LUMO} energy gap was negative for all compounds, indicating their stability. Interestingly, the band gap values, calculated by the difference of the energy values of HOMO and LUMO, were higher for the X_nI series as compared to the X_nII compounds (Figure 5). The higher band gap values indicate less electronic delocalisation and favour crystalline phase for the X_nI compounds. On the other hand, lower band gap for X_nII indicate enhanced anisotropic interactions, stabilising the nematic phase. Further, Frontier Molecular Orbital analysis (Figure 6) illustrates that the LUMO for X_nII compounds is more delocalised as compared to the X_nI compounds, with electron density extending to the additional ketone group in X_nII compounds, resulting in increased π -delocalisation and reduced LUMO energy. Notably, X_4II shows reduced LUMO delocalisation and higher degree of delocalisation in its HOMO as compared to X_6II , X_8II and $X_{10}II$. This leads to a relatively larger HOMO – LUMO gap for X_4II .

To provide a stronger structure–property rationale for the phase behaviour, we calculated the end-to-end molecular lengths and static isotropic polarisabilities (Table S1) for all compounds at the B3LYP/6–31+G(d,p) level of theory. The molecular length increases systematically with spacer extension, from 27.34 Å (X_4I) to 34.83 Å ($X_{10}I$), and from 28.16 Å (X_4II) to 35.81 Å ($X_{10}II$). A similar trend is observed for polarisability, which increases from 416.45 to 485.66 a.u. (61.7–72.0 Å³) for X_nI and from 403.00 to 435.07 a.u. (59.7–64.5 Å³) for X_nII . These values are consistent with enhanced molecular anisotropy and dispersive interactions in longer homologues. Overall, these observations indicate that

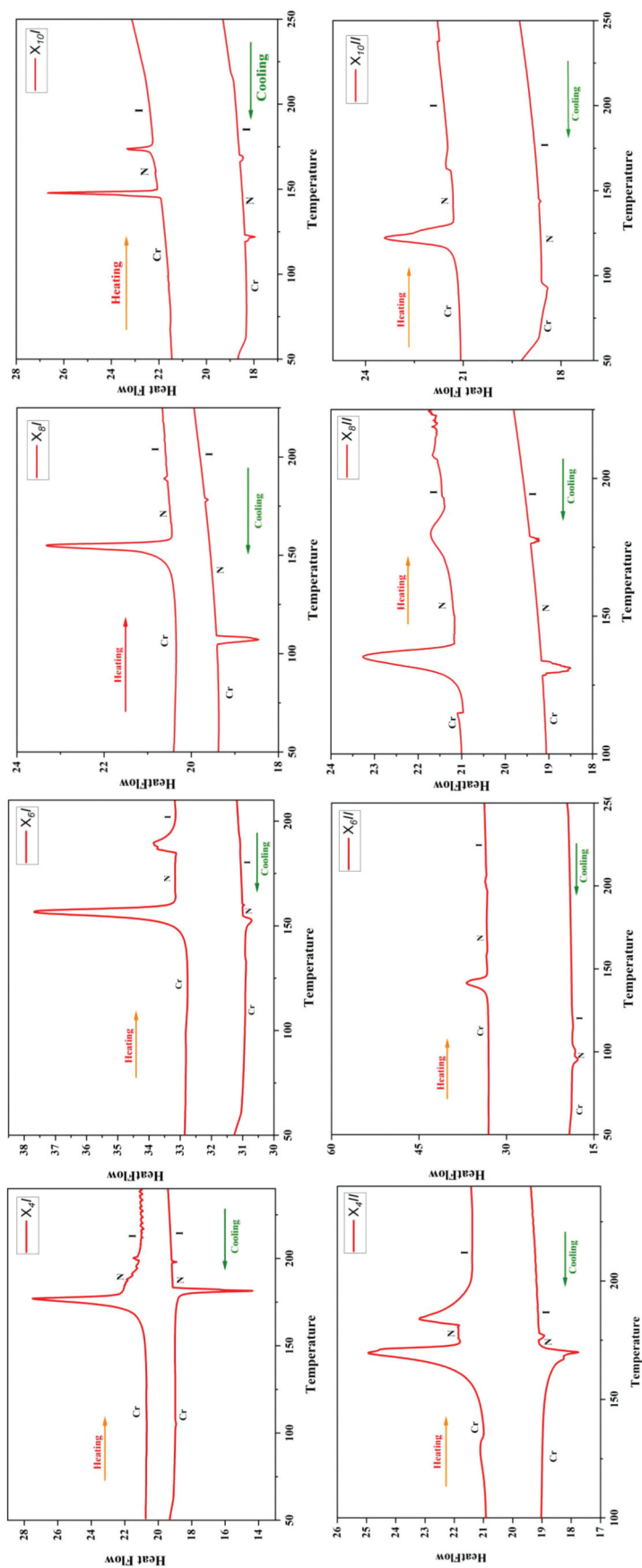


Figure 3. (Colour online) DSC thermogram of series X_d/I and $X_g/I/I$ (X_dI , X_dII , X_dI , X_dII , X_gII , X_gI , X_gII , X_gI).

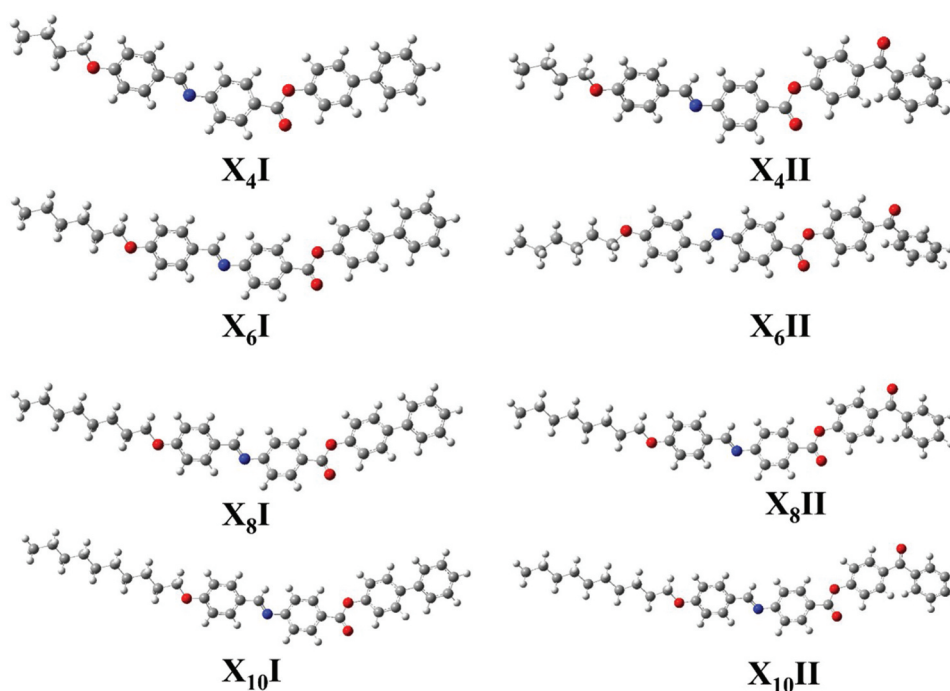


Figure 4. (Colour online) The geometry of X_{4I} , X_{6I} , X_{8I} , X_{10I} , X_{4II} , X_{6II} , X_{8II} , X_{10II} optimised at the B3LYP/6–31+G(d,p) level of theory.

Table 3. The calculated E_{HOMO} (kcal/mol), E_{LUMO} (kcal/mol), $E_{HOMO} - E_{LUMO}$ (kcal/mol) and dipole moment (Debye) for X_{4I} , X_{6I} , X_{8I} , X_{10I} , X_{4II} , X_{6II} , X_{8II} , X_{10II} compounds calculated at the B3LYP/6–31+G(d,p) level of theory.

	E_{HOMO} (eV)	E_{LUMO} (eV)	$E_{HOMO} - E_{LUMO}$ (eV)	Dipole Moment (Debye)
X_{4I}	−5.843	−1.968	3.874	6.44
X_{6I}	−5.841	−1.964	3.877	6.51
X_{8I}	−5.840	−1.961	3.879	6.55
X_{10I}	−5.839	−1.960	3.879	6.58
X_{4II}	−5.992	−2.128	3.864	6.15
X_{6II}	−5.985	−2.126	3.858	7.53
X_{8II}	−5.987	−2.124	3.864	6.30
X_{10II}	−5.986	−2.122	3.864	6.35

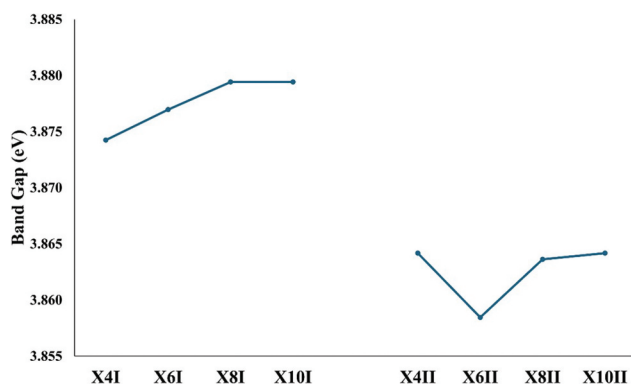


Figure 5. (Colour online) The band gap ($E_{HOMO} - E_{LUMO}$) values (eV) of X_{4I} , X_{6I} , X_{8I} , X_{10I} , X_{4II} , X_{6II} , X_{8II} , X_{10II} compounds as calculated at the B3LYP/6–31+G(d,p) level of theory.

the X_{nI} series, with higher band gaps and slightly lower electronic deformability, favours efficient molecular packing and crystalline phase formation.

4.6. Comparative study

The molecular structure of a liquid crystal compound significantly influences the characteristics of its mesophase. By analysing the geometry and configuration of the molecules, one can establish a connection between the phase transition process, the stability of the mesophase and the temperature range in which the mesophase exists. Table 4 summarises the phase transition temperatures, the temperature range of the nematic mesophase and the initiation of the nematic phase for the synthesised X_{8I} and X_{8II} compounds. For reference, comparative data for compound A [33] and compound B [32] are also included. The molecular structures of these comparison compounds are illustrated in Figure 7.

The data presented in Table 4 reveal that the nematic mesophase width and the N-I transition temperature for the X_{8I} compound are 11°C and 60°C lower,

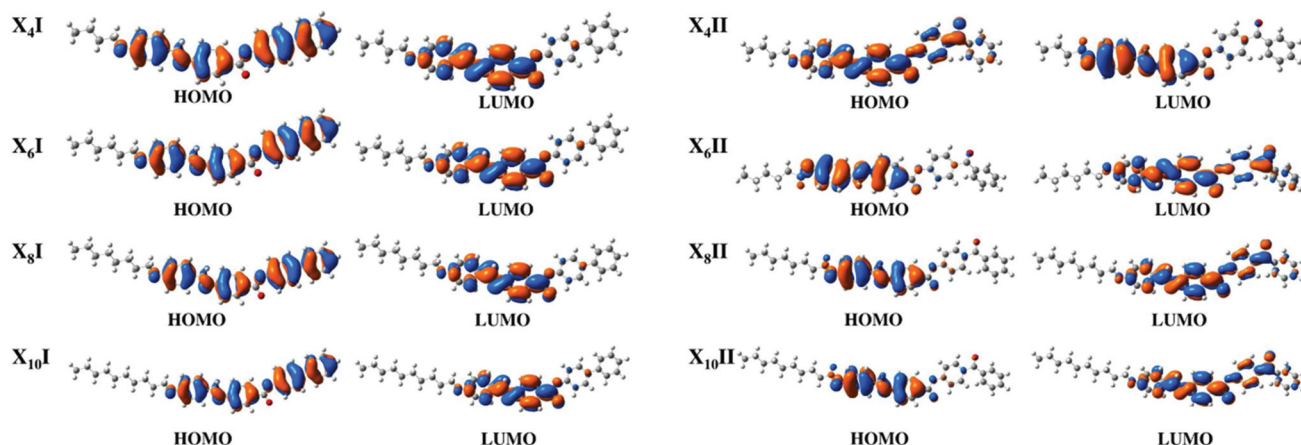


Figure 6. (Colour online) The HOMO and LUMO orbitals of X_4I , X_6I , X_8I , $X_{10}I$, X_4II , X_6II , X_8II , $X_{10}II$ compounds as calculated at the B3LYP/6-31+G(d,p) level of theory.

Table 4. Comparison of the phase transition temperatures, nematic mesophase range and comparative molecular structures of compounds X_8I , X_8II , **A** and **B**.

Compound	Nematic range	Isotropic range	Mesophase range/ $^{\circ}C$	Commencement of nematic phase
X_8I	155	189	34	C_8
X_8II	136	199	63	C_8
A	240	254	14	C_8
B	328	363	35	C_8

respectively, in comparison to compound **A**. This variation can be primarily ascribed to the structural differences between the X_8I and **A** compounds, which are confined to the linkages. X_8I compound terminates with an alkoxy substituent ($-OC_8H_{17}$), whereas **A** bears an alkoxy carbonyl ($-OOC-C_8H_{17}$) group attached through an additional ester linkage. The flexible alkoxy terminal group in X_8I promotes balanced molecular packing and mobility, making it superior to **A**, whose increased polarity and rigidity due to the terminal ester linkage restrict mesophase stability. Overall, although both compounds exhibit nematic mesophases, X_8I demonstrates a more favourable liquid crystalline behaviour with a broader mesophase range and better thermal stability of the nematic phase. Furthermore, the structural differences observed in compound **A** leads to a notable reduction of temperature to $104^{\circ}C$ in the width of the nematic mesophase for X_8II , as well as $55^{\circ}C$ decrease in the N-I transition temperature when compared to Series X_8II . Compound X_8II is more linear and rod-like, allowing better parallel alignment favourable for nematic phase formation. **A** compound is slightly bent because of the alkoxy carbonyl ($-OOC-C_8H_{17}$) linkage. This reduces the molecular aspect ratio and weakens nematic phase stability. The variation in functional group arrangement within compound **A** is pivotal in affecting these thermal properties, contributing to a reduction in stability.

Similarly, compound **B** exhibits variations in functional group arrangement, which results in a significant decline of $173^{\circ}C$ in the nematic mesophase width for compound X_8I , accompanied by a $174^{\circ}C$ decrease in the N-I transition temperature when compared to compound X_8I . This substantial difference can be attributed to structural rigidity and terminal substitution. The biphenyl terminal group in X_8I enhances molecular linearity, planarity and π - π stacking interactions, which favour nematic phase stability at lower temperatures. In contrast, the methoxy group in compound **B** introduces an electron-donating and sterically flexible moiety, disrupting coplanarity and increasing the temperature required for nematic ordering, thereby affecting the width of the nematic mesophase and the N-I transition temperature for the X_8II series, which are $192^{\circ}C$ and $164^{\circ}C$, lower than those of the **B** series, respectively. These differences can again be attributed to the terminal linkage variations between the molecules of X_8II and **B** compound.

X_8I and X_8II both compounds exhibit a nematic mesophase; however, their thermal behaviour shows a significant difference. Compound X_8I displays a nematic range from $155^{\circ}C$ to $189^{\circ}C$ with a mesophase width of $34^{\circ}C$, whereas X_8II shows a broader nematic range from $136^{\circ}C$ to $199^{\circ}C$, covering $63^{\circ}C$. The wider mesophase and higher clearing temperature of X_8II indicate greater thermal stability and stronger intermolecular

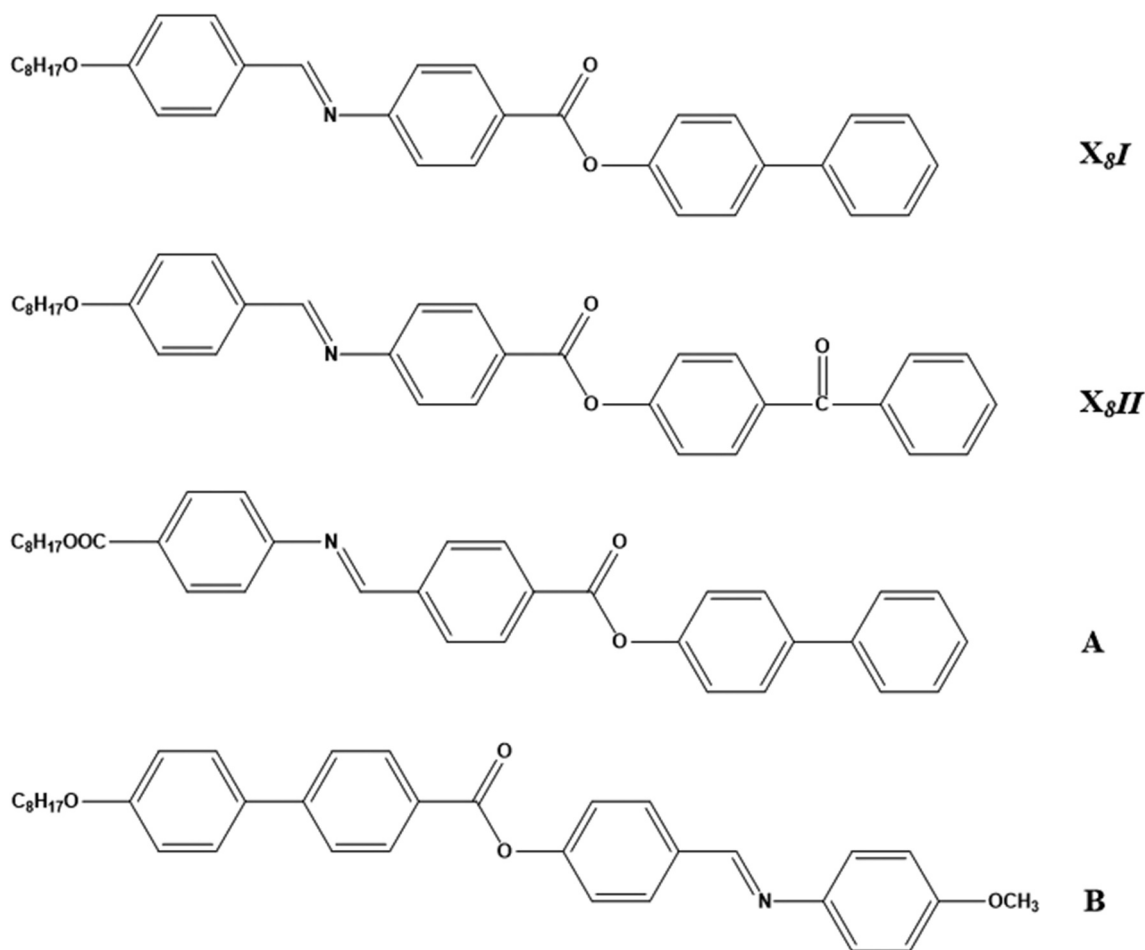


Figure 7. Comparative geometry of compounds **X₈I**, **X₈II**, **A** and **B**.

interactions. This improvement arises from the additional phenyl–carbonyl–phenyl linkage in **X₈II**, which enhances molecular polarity and rigidity. Thus, the new structural modification in **X₈II** extends the nematic phase stability compared to **X₈I**, demonstrating its potential for high-temperature liquid crystal applications.

5. Conclusion

A homologous series of [1,1'–biphenyl]–4-yl (E)-4-((4-*n*-alkoxybenzylidene) amino) benzoate (**X_nI**) and 4-benzoylphenyl (E)-4-((4-*n*-alkoxy) benzylidene) amino) benzoate (**X_nII**) were synthesised and investigated for their mesomorphic properties. Additionally, synthesised series **X_nI** and **X_nII** are characterised by IR, ¹HNMR and mass spectra. The homologous series of [1,1'–biphenyl]–4-yl (E)-4-((4-*n*-alkoxybenzylidene) amino) benzoate (**X_nI**) and 4-benzoylphenyl (E)-4-((4-*n*-alkoxy) benzylidene) amino) benzoate (**X_nII**) exhibited nematogenic behaviour. The compounds **X_nI** (ranging from **X₄I** to **X₁₀I**) demonstrated a nematic mesophase within the temperature interval of 177°C to

148°C, whereas the compounds **X_nII** (ranging from **X₄II** to **X₁₀II**) exhibited a nematic mesophase between 169°C and 122°C. Nematic phase was observed in series **X_nI** and **X_nII**. The temperature variation depends on tail. When the polarity of the compound increases it causes temperature variation. All compounds (**X₄I**, **X₆I**, **X₈I**, **X₁₀I**, **X₄II**, **X₆II**, **X₈II**, **X₁₀II**) were optimised using the DFT methods at B3LYP/6–31+G(d,p) level of theory. Interestingly, the band gap values, calculated by the difference of the energy values of HOMO and LUMO, were higher for the **X_nI** series as compared to the **X_nII** series compounds. Further, Frontier Molecular Orbital analysis illustrates that the LUMO for **X_nII** compounds is more delocalised than **X_nI** series compounds, with electron density extending to the additional ketone group in **X_nII** compounds.

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Author contributions

CRedit: **Jay C. Panchal**: Conceptualization, Methodology, Project administration, Writing – review & editing; **Meetkumar Y. Chaudhary**: Formal analysis; **Hemant N. Patel**: Conceptualization; **Shavi Thakur**: Software; **Vinod Ashtekar**: Formal analysis; **Sumit Mittal**: Software; **Tarun M. Patel**: Data curation; **Chetan B. Sangani**: Methodology.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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