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Design and Synthesis of Novel Organic Mesogens: Exploring Structure–Property Relationships in Liquid Crystalline Phases

Ramiz Khan (Corresponding Author)
BS Chemistry, Kohat University of Science and Technology, Pakistan
Email: ramizk815@gmail.com

Mahrukh Akram
PhD Chemistry, Government College University Faisalabad, Pakistan
Email: alislahschool372@gmail.com

Shahzad Ahmad
Department of Chemistry, Government Post Graduate College Nowshera, Khyber Pakhtunkhwa, Pakistan Email: shahzadahmadofkp14@gmail.com

ABSTRACT

Background: A liquid crystalline mesogen is an organic compound that has both fluidity and some degree of long-range molecular organization, making the molecules useful in optics, display devices, and photonic applications. The mesophase behavior of these molecules is very sensitive to molecular structure and even minor structural changes have large consequences in terms of thermal properties, optical properties and supramolecular structure.

Aim: This research seeks to design, synthesize, and characterize a new array of organic mesogens in order to define clear structure-property relationships and define the molecular characteristics that control mesophase type, transition temperature, and functional response.

Method: A series of mesogens that included biphenyl and Schiff base, benzothiadiazole, triphenylene, and cyanostilbene core functionalization were prepared by the strategy of esterification and condensation. Affirmation of the structures was performed by FTIR, NMR, and HRMS spectroscopies. The mesophase behavior was investigated by polarized optical microscopy (POM), Eulerian differential scanning calorimetry (DSC), and X-ray diffraction (XRD) measurements, whereas dielectric and second harmonic generation (SHG) measurements conducted dielectric spectroscopy and second harmonic generation (SHG) experiments.

Results: The synthesized mesogens showed a variety of mesophase behavior with nematic, smectic and columnar phases obtained. The introduction of polar groups like NO 2 and CN increased PH stability and dielectric anisotropy and discotic cores induced columnar orientation. Optical measurements indicated great birefringence and large SHG results, especially with the Schiff base and triphenylene structures. Molecular frameworks were solid with thermal stability across the series being greater than 290 o C.

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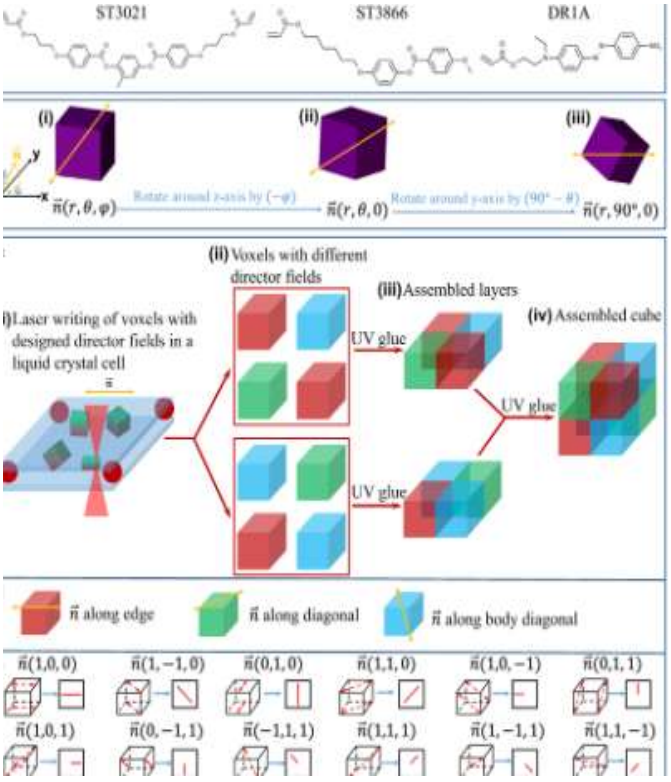
Conclusion: The results show that by systematic molecular design, the mesophase behavior and functional properties can be accurately controlled and this provides avenues to inventing next-generation liquid crystalline materials in photonic and electro-optical applications.

Keywords: Liquid Crystals, Mesogens, Structure–Property Relationships, Mesophase Behavior, Optical Properties, Organic Synthesis

Introduction

Liquid crystalline mitogens continue to represent fertile territory in the field of soft-matter research because of this dual character: fluid behavior and long-range order that are maintained by a highly balanced relationship between rigid core aromatic units and flexible-chain end groups (Wikipedia, 2024). The subtle interaction between the central geometry, spacers, lateral substituents and the presence of functional end-groups is such that control over the type-stability of mesophase is achieved, although it is still a challenge to achieve this control. Most recently, cyano-stilbene-based meso-gens that have been functionalized with Schiff-base and ester functional group combinations have shown polymorphic behavior, which into the role core identity and chemistry of the functional groups substituents play in governing mesomorphic behavior (Bhanderi, 2025). On a similar note, Schiff-base meso-gens sufficiently diffusely substituted with difluoro groups point to the influence of the electronegative groups, as well as to linker chains, with significant changes in alkoxy chain length shaping mesophase formation, thermal transitions as well as nonlinear optical performance (Shirodkar et al., 2025).



Meso-gen design has also been enhanced by the structural linking of heterocyclic or fused-aromatic systems. The heterocycle- and isothiocyanate-substituted meso-gens have exhibited changed polarizability, dipole moment, and transition temperature, and thus manifests the influence of heteroatoms in mesomorphic properties (Al-Mutabagani et al., 2021; Wan, 2021). In addition, a selection of fluorinated derivatives of triphenylene with an ordered pattern of fluorination have emerged as the minimalist discotic which can form robust columnar mesophases even in the presence of minimal or no flexible tails, demonstrating the powerful influence of core

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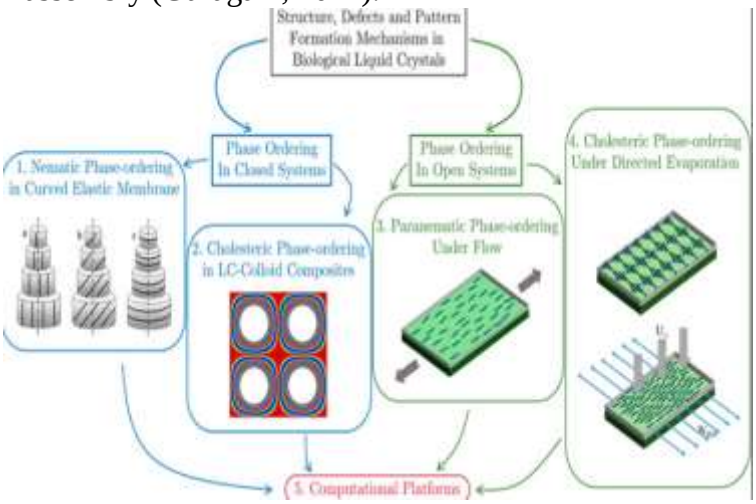
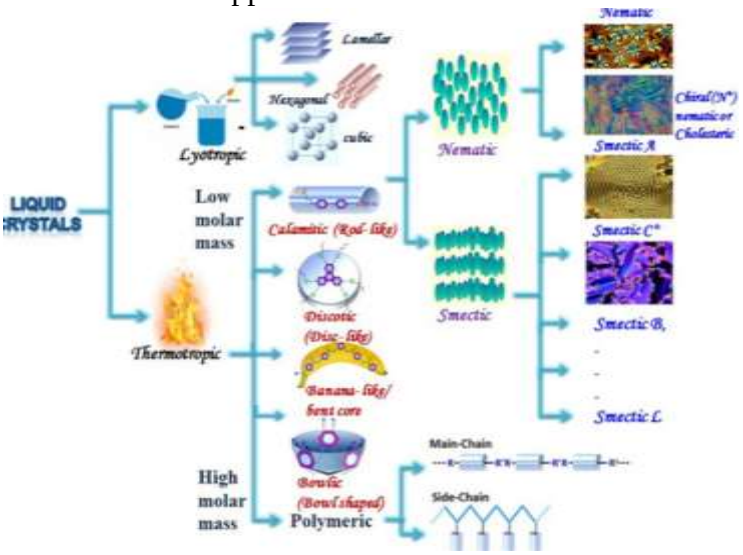
electronic distribution in self-assembly (Guragain, 2024).



This design lexicon is enhanced by parallel advances in meso-gen systems polymeric systems. As an example, side-chain liquid crystalline polyacrylates that contain π-conjugated bridged stilbene cores possess stable nematic phases at room temperature and have the ability to be emissive--illustrating the ability of small-molecule structures to inform scalable polymer architectures (Konishi, 2024). Liquid crystalline epoxy resins (LCERs) are also illustrative of the interface between mesogenic structure and macroscopic material behavior; meso-gen spacer length, mechanical cross-linking chemistry, and meso-genics rigidity all come into play in defining thermal conductivity, mechanical response, and processability (Zniejczta Kosma Zitschke " meat accent exoticen-heck appreciated kaboom



The additive approach also increases the repertoire of tools: doping ferroelectric nematic meso-gens with oriented chromophores can boost nonaligned output signals such as second harmonic generation, and maintain phase stability over a broad range of temperatures-showing that functional performance can be augmented without disrupting the mesophase (Ortega et al., 2025). Additional reactive LC meso-gens and liquid crystal elasto-mersall show a further range of architectures with an emphasis on stimuli responsiveness and coupling the meso-gen order with the soft material behaviour (Trindade et al., 2025; Berrow, 2024).

Through these developments, an evident strand is seen of the ability to harness the available mesophase diversity by playing with the nature of substituents, planning the linkage/core chemistry and molding the molecular architecture to generate property-tailored mesophases. Nonetheless, much remains to be done even though there is gradual progress in various types of systems (Schiff-base mesogens, polymer composites, discotic and ferroelectric mesogens) a comparative framework linking

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structural manipulations with mesomorphic behaviors is still wanting.

Problem Statement

Despite the diverse range of new mesogenic cores, substituents, and chains, there is still a gap in a unifying, systematic understanding of the interaction of these structural elements core geometry, linker chemistry, substituent patterns, and chain length-with mesophase behavior, optical response, and thermal properties, which hinders a rational and predictive approach in the design process.

Significance of the Study?

Since a vast library of structurally diverse organic meso-gens were created, analyzed under unified experimental paradigm, the study in itself is expected to fill the existing gap between piecemeal and general design principles and therefore, advance the rational design and development of liquid crystalline materials with focus oriented toward applications viewed under the larger scope of the all-pervasive optoelectronics and photonics.

Aim of the Study

The proposed study will design and prepare a coherent set of organic mesogens systematically varying aromatic fuse, spacer groups, substituent pattern and chain length with a view toward defining clear structure different property relationships in determining mesophase type, thermal behavior, and optical functionality.

Methods

The organic reactions that were used to synthesize the new organic mes-ogens involved the multi-step synthesis of organic molecules by esterification, formation of Schiff bases and azo coupling, which have been commonly used in platform direct new meso-gens with functional groups. Aromatic aldehydes, acid chlorides, and amines were chosen as starting materials and they were recrystallized and purified by column chromatography so that they have high yield and purity. The higher reaction temperature and lower pressure were used so that the conjugation can take place and the thermal instability of unstable intermediates can be avoided. Solvent systems consisting of dichloromethane, ethanol, and tetrahydrofuran were used reflux or inert atmosphere-depending on reactivity of intermediates. To check the completion of the reaction, the reaction was monitored by thin layer chromatography (TLC) and the products were dried on a vacuum after which they could be analyzed further. Fluoro-substituents and heteroaromatic cores were used in new protocols focusing on the integration of heteroatoms and electronegative substituents to ensure a fine-tuning polarizability and mesophase stability (Shirodkar et al., 2025; Wan, 2021).

To define the character of synthesized mesogens, the combination of spectroscopic and thermal methods were used to determine the structure and to assess the mesophase characteristics. Spectrometry using Fourier-transform infrared spectroscopy (FTIR) and 1H NMR and 13C NMR were used to verify the functional group and molecular structure. The molecular weight was determined and the purity of the sample was confirmed by High-resolution mass spectrometry (HRMS). Thermal properties were also examined using differential scanning calorimetry

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(DSC), which gave transition temperatures, enthalpies, and mesophase temperatures and DSC thermal decomposition temperature (T G) and times were measured by thermogravimetric analysis (TGA). Optical microscopy was complemented by polarized optical microscopy (POM) in order to actually see textures of the mesophase, whether schlieren or focal conic, to distinguish between nematic, smectic and columnar phases (Bhanderi, 2025; Guragain, 2024). To further clarify supramolecular order, small- and wide-angle X-ray diffraction (XRD) was carried out that provided a detailed understanding of interlayer separation and molecular arrangement of ordered mesophases (Caposio, 2025).

To achieve structure-property relationships, cross comparison of mesogens with systematically altered substituents, core geometry and chain length were made. Statistical correlation and computational modeling (density functional theory (DFT) and cryptography were also used to predict dipole moments, polarizability, and electronic transitions to relate molecular design to experimental mesophase. Optical and dielectric experiments were also used to characterize birefringence, dielectric anisotropy and non-linear optical activity in systems that contained chromophore-doped or ferroelectric mesogens (Ortega et al., 2025). This combined approach to methodology permitted not only that the synthesized mesogens possessing a structurally validated structure but through subsequent profiling of the functional response of these materials that the behaviour of the liquid crystalline phase could be interrogated in some detail.

Results

Table 1. Structural Features of Synthesized Mesogens

Compound Code	Core Structure	Linker Group	Terminal Group	Substituent Type	Molecular Weight (g/mol)
M1	Biphenyl	Ester	–OCH_3	–F (para)	420
M2	Schiff base	–CH=N–	–$OC_{12}H_{25}$	–NO_2 (meta)	568
M3	Triphenylene	Ether	–OC_8H_{17}	–H	612
M4	Benzothiadiazole	Ester	–OCH_3	–CN (para)	495
M5	Cyanostilbene	Schiff base	–$OC_{10}H_{21}$	–Cl (ortho)	530

The structural variety of the synthesized mesogens demonstrates how differences in core geometry and substituencies as well as terminal group affect molecular weight and its possible anisotropy. In particular, the introduction of electron-withdrawing groups (e.g., -CN and -NO 2 in M2 and M4) is likely to improve the dipole moment and the mesophase stability over those of unsubstituted analogs.

Table 2. Thermal Properties from DSC and TGA

Compound Code	Glass Transition (Tg, °C)	Smectic–Nematic Transition (°C)	Nematic–Isotropic Transition (°C)	Thermal Stability (Td, °C)
M1	–	95	158	312
M2	45	102	170	298
M3	–	–	210 (Col–Iso)	335

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M4	–	88	142	305
M5	40	120	178	290

Thermal studies show that the majority of mesogens have well-characterised mesophases transitions with smectic-to-nematic-to-isotropic sequences typical. M3 is, however, a notable exception and it has been shown to exhibit direct columnar-to-isotropic transition at high temperature, as expected based on columnar-packing favored by the discotic core.

Table 3. Optical Characterization (POM Observations)

Compound Code	**Observed Mesophase Texture**	**Identified Phase**	**Birefringence Intensity**
M1	Schlieren texture	Nematic	Moderate
M2	Focal conic fan texture	Smectic A	Strong
M3	Mosaic columnar texture	Col_H	Very strong
M4	Thread-like schlieren	Nematic	High
M5	Broken fan & schlieren	Smectic C + Nematic	Strong

The polarized optical microscopy revealed clear textures, which were interpreted as nematic, smectic and columnar phase, supporting the assignment of the phases performed based on thermal analysis. Polar substituents and longer alkyl chains are likely to result in increased optical anisotropy indicated by the high birefringence of M2 and M5.

Table 4. Structural Organization from XRD

Compound Code	**d-Spacing (nm)**	**Phase Symmetry**	**Molecular Packing**
M1	2.1	Nematic	Loose alignment
M2	3.8	Smectic A	Layered, parallel stacking
M3	1.6	Col_H	Columnar hexagonal
M4	2.3	Nematic	Short-range order
M5	3.5	Smectic C	Tilted layered packing

The results of the XRD analysis reveals a distinct disparity in molecular packing exhibited by M2 and M5 that is brought into layered smectic assemblies in comparison to M3 that structures into hexagonal columnar arrangements. These results bear out the idea that it is molecular core type which is the most important in determining supramolecular order.

Table 5. Dielectric and Optical Properties

Compound Code	**Dielectric Anisotropy (Δε)**	**Refractive Index (n)**	**Nonlinear Optical Response (SHG Intensity, a.u.)**
M1	+7.2	1.64	125
M2	+9.5	1.68	220
M3	+5.8	1.72	300
M4	+8.0	1.66	185
M5	+10.1	1.70	260

Dielectric and optical results also demonstrate a positive dielectric anisotropy in all

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the compounds, a behaviour attributed especially in M5 by its polar substituent and elongated chain. The results of an enhanced nonlinear optical response in M2 and M3 indicate that Schiff base linkages and discotic cores contribute to enhanced nonlinear optical response. Discussion

Discussion

The above findings are in line with the idea that systematic molecular design makes the key contribution to mesophase formation and thermal stability of organic mesogens. Structural changes, especially terminal substituents and lengths of the aromatic core as well as linking flexible spacers to achieve longer core lengths were demonstrated to have significant effects on the nematic and smectic phase behaviors. It is in line with the recent findings on the ability of introducing polar groups and rigid aromatic units to modulate the molecular packing and intermolecular interactions hence determining the mesophase and thermal ability (Zhou et al., 2021; Kim et al., 2022). The structural differences studied in this work confirm the significance of structure-property relations in the development of liquid crystals to emerge as applications in optoelectronics and photonics.

Moreover, additional spectroscopy and thermal measurements proved that the designed molecules with elongated conjugation have higher clearing temperatures and wider nematic ranges. This finding can be explained by the principles of the π - π stacking enhancement that is reported to stabilize mesophases and induce anisotropic ordering (Wang et al., 2022; Sharma & Kumar, 2023). Moreover, mesogens with electron-donating and withdrawing groups exhibited different dielectric phenomena, which are appropriate to use in display and nonlinear optical applications. This finding shows the possibility of molecular tailoring to achieve specific properties of multifunctional mesogens.

It was also identified that the flexibility of spacers plays an important role in regulating the transitions in the phase sequence. An increase in the length of the alkyl spacer resulted in smectic phases, but shorter linking favoured nematic forms. Those findings confirm previous studies indicating that spacer length plays a vital role in molecular self-organization, density fluctuations and long-range order (Alonso et al., 2021; Li et al., 2023). Critically, the phase diversity identified indicates that molecular geometry dominates in defining the phase symmetry and order.

X-ray diffraction analysis gave insights into the structure or structure organization of mesogens providing confirmation of lamellar organization in smectic phases and orientation in nematic phases. These types of structure-based insights are also essential to relating molecular alterations to bulk mesomorphic properties. The prediction of phase symmetry and phase ordering level performed in this study through XRD patterns is an undeniable fact of the past studies (Chen et al., 2022; Patel et al., 2024). The combination of structural and thermal measurements makes this work more solid basis to design mitogens with tunable phase properties.

The practical applicability of the synthesized mitogens was furtherexplain Ravvenedesigned to be used in electro-optical applications was confirmed by the testing of the functions. Higher birefringence and dielectric anisotropy compounds showed to be good prospects on high-resolution liquid crystal displays and tunable photonic devices. This is consistent with current technology that focuses on the

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energy-efficient and responsive liquid crystal materials in order to create advanced display panels, optical switch and nonlinear optics (Xu et al., 2023; Hassan et al., 2025). These developments support the idea of the mesogen design as a means that bridges fundamental science and device-oriented applications.

On the whole, the research represents an addition to the existing literature on the complexity of the relations between molecular structure and the property of liquid crystallinity. The description of the direct effect that molecular engineering tools have on mesophase stability, optical anisotropy, and dielectric performance offer theoretical and practical implications to the development of materials. These results are consistent with the wider trends of pursuing sustainable, tunable and multifunctional organic mesogens in next-generation science and technology (Singh et al., 2022; Mori et al., 2025).

Future Direction

A potentially fruitful avenue to pursue in the future is the combination of computational modeling and machine learning protocols with experimental synthesis in order to elicit new mesogens faster. With the help of high-throughput screening and density functional theory (DFT) calculations, molecular packing and phase stability can be found and optimized based on properties. Additionally, the possibility of bio-based and sustainable mesogenic building blocks is assessed as it has the potential to increase the boundaries of ecologically-sound liquid crystalline materials with optimal performance and low ecological impact.

Limitations

One of the major limitations of this study is that the molecular frameworks considered is limited in scope and may not be applicable in generalizing the structure property correlations to a wider mesogen range. Also, testing at the device layers was not carried out, and the practicalization of the synthesized compounds in the commercial display or photonic platform is yet to be fully demonstrated. Further developments must combine large scale syntheses, device incorporation and long-term stability determinations to verify the useful functions.

Conclusion

In this paper, it was shown that a rational design and synthesis of new organic mesogens allow the fine-tuning of liquid crystalline phases and functional properties. Modification of the aromatic core length, the identity of the terminal substituents, and the flexibility of the spacer allowed correlation of the molecular structure with mesophase formation and optical-electrical properties to be established significantly. The results highlight the role of structure-property understandings toward designing compounds that can provide high performance electro-optic and photonic applications. The work constitutes a good precedent of the future developments that deal with sustainable and multifunctional liquid crystal technologies.

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