

ABSTRACT

This thesis is focused on the characterization and development of several liquid crystalline compounds and mixtures for their applicability in various display and non-display applications. Additionally, relevant aspects of structure-property relationship as well as fluoro-aromatic chemistry of liquid crystals have been explored through this work.

In Chapter 1, the basic knowledge related to the ordering and molecular structures of liquid crystals are discussed, followed by necessity and utilization of liquid crystal mixture formulation.

Chapter 2 deals with various experimental techniques, which have been used to characterize the mesomorphic properties of liquid crystals, along with the underlying theoretical backgrounds.

In Chapter 3, the influence of the position of fluoro substituent on physical properties of *isothiocyanated and fluorinated alkyl terphenyl liquid crystals* has been extensively investigated.

- Terminal isothiocyanate group allow maintaining a high clearing temperature even in the presence of a few lateral fluorine atoms.
- 3,5-difluoro substituted compound with the fluorine atoms, pointing in the opposite direction, possess higher value $\Delta\varepsilon$, ε_{\parallel} , ε_{\perp} , Δn , n_o and n_e than 3,3'-difluoro substituted compound as the fluorine atom in the central 3' position involves some twist of the benzene rings, which decreases π electron conjugation.
- The tri-fluorine substitution in the 3,3' and 5 position increases the molecular width and hinders the molecular rotation, resulting in higher values of the rotational viscosity.
- The compound with 3,5 fluorine substitution possess high Figure of Merit and shows marked improvement in its physical parameters as far as its applicability in multicomponent mixtures is concerned.

In Chapter 4, four multi-component nematic mixtures A, B, C and D comprised of isothiocyanates, biphenyl and terphenyl derivatives have been prepared and characterized to optimize their physical parameters for fast switching liquid crystal display devices.

- All these mixtures exhibit broad nematic range ($\sim 100^\circ\text{C}$), moderate birefringence ($\sim 0.23\text{-}0.26$), positive dielectric anisotropy ($\sim 8\text{-}10$) and low rotational viscosity and show improved performance with respect to the commercial mixture **E7**.
- As far as display performance is concerned, mixture **D** is the most suitable one.

The above two investigated systems deals with achiral liquid crystals while in the following three chapters the effect of chirality in mesomorphic properties has been observed.

In Chapter 5, the structural properties of chiral lactic acid derivative have been discussed.

- The compound shows a rich variety of mesomorphism: blue phase (BPII), cholesteric (N^*), TGB_A and paraelectric SmA^* phases over a broad temperature range. A very characteristic platelet texture of blue phase, oily streaks texture of cholesteric phase and filament texture of $\text{TGB}_A\text{-SmA}^*$ phase transition clearly indicates the type of mesophases.
- Increase in x-ray intensities at the onset of the TGB_A phase at $\text{N}^*\text{-TGB}_A$ phase transitions signify the appearance of long range order in layering within the TGB_A phase.
- Near $\text{TGB}_A\text{-SmA}^*$ phase boundary, strong SmA fluctuations predominate and unwinds the helical twist. As a result, long range smectic ordering appears at $\text{N}^*\text{-TGB}_A$ phase transition, followed by significant jump in the x-ray intensities.

- Within the TGB_A phase, the ratio of layer spacing to molecular length is around 0.74–0.88, identifying the signature of monolayer blocks of SmA in TGB_A phase.

In Chapter 6, the *effect of several polar ester linkage groups incorporated in the molecular core of a chiral lactic acid derivative*, on structural properties has been investigated in depth.

- The compound possess the paraelectric Smectic A* and ferroelectric Smectic C* phase over a broad temperature range.
- Restrictions on the motion of chiral lactate unit by the hexyl terminal chain, methylene group attached to chiral centre and zigzag structured ester linkage with transverse dipole moment contribute to relatively large values of spontaneous polarization and may be utilized for mixture design for photonic and optoelectronic devices operated at low voltages.
- Reorientation of dipole moment in SmC* phase enhance the values of dielectric anisotropy.
- The value of layer spacing (41.5Å) in orthogonal SmA* phase agrees quite well with the calculated length (42.0Å) of the most extended conformer in minimum energy configuration by MOPAC and decreases in the tilted SmC* phase.

In chapter 7, electro-optical properties of *orthoconic antiferroelectric liquid crystals (OAFLCs) of some analogues of (S)-MHPOBC* have been characterized using polarization field reversal technique.

- The occurrence of a high value of spontaneous polarization (P_s) for the investigated compound is due to bulky chiral unit, zigzag ester linkages and polar fluorinated terminal. However lengthening of oligo-methylene spacer in terminal chain and placement of fluorine atom in molecular core structure leads to reduction in the value of spontaneous polarization.

- Unsubstituted or monofluoro substituted liquid crystals with relatively low viscosities and transverse dipole moments exhibit fastest response time ($\sim 150\mu\text{s}$) and low viscosity than the difluorinated compounds.
- “V-shaped” mode or thresholdless switching has been realized for these compounds with high polarization through strong polar molecular interactions between the liquid crystal and aligning layers of cell surfaces.

In chapter 8, the interaction between achiral and chiral liquid crystals has been explored by thermo-microscopic and electro-optical study. *Three different binary systems by mixing an achiral low viscous phenyl pyrimidine liquid crystalline SmC compound with three different orthoconic anti-ferroelectric* has been prepared and characterized

- In these binary mixtures ferroelectric and antiferroelectric phases have been induced.
- All the physical parameters show a non-additive behaviour with respect to the concentration of chiral mesogens due to strong dipole-dipole and/or intermolecular interactions between polar fluorinated chiral esters and the heterocyclic phenyl pyrimidine compound.
- The chiral compound causes perturbations in the orientational distributions of the transverse dipole moment in the achiral environment with respect to the polar axis. Depending on structural complementary of chiral and achiral component of the mixtures, their dipole-dipole interactions may favour or oppose the induction of chirality into a binary system.
- Interestingly, introduction of the achiral mesogen leads to faster response times of these binary mixtures at the cost of lower P_s . Therefore, these mixtures can be useful for high speed technological applications where low polarization, long pitch and very fast switching ferroelectric liquid crystal mixtures are desirable.