EXPERIMENTAL

3.1. Chemical and materials

All solvents were purified and dried using standard procedures. The materials were procured from Tokyo Kasei and Lancaster Chemicals. Silica (60-120 mesh) from Spectrochem was used for chromatographic separation. Silica gel G (E-Merck, India) was used for TLC.
3.2 Experimental techniques:

UV-visible spectroscopy:

UV visible absorption spectra of the compounds in CHCl₃ at different concentrations were recorded on a Shimadzu UV-1601PC spectrophotometer (λ_max in nm).

Infrared Spectroscopy:

IR spectra were recorded on a Perkin-Elmer L 120-000A spectrometer (λ_max in cm⁻¹) on KBr disks.

NMR:

The ¹H nuclear magnetic resonance spectra were recorded either on JEOL FX-90Q multinuclear spectrometer or Bruker DPX-300 spectrometer in CDCl₃ (chemical shift in δ) solution with TMS as internal standard.

CHN analysis:

The elemental analysis was carried out using PE2400 elemental analyzer.

Thermal Microscopy:

The thermal behaviour of the compounds is studied using a thin film of liquid crystalline material sandwiched between glass plate and a cover slip kept in the path of white light beam crossed with polarizers with a polarizing microscope (Nikon optiphot-2-pol) attached with Instec hot and cold stage HCS302, with STC200 temperature controller configured for HCS302. The accuracies in temperatures are 0.10°C. Since the sample is birefringent interference colors
appeared which resulted in beautiful textures characteristic of molecular arrangement. The phase transition temperatures were detected and associated textures of different liquid crystalline phases were observed. The textures were recorded using photo micrographic equipment attached with the polarizing microscope. The liquid crystalline properties were established by thermal microscopy and the phase transitions were confirmed by differential scanning calorimetry.

**Differential Scanning Calorimetry:**

The thermal behaviour of the compounds was examined using a Perkin-Elmer differential scanning calorimeter (DSC) Pyris-1 spectrometer.

**Magnetic susceptibility measurements:**

The magnetic susceptibility measurements were carried out at room temperature on Cahn-Faraday electrobalance using Hg[Co(NCS)₄] as the calibrant or the magnetic measurements were made using SQUID equipment.

**Photoluminescent measurements:**

Photoluminescence spectra were recorded on Shimadzu RF-53D1 PC. The fluorescence quantum yield was determined by using quinine bisulfate in 0.1N H₂SO₄) as standard or by dilution method using 9, 10- diphenyl anthracene as standard.

**DFT study:** Quantum chemical calculations were carried out using density functional theory (DFT) as implemented in DMol3 package.
**XRD study:** Variable temperature powder X-ray diffraction (PXRD) studies were carried out using an image plate detector (Mac Science, Japan) equipped with double mirror focusing optics, with the sample contained in a Lindmann capillary tube or Variable temperature powder X-ray diffraction (PXRD) of the samples were recorded on a Bruker D8 Discover instrument using Cu-Kα radiation.