



e-ISSN: 2319-8753 | p-ISSN: 2347-6710

# IJIRSET

International Journal of Innovative Research in  
**SCIENCE | ENGINEERING | TECHNOLOGY**



# INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH

IN SCIENCE | ENGINEERING | TECHNOLOGY

Volume 11, Issue 5, May 2022

**ISSN** INTERNATIONAL  
STANDARD  
SERIAL  
NUMBER  
INDIA

Impact Factor: 8.118

# Synthesis and Mesomorphic investigations of Novel Liquid Crystalline Hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxybenzylidene amino]-benzoate and its Nickel(II) complex

Madeeha Rashid, Sachin K Singh\*

Department of Chemistry, DDU Gorakhpur University, Gorakhpur, Uttar Pradesh, India

**ABSTRACT:** A new liquid crystalline ligand, hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate with dodecyloxy alkyl chain, and its nickel(II) complex have been synthesized. The ligand and its nickel(II) complexes are characterized by elemental analyses, fourier transform infrared (FT-IR), <sup>1</sup>H nuclear magnetic resonance (NMR) and ultraviolet (UV)-visible spectroscopy. The liquid crystalline properties of these compounds are investigated by polarizing optical microscopy (POM) studies. The ligand shows enantiotropic SmA phase with long temperature range. The square planar nickel(II) complex of the ligand shows only an isotropic phase at higher temperature and no mesogenic nature is observed. DFT calculations have been performed using GAUSSIAN-03 program at B3LYP level to obtain the stable electronic structure of the ligand.

**KEYWORDS:** liquid crystal, polarizing optical microscopy; calamitic phase, DFT

## I. INTRODUCTION

Liquid crystal phases are often referred to as a fourth state of matter. Various applications based on liquid crystal phases are of importance in everyday life. They are indispensable in biological systems (e.g. membranes) and are becoming part of high-tech processes [1]. Investigations on the mesomorphic properties of 4-alkoxy benzaldehydes with ester substituted moiety without lateral hydroxyl group [2] and with lateral hydroxyl group [3] and their Ni(II) and Cu(II) complexes were discussed [4]. On the basis of these mesomorphic investigations on ester containing liquid crystals and also all the previous few investigations on this work [5], it is concluded that all these reports are based on condensation of simple alkoxy benzylidenes with different ester compounds (Figure-1). No report on mesomorphic properties and structure-property relationship of *o*-substituted benzylidines are found till date. The present work describes our results of synthesis, characterisation and mesomorphic properties of hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate with dodecyloxy alkyl chain, and its nickel(II) complex. The influence of substitution on mesomorphic properties in terms of the relationship between molecular structure and the thermal stability of the mesophases is also discussed.

Further, in order to explore further the factors which govern the thermal stability of liquid crystals with a Schiff's base core, and the relationship with its molecular structures, we carry out the investigations in a more comprehensive manner wherein a dodecyloxy benzoate ester group into the aldehyde fragment of benzylideneaniline compound and hexoxybenzoate group as terminal fragment are introduced through the preparation of the new mesogenic ligand and its nickel(II) complex. The molecular structures of the title compounds were characterized by elemental analyses, FTIR and NMR techniques. Their liquid crystal properties were investigated by polarizing optical microscopy (POM).

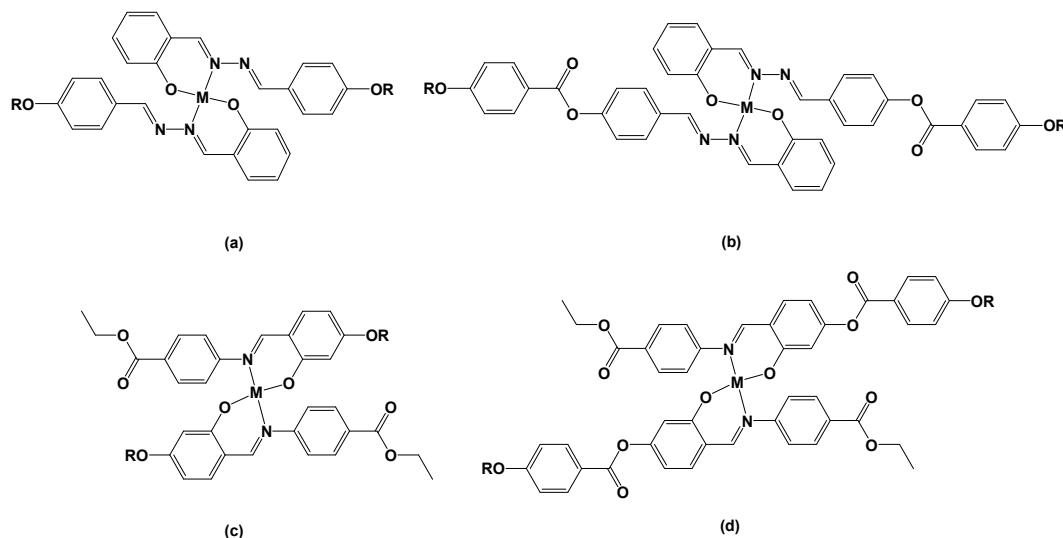


Figure 1. Structure of Schiff's base containing metal complexes

## II. EXPERIMENTAL

### 2.1 Materials

Hexyl 4-aminobenzoate, 4-hydroxybenzoic acid, 2,4-dihydroxy benzaldehyde, bromododecane, thionyl chloride, nickel(II) acetate purchased from Aldrich Chemicals, USA were used as received. All other solvents and reagents were purchased from Merck. The solvents were dried using standard methods [7,8] when required.

### 2.2 Techniques

All the characterization techniques used for the samples as used in copper(II) complexes of butyl-ester derivatives [5]. Elemental analyses were performed on a CE-440 Exeter Analytical CHN analyser. IR spectra ( $4000\text{--}100\text{ cm}^{-1}$ ) were recorded on a Varian 3100 FT-IR Excalibur series spectrophotometer.  $^1\text{H}$  NMR spectra were obtained on a JEOL FT-NMR AL 300 MHz spectrometer using tetramethylsilane as the internal standard. UV-visible spectra were recorded on an (UV)-1700 Pharma Spec. Shimadzu UV-visible spectrophotometer. The mesophase type was identified by visual comparison with known phase standards using an Optica polarizing optical microscope fitted with a hot stage with temperature controlling accuracy of 0.1 K. Quantum chemical calculations was carried out using density functional theory (DFT) as implemented in GAUSSIAN-03 package.

### 2.3 Synthesis

All the synthetic steps used for the work were performed as reported earlier [5,7,8]. The description of all the steps is given below for further understanding (Scheme-1)

#### 2.3.1 Synthesis of 4-dodecyloxybenzoic acid

Ethanol solution (25ml) of KOH (1.235g, 22mmol) was dissolved in 4-hydroxybenzoic acid (1.381g, 10mmol). To this, 1-bromododecane (2.33, 10mmol) was added drop by drop and with constant stirring and was refluxed for 6h. The potassium salt thus obtained was hydrolysed with HCl (pH 3.5), which yielded a white precipitate. The precipitate was filtered off, washed with water and recrystallized from glacial acetic acid and toluene, three times each.

Yield: 77%; IR (KBr,  $\text{cm}^{-1}$ ): 3450 (OH), 2936, 2857 (aliphatic C-H), 1696 (C=O), 1605, 1514 (Ph), 1314, 1257 (-OPh);  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ,  $25^\circ\text{C}$ ): 11.79 (s, 1 H, -OH), 8.11–8.03 (d, 2 H, ArH), 6.93–6.90 (d, 2 H, ArH), 4.04–4.01 (t, 2 H, -OCH<sub>2</sub>), 1.80–1.39 (m, 20 H, -[CH<sub>2</sub>]<sub>8</sub>), 0.89–0.87 (t, 3 H, -CH<sub>3</sub>);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ,  $25^\circ\text{C}$ ):  $\delta_c$  171.96, 163.65, 132.30, 121.30, 114.12, 77.01, 68.25, 31.90, 29.34, 29.23, 29.30, 29.05, 25.94, 22.66, 14.11. Elemental analyses: calculated for  $\text{C}_{19}\text{H}_{30}\text{O}_3$  (%), C, 74.47; H, 9.87; Found, C, 74.43; H, 9.89.

#### 2.3.2 Synthesis of 4-(4'-dodecyloxy)benzoyloxy-2-hydroxybenzaldehyde:

4-dodecyloxybenzoic acid (5.0 mmol, 1.41 g) dissolved in dry chloroform (20 ml) was heated under reflux with thionyl chloride (15.0 mmol, 1.10 ml) for 6h. The solvent was removed under reduced pressure to give yellow oil. It was further treated with a solution of 2, 4-dihydroxy benzaldehyde (5.0 mmol, 0.69 g) in dry chloroform (35 ml) in

presence of 2–3 drops of pyridine. The mixture was then refluxed for 5h. A light yellow solution was obtained. It was washed with water (2x25 ml), dried over anhydrous  $\text{MgSO}_4$ , and then concentrated to form cream coloured crystals of 4-(4'-decyloxybenzoyloxy)-2-hydroxybenzaldehyde.

Yield: 61%; IR (KBr,  $\text{cm}^{-1}$ ): 3418(-OH), 2924, 2854(aliphatic C-H), 1716(ester, C=O), 1679 (aldehyde, C=O), 1604, 1511 (Ph), 1303, 1254 (-OPh);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS)  $\delta_{\text{H}}$  (ppm): 11.24(s, 1H, -OH), 9.88(s, 1H, -CHO), 8.12-6.86(m, 7H, ArH), 4.04-4.01(t, 2H, -OCH<sub>2</sub>), 1.84-1.27(m, 20H, -[CH<sub>2</sub>]<sub>10</sub>), 0.90-0.84(t, 3H, -CH<sub>3</sub>);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ , 25°C):  $\delta_{\text{C}}$  194.46, 163.92, 163.18, 134.91, 132.465, 118.57, 114.42, 114.15, 110.86, 68.42, 31.91, 29.62, 29.58, 29.53, 29.33, 29.32, 29.05, 25.94, 22.64, 14.11. Elemental analyses: calculated for  $\text{C}_{26}\text{H}_{34}\text{O}_5$  (%), C, 73.21; H, 8.03; Found, C, 73.20; H, 8.09.

### 2.3.3 Synthesis of Hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate:

4-(4'-dodecyloxy)benzoyloxy-2-hydroxybenzaldehyde (2.03, 5mmol) and hexyl-4-aminobenzoate (1.10g, 5 mmol) were mixed together in ethanol (20 ml) followed by the addition of 8-10 drops of glacial acetic acid. The reaction mixture was refluxed for 4h. The yellow precipitate that formed on cooling was filtered off. Washed with cold ethanol and recrystallized from ethanol-chloroform(1/1, v/v) mixture.

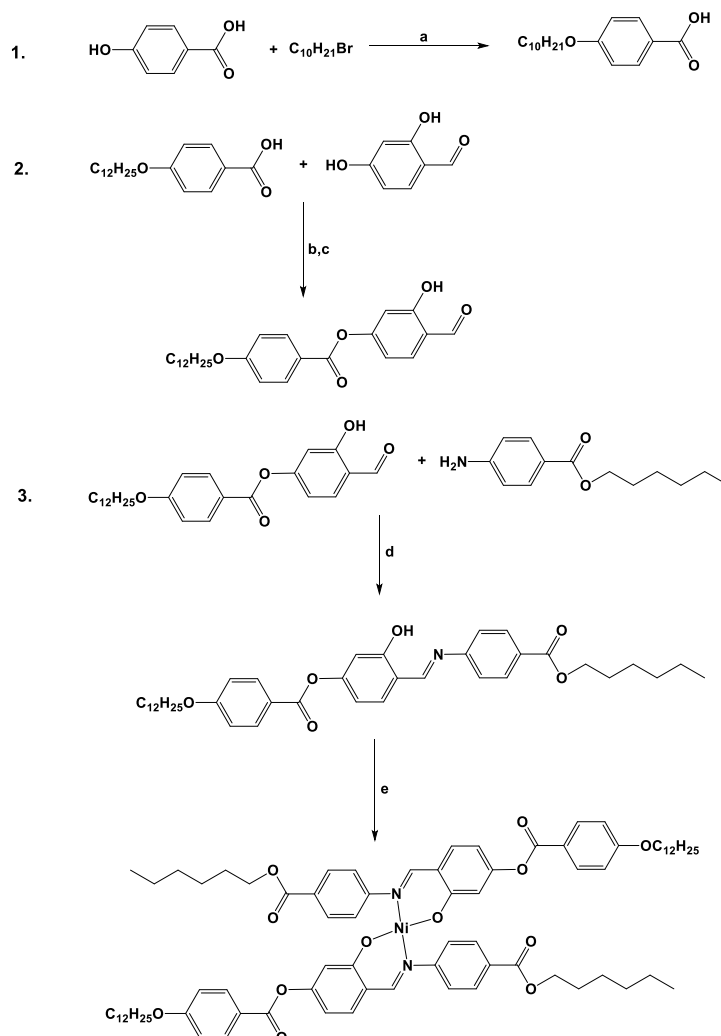
Yield: 78%; IR (KBr,  $\text{cm}^{-1}$ ): 3421(OH), 2924-2854(aliphatic C-H), 1716(ester, C=O), 1636 (-C=N), 1605-1509 (Ph), 1321, 1255 (OPh);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , TMS)  $\delta_{\text{H}}$  (ppm): 13.23(s, 1H, -OH), 8.63(s, 1H, -CH=N), 8.11-6.84(m, 11H, ArH), 4.35-4.32(t, 2H, COOCH<sub>2</sub>-), 4.06-4.01(m, 2H, -OCH<sub>2</sub>), 1.84-1.27 (m, -[CH<sub>2</sub>]<sub>n</sub>), 1.02-0.94(t, 3H, -CH<sub>3</sub>), 0.90-0.86(t, 3H, -CH<sub>3</sub>). Elemental analyses: calculated for  $\text{C}_{39}\text{H}_{51}\text{NO}_6$  (%), C, 74.37; H, 8.16; N, 2.22; Found, C, 74.30; H, 8.14; N, 2.16.

### 2.3.4 Synthesis of nickel (II) complex of hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate:

To a solution (20 ml) of hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate (1.23g, 2 mmol) in hot methanol/chloroform(1/1, v/v), stirred at room temperature was added nickel acetate (1.78 g, 1 mmol) in methanol (12 ml). The mixture was stirred at room temperature for 6h. The resulting brown solid was filtered off, washed with methanol and recrystallized from chloroform-ethanol (1/1, v/v).

Yield: 43%; IR (KBr,  $\text{cm}^{-1}$ ): 1716(ester, C=O), 2924-2853(aliphatic C-H), 1605(-C=N and Ph merge together), 1544, 1512(Ph), 1281, 1256(OPh); UV-visible: (nujol):  $\lambda_{\text{max}}$  = 412, 378, 368, 355, 295, 280, 267, 210; Elemental analyses: calculated for  $\text{C}_{78}\text{H}_{100}\text{N}_2\text{O}_{12}\text{Ni}$  (%), C, 71.17; H, 7.66; N, 2.13; Found, C, 71.11; H, 7.58; N, 2.08.





**Scheme 1.** Reactions and reagents: (a)  $\text{C}_{12}\text{H}_{25}\text{Br}$  (1.0 equiv.), KOH (3.0 equiv.), refluxing in EtOH, 8 h, 77% (b)  $\text{SOCl}_2$  (3.0 equiv.), refluxing in dry chloroform, 7h (c) 2,4 dihydroxy-benzaldehyde (1.0 equiv.), pyridine (catalyst), refluxing in dry DCM, 61%. (d) acetic acid (3 drops), refluxing in EtOH, 4 h, 78%. (e)  $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$  (0.5 equiv.), refluxing in  $\text{MeOH}/\text{CHCl}_3$  (1:1), 6 h, 43%.

### III. RESULTS AND DISCUSSION

#### 3.1 Synthesis and Characterization

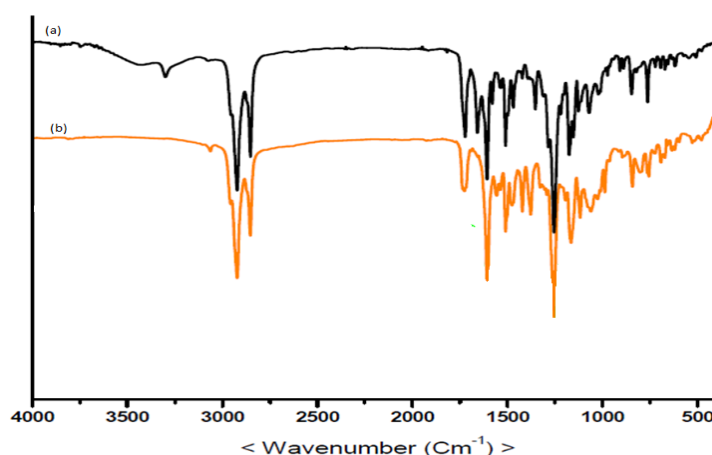
The synthetic route for preparation of calamitic liquid crystalline compound hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate and the nickel(II) complex is outlined in Scheme 1. Alkylation of 4-hydroxybenzoic acid with dodecyl bromide in presence of strong base in ethanol allowed yield of 4-dodecyloxybenzoic acid, which on further esterification with 2, 4-dihydroxy benzaldehyde gave the desired ligand. The Schiff base was obtained by the condensation of hexyl 4-aminobenzoate with 4-(4'-dodecyloxy)benzoyloxy-2-hydroxybenzaldehyde in refluxing ethanol.

The metal complex, Ni(II) was prepared by the reaction of hexyl-[4-(4'-decyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate with nickel acetate in refluxing ethanol. The complex was then isolated as orange crystals by recrystallisation from absolute ethanol in good yield.

The ligand and its nickel(II) complex were characterized by all the standard spectroscopic techniques. The IR spectrum of 4-(4'-dodecyloxy)benzoyloxy-2-hydroxybenzaldehyde shows absorption bands at 3418, (2924, 2854), 1716, 1679, (1604, 1511), (1303, 1255)  $\text{cm}^{-1}$  assigned to  $\nu$  (OH),  $\nu$  (aliphatic C-H stretch),  $\nu$  (C=O phenyl ester),  $\nu$

(C=O aldehyde),  $\nu$  (Ph), and  $\nu$  (OPh), respectively. The IR spectrum of hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate shows absorption bands at 3421, (2921, 2854), 1716, 1636, (1605, 1509) and (1321, 1255) which are assigned to  $\nu$  (OH),  $\nu$  (aliphatic C-H),  $\nu$  (C=O) of phenyl ester,  $\nu$  (C=N),  $\nu$  (Ph) and  $\nu$  (OPh) modes, respectively. The disappearance of the band at  $1679\text{ cm}^{-1}$  due to  $\nu$  (CH=O) and appearance of a new band at  $1636\text{ cm}^{-1}$  due to  $\nu$  (C=N) indicate condensation of aldehyde with amine forming Schiff base (Figure-2). The proton NMR of 4-(4'-dodecyloxy)benzoyloxy-2-hydroxybenzaldehyde exhibit peaks  $\delta$  11.24 (s), 8.63, 9.88, 8.12-6.86 (m), 4.04-4.01 (t), 1.84-1.27 (m), and 0.90-0.84 (t) ppm which are assigned to -OH, -CHO, ring, -OCH<sub>2</sub>-, -[CH<sub>2</sub>]<sub>n</sub> and -CH<sub>3</sub> protons, respectively. The proton NMR spectrum of hexyl-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylideneamino]-benzoate exhibits peaks at  $\delta$  13.23 (s, 1 H, -OH), 8.63 (s, 1 H, -CH=N), 8.11-6.84 (m, 11 H, ring), 4.35-4.32 (t, 2H, COOCH<sub>2</sub>-), 4.06-4.01 (t, 2H, -OCH<sub>2</sub>), 1.84-1.27 (m, 20H, -[CH<sub>2</sub>]<sub>n</sub>), 1.02-0.94 (t, 3H, -CH<sub>3</sub>) and 0.90-0.86 (t, 3H, -CH<sub>3</sub>) ppm, respectively. The signals due to Schiff base formation is observed at 8.63 ppm which corresponds to o-hydroxy benzylidene. The signals of three rings overlap and are observed at  $\delta$  8.14-6.84. The length of alkyl chain has no significant effect on the position of the signals due to -OH, -CH=N, ring, -OCH<sub>2</sub>-, -[CH<sub>2</sub>]<sub>n</sub>, and -CH<sub>3</sub> protons, respectively.

The IR spectrum of nickel(II) complex shows absorption bands at (2924, 2853), 1716, 1605 and (1281, 1256) which are assigned to  $\nu$  (aliphatic C-H),  $\nu$  (C=O) of phenyl ester,  $\nu$  (Ph, C=N) and  $\nu$  (OPh) modes, respectively. The disappearance of the band  $3421\text{ cm}^{-1}$  due to  $\nu$  (OH) and considerable shift in  $\nu$  (C=N) mode indicates coordination of ligand to nickel(II) ion. The electronic-spectrum of the orange coloured nickel(II) complex shows transitions at 412, 378, 368, 355, 295, 280, 267, 211 nm. The first band can be assigned to the transition,  $^1A_{1g} \rightarrow ^1B_{1g}$ , in a square planar environment of the metal ion [12]. The remaining bands are attributed to the  $\pi$ - $\pi^*$  and  $n$ - $\pi^*$  transitions of the ligand.



**Figure 2.** Infrared Spectra of mesogenic ligand (upper spectra) and it's nickel(II) complex (lower one)

### 3.2 DFT study

The GAUSSIAN-03 program [9] package was employed to carry out DFT [10-15] calculations at the Becke's three parameter functional and Lee, Yang and Parr correlation functional (B3LYP) level [15-18] of calculation and 6-31G(d) basis set [19] was used for ground state geometry optimization and frequency calculations of the ligand with dodecyloxy alkoxy chains. The internal coordinates of the system, which is used as input for GAUSSIAN-03 program was generated by the GAUSS VIEW 4.1 program [20]. The absence of any imaginary frequencies in the calculated vibrational frequencies ensures that the optimized geometry corresponds to a true energy minimum. The length of fully extended ligand is found to be  $35.50\text{ \AA}$ , from DFT calculations. All the three phenyl rings are twisted with respect to central ring. The calculated dihedral angle between C(2)-C(3)-C(14)-C(15) and C(19)-C(21)-C(30)-C(32) are  $131.24^\circ$  and  $147.34^\circ$  respectively, implying the twist of two outer most phenyl rings with respect to central ring. The DFT study also indicates that three phenyl rings are although twisted with respect to each other but shape of the compound is calamitic (rod like) in nature. The space filling diagram of the ligand indicates that non coplanarity of the dodecyloxy chain containing ester ring is very high with central ring. This non-coplanarity may play a considerable role in broadening of the molecule and therefore affects the mesomorphic behaviour of the molecule.

### 3.3. Liquid Crystalline behavior

The liquid crystalline property of ligand and its nickel(II) complex were investigated by polarizing optical microscopy using a heating and cooling stage and the phase transition temperatures. The texture of the mesophase seen through polarizing microscope as shown in Figure 3 revealed that it is a SmA mesophase, having a fluid property with higher viscosity and stratified structures with well defined interlayer spacing. The interlayer attractions are weak and the layers are able to slide over one another relatively easily. The flexibility of the layers leads to distortions, which give rise to beautiful optical patterns known as the focal-conic texture [1-3]. The systematic observation of textural pattern can be seen through POM studies which indicates that the ligand is enantiotropic in nature, it is showing liquid crystalline behaviour in heating and cooling cycle both. The SmA mesophase shown in both cycles have a beautiful observations of different colour bands which are actually due to thermochromic behaviour of the molecule on POM hot stage and indicates its possible application for temperature sensor after suitable chemical modifications. The nickel(II) complex was found as non-mesogenic in nature as indicating by POM studies.

Thus, on comparison of Schiff base mesogens with ethoxy end group and their copper(II) complexes [5]; the present ligand with dodecyloxy chain length and hexyloxy end group is although mesogenic in nature showing same mesophase behaviour (SmA) with focal conic texture in both heating and cooling cycle, its nickel(II) complex is non-mesogenic. This is probably due to fact that presence of substituted (ester containing) aryl ring in imine moiety, considerably broadens the molecular width. Moreover, the ester containing benzylidene ring is not coplanar with the central ring containing metal ion. This broadening of molecular width and the non coplanarity of the imine ring is less favorable for exhibiting liquid crystal properties.



**Figure 3.** Optical textures of ligand under a polarizing optical microscope

## IV. CONCLUSIONS

A new mesogenic ester containing Schiff's base having terminal dodecyloxy chain and hexyloxy benzoate as end group and its nickel(II) complex, have been synthesized and characterized. The mesomorphic properties of the compounds were characterized by polarizing optical microscopy. The ligand shows enantiotropic SmA mesophase and nickel(II) complex is non-mesogenic in nature. Thus, addition of ester bond at benzylideneaniline ring although helps in introducing mesogenic property in ligand but it is unfavourable for metallomesogen formation due to non-coplanarity of the benzoate ring which broadens the width of the metal containing molecule leading to transition of the molecule in higher order state i.e. solid state.

### Acknowledgements

The authors thank Department of Chemistry, Banaras Hindu University, Varanasi, India for providing characterization facilities.

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