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"Effect of the linking unit on the calamitic-shaped liquid crystal: a comparative study of two homologous series of benzoate and cinnamate linked compounds"

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ABSTRACT

Two homologous series based on three linking groups have been synthesized and well characterized by elemental analyses and spectroscopic techniques such as Fourier transform infrared [FT-IR] and proton magnetic resonance magnetic resonance [¹H NMR] spectroscopy. The mesomorphic properties of these compounds were observed by using optical polarized microscopy (POM) and confirmed by differential scanning calorimetry (DSC) analysis. In this present investigation, we have synthesized two homologous series viz. (E)-4-(3-(4-(tetra decanoyloxy) phenyl) acryloyl) phenyl-4-n-alkoxy benzoate (Series-1) and 4-((E)-3-(4-(((E)-3-(4-n-alkoxy phenyl) acryloyl) oxy) phenyl)-3-oxo prop-1-en-1-yl) phenyl tetradecanoate (Series-2). Both of the series are differing with respect to the first linking group. All the homologous in following series displays LC properties on heating as well as cooling condition except first four homologous (C_1 to C_4) in series-1 and six homologous (C_1 to C_6) in series-2. To get more insights, the HOMO, LUMO studies are carried out which supports intramolecular charge transfer interactions in this class of mesogens.



Liquid crystals; SmC; chalcone; nematic



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1. Introduction

Thermotropic liquid crystals are an important class of self-organized molecular entities which are in dynamic motion yet possessing a long range orientational order [1,2]. A Thermotropic LC molecule consists a core, which is usually a linker rod like to link aromatic ring by different linker units and tail part which are either straight alkyl or alkoxy chains whose terminal unit is obviously a polar substituent to providing flexibility to stabilize the molecular alignment. Based on the type of the substituents and their combinations, both nematic and smectic mesophases may be formed [3–5]. Study of liquid crystalline state is a multidisciplinary subject and useful to mankind and various industrial applications [6–9] due to its unique property to flow as liquid and optical properties as crystals. The construction of liquid crystalline molecules is usually carried out by adopting a covalent strategy [10].

A number of shaken, having reported to exhibit a broad spectrum of anti-bacterial, antifungal, antiulcer, antimalarial, antitumor, anticancer, anti-inflammatory and antitubercular activity [11,12]. Remarkably, when shaken group is linked to another linking group it becomes conductive to bring thermally stable mesophase. Liquid crystals in the nematic group are most widely used in production of liquid crystal displays (LCD) mainly due to their unique physical properties as well as a wide range of temperature [13]. In the literature studies, there are several reports of mesogenic compounds having chalcone linkage group [14–19].

Chudghar and his co-workers reported a homologous series containing on ester-chalcone linkages [20]. Yeap et al. have also synthesized mesomorphic compounds containing on ester-chalcone linkage [21]. Thaker et al. reported homologous series based on schiff base and chalconyl linking group [22]. Many homologous series based on single chalcone linkage group were reported by Sharma et al. [23–25]. Earlier, Yellamaggad et al. reported the bent-core unsymmetrical dimers in which cholesteryl ester and chalconyl moiety are present, which enhances the biaxiality and chirality of the system [26]. Later, Gallardo and his group reported polycatenar liquid crystals series based on bent shaped chalcone based LCs compounds possessing a short alkyl chain at one end and other end with varying chain lengths. These derivatives were reported to exhibit SmC, SmA and nematic phase [28]. Sharma et al. reported various homologous series based on chalconyl linking group [29–35]. Recently, Goodby et al. reported reviews based on structure property relationship in low molar mass materials [36].

Thus, the main object of this present work to synthesized and studied the effect of linking group and variable side chain on mesomorphic properties. Here, we have introduce some new calamitic liquid crystal based on ester and vinyl ester linked with chalconyl (-CO-CH = CH-) group. We have compared the thermal stability of mesophase in both series-1, -2. Furthermore, density functional theory (DFT) based HOMO, LUMO studies are carried out which supports charge transfer interactions in presently synthesized LCs compounds.

2. Experimental

2.1. Materials

For present synthesized homologous series required materials: 4-hydroxy acetophenone, Lauric acid, 4-hydroxy benzaldehyde, 4-hydroxy benzoic acid were purchased from

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(S.R.L, Mumbai). N, N-dimethyl amino pyridine (DMAP) and Dicyclohexyl carbodiimide (DCC) was purchased from (Fluka Chemie, Switzerland). R-Br was purchased from (S.R.L. Chemicals, Mumbai). The solvents were dried and purified by standard method prior to use.

2.2. Measurements

Melting points were taken on Opti-Melt (Automated melting point system). The FT-IR spectra were recorded as KBr pellet on Shimadzu in the range of 3800-600 cm⁻¹. Microanalysis was performed on a Perkin-Elmer PE 2400 CHN analyzer. The texture images were studied with a Trinocular optical polarizing microscope (POM) equipped with a heating plate and digital camera. ¹H NMR was recorded on a 400 MHz in Bruker Advance in the range of 0.5 ppm-16 ppm using CDCl₃ solvent. The phase transition temperatures were measured using Shimadzu DSC-50 at heating and cooling rates of 10 °C min⁻¹. The texture image of nematic phase was determined by miscibility method. Thermodynamic quantities enthalpy (Δ H) and entropy (Δ S = Δ H/T) are qualitatively discussed. For the POM measurement, the newly synthesized compound is sandwiched between glass slides and cover slip and heating and cooling rate is (2°C/min) respectively.

3. Result and discussion

The mesomorphic behavior of the present compounds was analyzed by using a polarizing optical microscope (POM), differential scanning calorimetry (DSC), and high temperature X-ray diffraction (XRD).

3.1. Synthesis and characterization

The synthetic route for the preparation of the target molecules is outlined in scheme 1 and scheme 2. The synthesis of 4-formyl phenyl tetradecanoate (1a) is prepared by Steglich esterification reaction from 4-hydroxy benzaldehyde and tetradecanoic acid [37]. Comp.3a is prepared by treating of camp. 1a with 4-hydroxy acetophenone in ethanol [37]. Form FT-IR, the peak of at $1650 \,\mathrm{cm}^{-1}$ confirm the presence of a ketone group in chalcone. 4-n-alkoxy benzoic acid (3c) is prepared by reporting method [38]. 4-n-alkoxy benzaldehyde (4a) is prepared by condensation of 4-hydroxy benzaldehyde with various alkyl bromides (R-Br) in the presence of any. K_2CO_3 and dry acetone [39]. Trans 4-n-alkoxy cinnamic acid is prepared by knoevenagel condensation reaction reported in literature [40]. The final target compounds of series-1 and series-2 were prepared by modifying method using DCC and DMAP in dichloromethane for 24 hours. to get the final compounds [36]. The resultant crude residue was purified by using column chromatography on silica gel eluting with chloroform: methanol as eluent (4:2). FT-IR results show a peak at 1730 to $1760 \,\mathrm{cm}^{-1}$ in the presence of two ester group and 1660 cm-1 for ketone group existence in present series-1 while in series-2, the peaks arise at 1740 to 1750 cm^{-1} and 1630 to 1660 cm⁻¹ which confirms the presence of ester



Scheme 1. (ia) DCC/DMAP, DCM, 48 hr. stirring (rt.); (iia) KOH, EtOH, 24 hr. stirring (rt); (iiia) MeOH, conc.H₂SO₄, 1 hr. reflux; (iiib) R-Br, KOH, MeOH, 4 to 5 hr. reflux; (iiic) KOH, EtOH, 2 hr. reflux; (iva) DCC/DMAP, DCM, 48 hr. stirring (rt); (iva) R-Br, Anhydrous K₂CO₃, dry acetone, reflux; (ivb) Malonic acid, piperidine, pyridine, 1 to 2 hr. reflux.

group and The ¹H NMR results also well supported to the corresponding structures of comp.C₁-I, C₂-l, C₆-l, C₇-l, C₃-ll, C₅-ll, C₇-ll, C₁₂-ll and C₁₄-ll are mention in ESI.

3.2. Mesomorphic behavior study

Here in the present study, we have synthesized novel liquid crystalline compounds having two ester and chalcone as central linking group, joint via three phenyl rings and variable side chain from small alkyl spacer (C_1) to high alkyl spacer (C_{18}) in alkoxy side



Scheme 2. (1) 3C, DCC/DMAP, DCM, 24 hr. stirring (rt.); (2) 4b, DCC/DMAP, DCM, 12 hr. stirring.

group (-OR) with the unchanged tetradecyl group at the right terminal side through both of the series. A newly ester-chalcone-ester linking group based homologous series-1 & series-2 were synthesized from condensation of 4-n-alkoxy benzoic acid (**3c**) and *Trans* 4-n-alkoxy cinnamic acid (**4b**) with (*E*)-4-(3-(4-hydroxy phenyl)-3-oxoprop-1-en-1-yl) phenyl tetradecanoate (**2a**) (chalcone) is synthesized and studied their mesogenic properties. The thermotropic mesophase behavior of all newly synthesized compounds was investigated by using a polarizing optical microscope (POM). The exact temperature of phase transition and associated enthalpy values were determined by differential scanning calorimetry (DSC) analysis. The presence of SmC phase is confirmed by high temperature XRD technique. We have prepared thirteen compounds in each series from the lower member (C₁) to higher member (C₁₈). In series-1, comp. C₁-l to C₅-l and comp.C₁-ll to C₆-ll in series-2 shows the non LCs property, whereas comp.C₅-l to C₁₈-l in series-1 and comp.C₇-ll to C₁₈-LL shows enantiotropic nematic phase. Higher numbers of both the series show enantiotropic smectic C phase.

3.2.1. POM study

We have studied the effect varying alkoxy group and also the effect of linking group on mesogenic property of liquid crystalline compounds. In the present study, we have prepared two newly homologous series based on ester-chalcone and vinylester-chalcone linking group. The transition temperature of present series-1 and series-2 are mentioned in Table 1. Comp.C₁ to C₄ in series-1 and comp.C₁ to C₆ displays non liquid crystalline properties and directly transform solid state to isotropic state without exhibiting LCs properties. Higher member compounds in both series exhibited smectic C phase enantiotropic manner while middle members of both the series show enantiotropic nematic mesophase. Mesophase formation was found to be dependent on the number, position and the molecular length of the side alkyl chain which alter the flexibility of molecules. As shown in Table 1, present synthesized chalconyl-ester and chalconyl-vinylester series shows a wide temperature range of marsupials.

The bar graph of series-1 and series-2 shows the phase behavior of Cr-SmC, Cr/ SmC-N and Cr/N-I transition are listed in Figure 1. It can be seen that, as series

Comp.	Transition	Heating scan(°C)	Cooling scan(°C)	∆H (kJmol ⁻¹)	∆H (kJmol ⁻¹)	ΔS (Jk ⁻¹ mol ⁻¹)	ΔS (Jk ⁻¹ mol ⁻¹)
C ₁ -I	Cr-l	161.1	159.3	7.54	3.56	0.0173	0.0082
C ₂ -I	Cr-I	155.4	153.8	8.65	5.35	0.0192	0.0125
C ₃ -I	Cr-I	154.8	152.5	6.75	7.54	0.0157	0.0177
C ₄ -I	Cr-I	153.4	149.5	5.45	6.43	0.0127	0.0152
C₅-I	Cr-N	139.5	136.9	6.75	5.78	0.0163	0.0141
	N-I	148.9	147.6	11.32	9.87	0.0268	0.0234
C ₆ -I	Cr-N	137.5	135.4	5.65	3.65	0.0137	0.0089
	N-I	144.6	142.5	9.86	10.43	0.0236	0.0251
C ₇ -I	Cr-N	129.6	128.7	6.64	5.64	0.0164	0.0140
	N-I	143.5	142.4	12.43	9.76	0.0298	0.0234
C ₈ -I	Cr-N	124.3	121.5	6.75	4.64	0.0169	0.0117
	N-I	139.8	136.6	14.65	8.97	0.0354	0.0218
C ₁₀ -I	Cr-SmC	108.1	110.1	5.82	1.42	0.0151	0.0037
	SmC-N	121.3	119.9	13.24	8.54	0.0335	0.0217
	N-I	130.4	132.6	6.31	5.67	0.0032	0.0213
C ₁₂ -I	Cr-SmC	102.2	106.6	4.81	3.92	0.0128	0.0103
	SmC-N	120.2	123.7	14.95	4.63	0.0380	0.0116
	N-I	130.1	133.8	9.42	7.85	0.0233	0.0214
C ₁₄ -I	Cr-SmC	95.01	91.92	3.32	5.01	0.0090	0.0137
	SmC-N	103.8	101.3	9.54	10.83	0.0253	0.0289
	N-I	124.1	126.4	4.93	6.42	0.0124	0.0142
C ₁₆ -I	Cr-SmC	93.72	91.67	6.87	3.87	0.0187	0.0106
	SmC-N	107.4	106.8	12.75	9.45	0.0335	0.0248
	N-I	123.5	119.8	9.56	6.86	0.0241	0.0174
C ₁₈ -I	Cr-SmC	79.21	80.54	1.98	4.03	0.0056	0.0113
	SmC-N	101.7	97.02	12.83	14.94	0.0342	0.0403
	N-I	110.2	112.4	7.92	6.78	0.0206	0.0213
C₁-II	Cr-I	193.5	189.4	6.56	5.35	0.0140	0.0115
C ₂ -II	Cr-I	183.5	188.6	8.65	5.87	0.0187	0.0128
C ₃ -II	Cr-I	183.3	186.7	9.45	5.98	0.0205	0.0131
C ₄ -II	Cr-I	173.9	177.3	8.54	6.54	0.0188	0.0146
C ₅ -II	Cr-I	171.4	173.7	9.65	8.75	0.0214	0.0197
C_6 -II	Cr-I	169.8	172.3	7.54	6.98	0.0169	0.0158
C ₇ -II	Cr-N	151.6	154.7	2.76	5.21	0.0064	0.0121
-	N-I	166.9	169.4	4.65	8.64	0.0105	0.0197
C ₈ -II	Cr-N	141.6	143.5	6.98	6.43	0.0249	0.0155
0	N-I	162.8	165.9	9.87	8.96	0.0225	0.0206
C ₁₀ -II	Cr-N	139.5	131.4	7.86	6.54	0.0190	0.0161
	N-I	156.6	159.8	12.65	9.76	0.0293	0.0228
C ₁₂ -II	Cr-SmC	124.21	122.90	5.74	9.01	0.0144	0.0227
	SmC-N	138.92	134.52	12.01	10.56	0.0291	0.0259
	N-I	148.9	150.2	3.74	6.87	0.0088	0.0162
C14-II	Cr-SmC	115.2	117.6	8.73	7.82	0.0224	0.0200
	SmC-N	135.1	138.7	13.04	8.43	0.0319	0.0205
	N-I	140.6	142.6	5.52	7.42	0.0133	0.0175
C ₁₆ -II	Cr-SmC	110.6	108.1	10.45	8.21	0.0272	0.0215
-10	SmC-N	127.4	129.3	12.83	10.45	0.0320	0.0259
	N-I	139.3	141.5	9.01	6.54	0.0218	0.0157
C19-II	Cr-SmC	105.6	109.1	7.32	4.42	0.0193	0.0115
~10 "	SmC-N	121.8	123.6	20.21	9.75	0.0512	0.0245
	N-I	130.6	134.1	7.21	5.67	0.0178	0.0138

Table 1. Transition temperature (°C) and enthalpy (kJ mol⁻¹) and entropy change (J k⁻¹mol⁻¹) by DSC measurement.

(Cr-SmC = solid crystal to SmC; SmC-N = SmC to nematic; N-I = nematic to isotropic transition)

increases from the lower member (C_1) to higher member (C_{18}) , the isotropic temperature gradually decreases. The decreasing tendency in melting and clearing temperature could be due to the lowering the vander waals interactions between aromatic phenyl cores and also the flexibility due to the presence of long alkyl chain in alkoxy group at left terminal part and also the presence of hexadecyl chain inbuilt with the ester group



Figure 1. Bar graph showing thermal behaviour of series-1 and Series-2.

at the right terminal side group [42]. Higher alkyl chain substituted compounds in both the series form a lamellar packing type of arrangement of molecules to induce smectic C mesophase.

3.2.2. Textural study

The crystalline compounds placed on a clear glass slide sheltered by coverslip were heated to the isotropic state and heating and cooling rate is $(2 \degree C/min)$ respectively and observing mesophase texture images. Microphotographs of the textures studied for compounds C₆-l, C₁₄-l, C₁₂-l, and C₁₆-l is shown in Figure 2. Comp.C₆-l display schlieren type texture image of nematic phase at 134.0°C on heating condition. Comp. C₁₄-l shows broken fan type, texture image of smectic C phase at 118.0°C on cooling condition. Comp.C₁₂-l exhibits broken fan type, texture image of smectic C phase at 108°C on heating, condition while comp.C₁₆-ll display schlieren type texture image of nematic phase at 124°C on heating condition. It can be noted that, presence of mesophase in present both series are enantiotropic type.

3.2.3. Comparative study

Figure 3 shows the geometrical structure of both the series which is generally calamitic rod type. Both the series-1 and series-2 having three phenyl rings joint via three linking groups and unchanged tetradecyl ester group while differ at the first linking group with respect to each other. The presence of ester linking group favors the formation of lamellar packing arrangement due to the dipole–dipole interaction which eventually generated the smectic mesophase [43]. The presence of polar flexible methylene parts in the variable alkoxy chain (-OR) and also presence of the tetradecyl ester group at the right terminal part which increases the polarity and flexibility of molecule to exhibit liquid crystalline property. The space-filling diagram of both the series suggest the molecular length of series-2 is higher as compared to series-1 due to the presence of ethylene group in cinemas linkage which is mentioned in Figure 4 respectively.



Figure 2. Optical photomicrographs on cooling; (a) nematic (comp. C_6 -I) at 134°C; (b) smectic C (comp. C_{14} -II) at 118°C; (C) smectic C (C_{12} -I) at 108°C; (d) nematic (comp. C_{16} -II) at 124°C.



Figure 3. Geometrical shape of series-1 and series-2.

3.2.4. Frontier molecular orbital (FMO) distribution

The calculated frontier molecular orbital (FMO) distributions of comp.C₆-l, comp.C₃-l, comp.C₆-ll and comp.C₃-ll are presented in Figure-S₁ to Figure-S₄. The energy difference between the HOMO and LUMO is termed as HOMO-LUMO gap which provide the knowledge about the molecular length of conjugation and also the band gap level. The theoretical band gaps for comp.C₆-l, C₃-l, C₆-ll and C₃-ll were found to be 5.05 eV, 5.06 eV, 5.03 eV and 5.04 eV respectively. The reactivity and stability of series-2 is higher as compared to series-1 due to the presence of the small band gap. In series-1, close examinations of these orbits reveal that the HOMO is predominantly localized on the second phenyl ring inbuilt with a choking linkage group while the LUMO is mostly concentrated on chalcone group inbuilt with two phenyl rings. Presence of varying



Figure 4. Space-filing diagram of (a) comp.C₆ (series-1); (b) comp.C₆ (series-2).

Table 2.	Average	thermal	stability	in	°C
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Series	Series-1	Series-2
Cr-N	131.2 (C ₅ -C ₈)	147.5 (C ₇ -C ₈)
SmC-N	109.8 (C ₁₀ -C ₁₈)	130.2 (C ₁₂ -C ₁₈)
Cr-SmC	98.6 (C ₁₀ -C ₁₈)	115.0 (C ₁₂ -C ₁₈)
N-I	132.3 (C ₅ -C ₁₈)	148.5 (C ₇ -C ₁₈)

(Cr-N = solid to nematic; SmC-N = smectic C to nematic; Cr-SmC = solid to smectic C; N-I = nematic to isotropic)

alkoxy side chain (-OR) and hexadecyl ester group in both terminal side shows some significant influence on the HOMO and LUMO orbitals. Thus, it can be concluded that the electronic properties of present synthesized compounds could have originated from the phenylic-chalcone group in a series-1 and vinyl-ester contain phenolic chalcone in series-2.

3.2.5. Thermal stability and temperature range

Thermal stability of present novel synthesized series is listed in Table 2. From the Table 2, presently series display smectic C and nematic phase with good thermal stability. SmC-I transition curve shows higher thermal stability as compared to other phase transition. Mesophase commences from C_3 homologue in present both series. Temperature range of mesophase in series-1 is higher as compare to series-2 respectively.

Figure 5 represents the proposed mechanism to indicate the arrangement of lamellar packing in molecules to show SmC and on further heating transform into nematic phase. In Figure 5, we have compared the structural arrangement of comp. C_4 and C_{14} in which comp. C_4 shows only smectic C phase while comp. C_{14} display only nematic phase. Both of the compounds show mesophase on heating and cooling conditions. The molecular length of comp. C_{14} is higher as compared to camp. C_4 due to the presence of long alkyl chain which increases the flexibility and polarity of molecule and does not exist any lamellar packing type arrangement of molecules to exhibit smectic mesophase.

3.3. DSC analysis

The phase transition temperatures and enthalpies were measured by carrying out DSC thermal analysis. All compounds are thermally stable as confirmed by the reproducibility



Figure 5. Propose mechanism of present series-1 and series-2.

of thermograms on several heating and cooling cycles. In Figure 6(a), comp.C₁₀-l exhibits three endothermic peaks at 108.1°C, 121.3°C and 130.4 °C on heating cycle, which corresponds to the presence of crystal to smectic C and smectic C to nematic phase transition while on cooling condition, it appears at 132.6 °C, 119.9 °C and 110.2 °C which was further confirmed by POM analysis. Comp. C12-l shows three endothermic peaks at 102.2 °C, 120.2 °C and 130.1 °C on heating cycle and on cooling cycle, it again appears at 106.2 °C, 123.7 °C and 133.8 °C. Comp. C8-ll shows two endothermic peaks at 141.6 °C and 162.8 °C on heating condition and again reappears at 143.5 °C and 165.9 °C on cooling condition which confirm the results obtained by POM study. Comp.C₁₄-ll exhibits two endothermic peaks at 115.9 °C and 135.1 °C on heating cycle and on cooling cycle, these exothermic peaks traced at 117.62°C and 138.07°C to confirm the presence solid to smectic C and smectic C to nematic phase transition. Comp.C₁₈-ll shows three endothermic peaks at 105.6°C, 121.8°C and 130.6°C in heating condition while on cooling condition; it trace at 109.18°C, 123.63°C and 135.01°C. The phase transition temperatures, enthalpy and entropy values for the present synthesized series are summarized in above Table 1.

4. Conclusion

A new calamitic chalconyl ester derived LCs compounds based on three phenyl rings as rigid core possessing three linking unit having lauryl side group at right end and other



Figure 6. DSC thermograms of compound (a) comp. C_{10} -I; (b) comp. C_{12} -I; (c) comp. C_{14} -II; (d) comp. C_{18} -II on heating and cooling cycles.

end with a variable alkyl chain length in an alkoxy group (-OR). The liquid crystalline properties of the synthesized mesogens are carried out by POM and DSC methods which revealed the occurrence of enantiotropic nematic as well as the addition of smectic C phase in comp. (C_7 to C_{12}). The lower member comp. (C_1 , C_2) shows non liquid crystalline nature due to the presence of short alkyl spacer in the right end alkoxy group. Comp. (C_3 to C_6) shows only enantiotropic smectic C phase while comp. (C_7 to C_{12}) shows smectic C and nematic phase with higher value of temperature range and thermal stability. Comp. (C_{14} to C_{18}) shows nematic phase without displaying any smectic phase on heating and cooling condition. The group efficiency order derived on the basis of (a) mesophase thermal stability, (b) early or late commencement of mesophase, (c) Temperature range of mesophase. The HOMO-LUMO calculations indicated the intermolecular charge transfer interactions and revealed the electronic properties of present synthesized newly compounds were originated from second and third phenyl to chalcone moiety.

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