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Novel Series of 1,3,4- Oxadiazole Derivatives: Evaluation of Thermal Properties and Antibacterial Activity

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Abstract: A new series of 1,3,4-oxadiazole derivatives were synthesized **6(a-i)** by the reaction between respective aliphatic acid hydrazides with *p*-alkoxy aldehydes using chloramine-T (CAT). The synthesized compounds were evaluated for their thermal properties using Polarising Optical Microscopy (POM), Differential Scanning Calorimetry (DSC), and variable temperature Powder X-RD (PXRD). The compounds exhibited spherulitic textures associated with the crystal to isotropic phase. No mesophase was detected upon heating or cooling cycles. Also, the synthesized compounds showed moderate to good antibacterial activity.

Keywords: 1,3,4-oxadiazole;spherulitic;chloramine-T;polarising optical microscope; antibacterial activity.

1. Introduction

Liquid crystallinity is an intermediate property between solid and liquid properties viz., crystallinity and fluidity; this property is exploited for various device technologies. Its design is greatly influenced by the shape of the moiety and often enhanced by linear terminal groups. Molecular geometry and dipole-dipole interactions also play an important role in designing materials to exhibit liquid crystalline properties [1]. Many rod-like mesogens possess para-substituted phenyl ring hasbeen reported [2-4]. The molecule provides polarizability and structural linearity, thereby enhancing the LC properties. Of late, interest has been growing towards incorporating-heterocycles as a mesogenic core in thermotropic liquid crystals. They are electron deficient and would contribute to effective electron-transporting properties, thereby developing self-organization of liquid crystals (LCs) [5-12].

Interest towards oxadiazole derivatives as the mesogenic core has increased linearly since its first report by Zaschke [13] due to its mesomorphic properties and application as potential display materials of electronic devices [14-17].1,3,4-oxadiazoles with varied molecular shapes viz., disk-like [18,19],rod-like [20-24], boomerang-shaped [25], star-like [26], have been studied and also few molecules containing oxadiazole as their mesogenic core have been reported [27-41]. There have also been reports wherein 1,3,4-oxadiazole is nonmesogenic and did not exhibit LC properties due to the great distortion brought about in the molecules' linearity [42]. This destabilization of mesophases is mainly attributed to the

strong bend of the 134^{o} angle. In the interim, 1,3,4-oxadiazoles have been studied by many researchers due to their chemical and thermal stability and their ability to exhibit mesomorphic behavior based on the changes in the groups linked to it. On the other hand, these heterocyclic frameworks are present in several natural products. 1,3,4-oxadiazoles derivatives have a variety of biological applications viz., antibacterial, antifungal [43], anti-inflammatory, analgesic, antitubercular [44], antitumor [45], and anticonvulsant activity [46]. In this regard, we decided to synthesize rod-like mesogens comprising oxadiazole core by varying the terminal chain length to study the structure-property correlations. In this paper, we have reported the synthesis of 1,3,4-oxadiazole derivatives **6(a-i)** using CAT. The reaction conditions and the synthetic route are shown in Scheme 1. We decided to study the effect of the presence of phenyl ring linked to a 1,3,4-oxadiazole ring on one side, and the other side was substituted with the aliphatic group. All the synthesized molecules have the same conjugated core possessing one different terminal groups. The synthesized compounds were evaluated for thermal properties using variable temperature PXRD, POM, and DSC. Besides, antibacterial activities of the synthesized compounds are also reported.

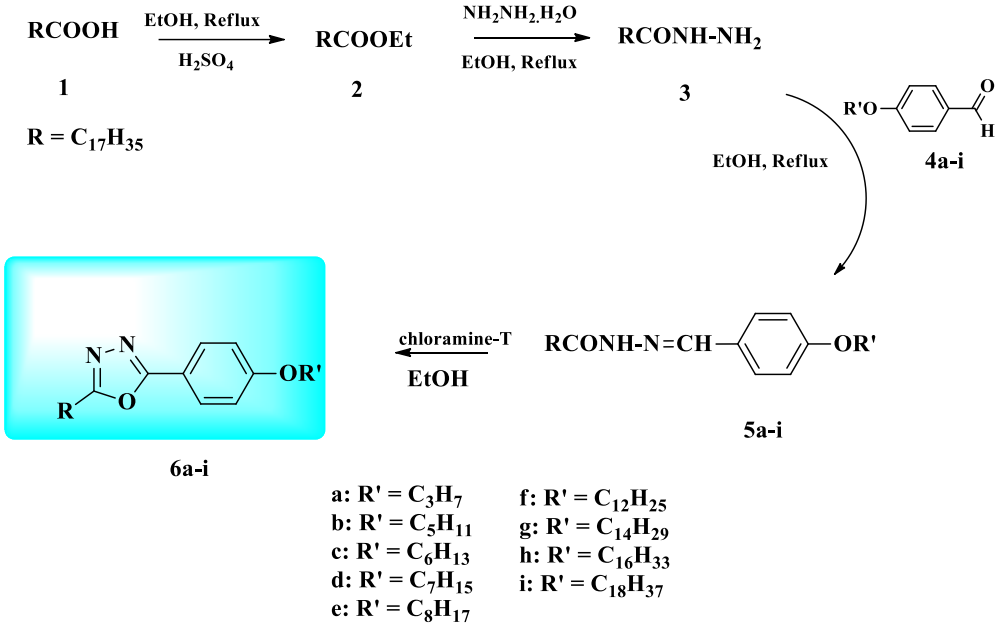
2. Materials and Methods

2.1. Materials and methods.

The chemical ingredients, viz., stearic acid, 4-hydroxy benzaldehyde, n-bromo alkyl halides (for n = 3, 5, 6, 7, 8, 12, 14, 16, and 18), and chloramine-T were procured from LOBA Chemie, India. Hydrazine hydrate was procured from SRL, India. Sulphuric acid, potassium carbonate, dimethylformamide, and diethyl ether were procured from RANKEM, India. Ethanol was procured from CHANGSHU YANGYUAN CHEMICAL, China. Anhydrous sodium sulfate was procured from SDFCL, India. The proposed structure for the intermediate compounds and the final compound is confirmed by the ^{1}H-NMR spectra obtained using an AGILENT (400 MHz) NMR spectrometer. The ^{1}H, ^{13}C NMR, and IR spectra were used to confirm the molecular structure, hydrogen bonding, and the purity of the sample. DSC thermograms were obtained using a Perkin-Elmer DSC 7, with a TAC 7/PC interface and a controlled cooling accessory. The heating rate was 1^{o}C min^{-1}. The textural studies were carried out using an Olympus BH-2 polarizing microscope, fitted with a Mettler FP52 hot stage and a Mettler FP5 controller. Samples were prepared as thin films between a glass slide and a glass coverslip. Thin-layer chromatography (TLC) was carried out on aluminum sheets coated in Merck Kieselgel silica gel 60, eluting with petroleum ether and ethyl acetate (20%).

The antibacterial activity of the synthesized compounds was assessed by the agar well diffusion method. The bacterial strains used in this study were gram-negative bacteria such as *Klebsiella pneumonia* (MTCC 661), *Escherichia coli* (MTCC 1698), gram-positive bacteria such as *Bacillus subtilus* (MTCC 121), *Staphylococcus aureus* (MTCC 6908). 100 mL of Nutrient Agar and cotton swaps were prepared and sterilized. 20mL agar was poured into each clean petri-dish and was placed in a laminar airflow chamber. After solidification, 0.1 mL of the human pathogenic bacteria was spread in the agar plates using the cotton swabs. A well of 10 mm diameter was then formed in the agar plates using a good puncture apparatus. The prepared compounds were poured into the well with 1mg/mL concentration, and the sample volume being 75µL. The plates were kept for incubation at 37°C for 24 hrs. After incubation, the zone of inhibition was measured. Absolute alcohol (solvent), which acts as a negative

control, was added in one well. In the other well, positive control as *Gentamicin Sulphate* (HIMEDIA) was added to the plates.



a: R' = C_3H_7 **b:** R' = C_5H_{11} **c:** R' = C_6H_{13} **d:** R' = C_7H_{15} **e:** R' = C_8H_{17} **f:** R' = $C_{12}H_{25}$ **g:** R' = $C_{14}H_{29}$ **h:** R' = $C_{16}H_{33}$ **i:** R' = $C_{18}H_{37}$

Scheme 1. Scheme of synthesis.

2.2. General procedure for the synthesis of 2.

Stearic acid (1g, 3.5mmol) was taken in 10mL of ethanol and stirred under reflux using a catalytic amount of H_2SO_4. The reaction's progress was monitored using thin thin-layer chromatography; after completing the reaction, ethanol was evaporated. The solid product was washed using sodium bicarbonate and extracted into an ether layer, and it was dried over anhydrous Na_2SO_4.

2.3. General procedure for synthesis of 3.

A mixture of stearate 2 (1g, 3.20mmol) and hydrazine hydrate (0.3mL, 6mmol) in ethanol was stirred under reflux conditions for 6hours. After the completion of the reaction, the mixture was poured into the crushed ice. The precipitate was filtered and washed with water and recrystallized using ethanol.

2.4. General procedure for the synthesis of 4a

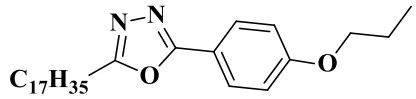
A mixture of *p*-hydroxy benzaldehyde (1g, 8mmol) and *n*-bromopropane (1 mL, 8mmol) and K_2CO_3 (3.3g, 24mmol) in dimethylformamide (20 mL) were stirred for 8 hours at room temperature 25 ^oC. The solid product was extracted into the ether layer, and it was dried over anhydrous Na_2SO_4.

2.5. General procedure for the one-pot synthesis of 6a [47].

A mixture of **3** (1g, 6mmol) and **4a** (1.81g, 6mmol) was dissolved in ethanol and was refluxed for 4 hours, which generates **5a** *in situ. To* it, chloramine-T (3.4g, 12mmol) was added and continued to reflux for 8hours. The completion of the reaction was monitored by TLC. After completion, sodium chloride formed was filtered off and washed with ethanol (15 mL). Filtrate and washing were combined, and the solvent was evaporated in a vacuum. The residue was extracted with ether (25mL × 3), the extract was washed successively with water (15mL ×

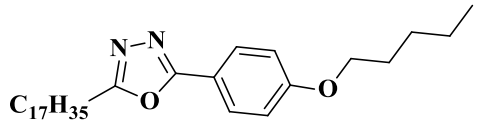
2), 10% NaOH (15mL × 2), and saturated brine solution (10 mL). The organic layer was dried over anhydrous Na_2SO_4. The obtained crude product was purified by recrystallization using methanol.

2.6. Spectral data.

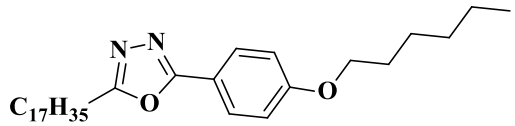


2-heptadecyl-5-(4-propoxyphenyl)-1,3,4-oxadiazole 6a

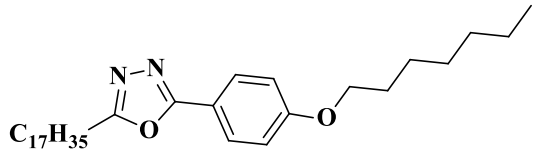
Yield: 78% mp: 167ºC. IR: *v* 2956 cm^{-1} (Ar C-H), 1625 cm^{-1} (Ar C=N), 1616 cm^{-1} (C=C), 1090 cm^{-1} (Ether C-O). ^{1}H NMR (400MHz, $CDCl_3$) *δ*: 7.93 (d, 2H, ArH, *J* = 8.8 Hz), 6.97 (d, 2H, ArH, *J* = 8.8 Hz), 3.99 (t, 2H, OCH_2), 2.90 (t, 2H, CH_2), 1.46-1.24 (m, 32H, CH_2), 1.06 (t, 3H, CH_3), 0.88 (t, 3H, CH_3).^{13}C NMR (100MHz, $CDCl_3$) *δ*: 166.44, 164.61, 161.74, 129.53, 128.42, 128.36, 116.45, 114.88, 69.70, 31.88, 29.64, 29.60, 29.52, 29.48, 29.37, 29.30, 29.08, 28.99, 28.80, 26.60, 25.40, 24.32, 22.63, 22.44, 14.04, 10.40. Anal. Calcd for $C_{28}H_{46}N_2O_2$ C - 75.97; H - 10.47; N - 6.33%; Found: C - 75.56; H - 10.27; N- 6.11%. LCMS [M+1]: 443.24.



2-heptadecyl-5-(4-(pentyloxy)phenyl)-1,3,4-oxadiazole 6b Yield: 81% mp: 154ºC. IR: *v* 2917 cm^{-1} (Ar C-H), 1615 cm^{-1} (Ar C=N), 1605 cm^{-1} (C=C), 1040 cm^{-1} (Ether C-O). ^{1}H NMR (400MHz, $CDCl_3$): *δ* 7.98 (d, 2H, ArH, *J* = 8.4 Hz), 6.96 (d, 2H, ArH, *J* = 8.4 Hz), 4.02(t, 2H, OCH_2), 2.88 (t, 2H, CH_2), 1.81-1.19 (m, 36H, CH_2), 0.89 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): *δ* 166.41, 164.51, 161.73, 129.51, 116.44, 114.87, 69.71, 31.87, 29.64, 29.53, 29.51, 29.49, 29.30, 29.09, 29.00, 28.98, 28.89, 28.81, 28.79, 28.52, 28.11, 26.59, 25.40, 22.63, 22.38, 14.04, 10.42. Anal. Calcd for $C_{30}H_{50}N_2O_2$ C - 76.55; H - 10.71; N - 5.95%; Found: C - 76.25; H - 10.16; N - 5.26%. LCMS [M+1]: 471.27.



2-heptadecyl-5-(4-(hexyloxy)phenyl)-1,3,4-oxadiazole 6c Yield: 79% mp: 130ºC. IR: *v* 2955 cm^{-1} (Ar C-H), 1682 cm^{-1} (C=N), 1574 cm^{-1} (C=C), 1070 cm^{-1} (Ether C-O). ^{1}H NMR (400MHz, $CDCl_3$): *δ* 7.93 (d, 2H, ArH, *J* = 8.8 Hz), 6.96 (d, 2H, ArH, *J* = 8.8 Hz), 4.02(t, 2H, OCH_2, 2H), 2.87 (t, 2H, CH_2), 1.83-1.28 (m, 38H, CH_2), 0.89 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): *δ* 166.42, 164.51, 161.72, 129.50, 116.45, 114.86, 69.70, 31.89, 29.64, 29.54, 29.53, 29.51, 29.49, 29.31, 29.08, 29.00, 28.98, 28.87, 28.83, 28.78, 28.54, 28.12, 26.57, 25.41, 22.61, 22.37, 14.03, 10.41. Anal. Calcd for $C_{31}H_{52}N_2O_2$ C - 76.17; H - 10.12; N - 5.22%; Found: C - 76.81; H -10.81; N - 5.78%. LCMS [M+1]: 485.48.

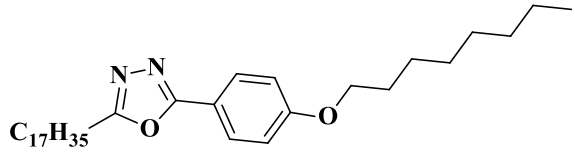


2-heptadecyl-5-(4-(heptyloxy)phenyl)-1,3,4-oxadiazole 6d Yield:76% mp: 122ºC.

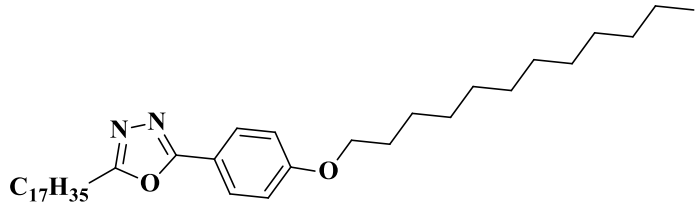
IR: *v* 2917 cm^{-1} (Ar C-H), 1550 cm^{-1} (C=N), 1540 cm^{-1} (C=C), 1034 cm^{-1} (Ether C-O).

^{1}H NMR (400MHz, $CDCl_3$): *δ* 7.93 (d, 2H, ArH, *J* = 8.8 Hz), 6.96 (d, 2H, ArH, *J* = 8.8 Hz), 4.02 (t, 2H, OCH_2), 2.72 (t, 2H, CH_2), 1.83-1.24 (m, 40H, CH_2), 0.87 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): *δ* 166.40, 164.52, 161.71, 129.51, 116.44, 114.88, 69.70, 31.88, 29.67, 29.54, 29.52, 29.49, 29.47, 29.30, 29.09, 29.01, 28.97, 28.88, 28.83, 28.77, 28.54, 28.10, 26.57,

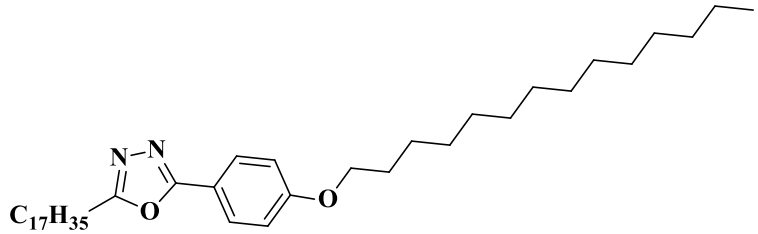
25.41, 22.64, 22.37, 14.02, 10.41. Anal. Calcd for $C_{32}H_{54}N_2O_2$: C - 77.06; H - 10.91; N - 5.62%; Found: C - 77.41; H - 10.22; N - 5.14%. LCMS [M+1]: 499.44.



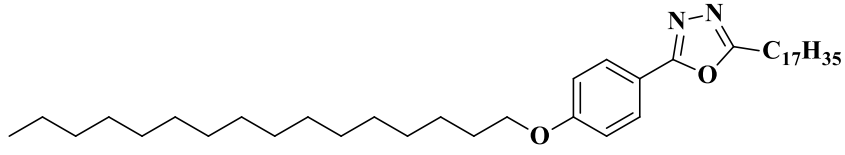
2-heptadecyl-5-(4-(octyloxy)phenyl)-1,3,4-oxadiazole 6e Yield:81%mp: 120ºC. IR: *v* 2956 cm^{-1} (Ar C-H), 1625 (C=N), 1616 (C=C), 1080 (Ether C-O). ^{1}H NMR (400MHz, $CDCl_3$): *δ* 7.93 (d, 2H, ArH, *J* = Hz), 6.96 (d, 2H, ArH, *J* = Hz), 4.02 (t, 2H, OCH_2), 2.88 (t, 2H, CH_2), 1.46-1.24 (m, 42H, CH_2), 0.87 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): *δ* 166.41, 164.50, 161.71, 129.50, 116.45, 114.88, 69.72, 31.88, 29.65, 29.55, 29.53, 29.47, 29.31, 29.27, 29.10, 29.07, 28.97, 28.88, 28.80, 28.78, 28.51, 28.10, 26.57, 25.41, 22.61, 22.37, 14.05, 10.40. Anal. Calcd for $C_{33}H_{56}N_2O_2$: C - 77.29; H - 11.01; N - 5.46%; Found: C - 77.12; H - 11.03; N - 5.21%. LCMS [M+1]: 513.23.



2-heptadecyl-5-(4-(dodecyloxy)phenyl)-1,3,4-oxadiazole 6f Yield:71% mp: 116ºC. IR: *v* 2955 cm^{-1} (Ar C-H), 1711 cm^{-1} (C=N), 1575 cm^{-1} (C=C), 1045 cm^{-1} (Ether C-O). ^{1}H NMR (400MHz, $CDCl_3$): *δ* 7.94 (d, 2H, ArH, *J* = 8.8 Hz), 6.98 (d, 2H, ArH, *J* =8.8 Hz), 4.02(t, 2H, OCH_2), 2.88 (t, 2H, CH_2), 1.84-1.24 (m, 50H, CH_2), 0.87 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): *δ* 166.40, 164.51, 161.70, 129.51, 116.46, 114.89, 69.71, 31.80, 29.60, 29.54, 29.41, 29.37, 29.33, 29.28, 29.11, 29.09, 28.96, 28.89, 28.81, 28.77, 28.50, 28.11, 26.53, 25.40, 22.62, 22.34, 14.06, 10.41. Anal. Calcd for $C_{37}H_{64}N_2O_2$: C - 78.11; H - 11.34; N - 4.92%; Found: C - 78.08; H - 11.14; N - 4.01%. LCMS [M+1]: 569.51.

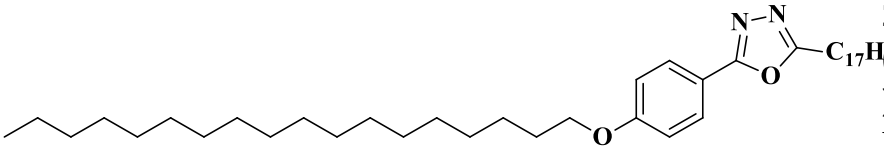


2-heptadecyl-5-(4-(tetradecyloxy)phenyl)-1,3,4-oxadiazole 6g Yield: 77% mp: 105ºC. IR: *v* 2956 cm^{-1} (Ar C-H), 1614 cm^{-1} (C=N), 1574 cm^{-1} (C=C), 1057 cm^{-1} (Ether C-O). ^{1}H NMR (400MHz, $CDCl_3$): *δ* 7.93 (d, 2H, ArH, *J* = 8.8 Hz), 6.96 (d, 2H, ArH, *J* = 8.8 Hz), 4.02 (t, 2H, OCH_2), 2.88 (t, 2H, CH_2), 1.83-1.24 (m, 54H, CH_2), 0.86 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): *δ* 166.44, 164.52, 161.69, 129.52, 116.48, 114.84, 69.70, 31.88, 29.64, 29.56, 29.54, 29.52, 29.48, 29.44, 29.10, 29.07, 28.97, 28.88, 28.80, 28.78, 28.64, 28.41, 26.54, 25.41, 22.64, 22.36, 14.07, 10.40. Anal. Calcd for $C_{39}H_{68}N_2O_2$: C - 78.12; H - 11.16; N - 4.15%; Found: C - 78.47; H - 11.48; N - 4.69%. LCMS [M+1]: 597.53.



2-heptadecyl-5-(4-(hexadecyloxy)phenyl) -1,3,4-oxadiazole 6h Yield: 72% mp: 98ºC. IR: *v* 2917 cm^{-1} (Ar C-H), 1692 cm^{-1} (Ar C=N), 1555 cm^{-1} (Ar C=C), 1030 cm^{-1} (Ether C-O). ^{1}H NMR (400MHz, $CDCl_3$): *δ* 7.94 (d, 2H, ArH, *J* = 8.8 Hz), 6.97 (d, 2H, ArH, *J* = 8.8 Hz), 4.02(t, 2H, OCH_2), 2.88 (t, 2H, CH_2), 1.84-1.25 (m,

58H, CH_2), 0.87 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): δ 166.44, 164.61, 161.74, 129.53, 128.42, 128.36, 116.45, 114.88, 69.70, 31.88, 29.64, 29.61, 29.53, 29.51, 29.37, 29.30, 29.10, 29.00, 29.60, 26.59, 25.96, 25.41, 22.63, 14.04, 10.40. Anal. Calcd for $C_{41}H_{72}N_2O_2$: C - 78.22; H - 11.14; N - 4.12%; Found:C - 78.79; H - 11.61; N - 4.48%. LCMS [M+1]:625.28



2-heptadecyl-5-(4-octadecyloxy)phenyl)-1,3,4-oxadiazole 6i

Yield: 82% mp:93°C. IR: 2917 cm^{-1} (Ar C-H), 1693 cm^{-1} (Ar C=N), 1595 cm^{-1} (Ar C=C), 1020 (Ether C-O). ^1H NMR (400MHz, $CDCl_3$): δ 7.94 (d, 2H, ArH, J = 8.8 Hz), 6.97 (d, 2H, ArH, J = 8.8 Hz), 4.04 (t, 2H, OCH_2), 2.42 (t, 2H, CH_2), 1.81-1.24 (m, 62H, CH_2), 0.88 (t, 6H, CH_3). ^{13}C NMR (100MHz, $CDCl_3$): δ 166.43, 164.60, 161.73, 129.54, 128.41, 128.37, 116.47, 114.87, 69.72, 31.86, 29.67, 29.61, 29.54, 29.50, 29.36, 29.31, 29.14, 29.01, 29.61, 26.58, 25.98, 25.40, 22.64, 14.02, 10.41. Anal. Calcd for $C_{43}H_{76}N_2O_2$: C - 79.08; H - 11.73; N - 4.29%; Found: C - 79.01; H - 11.42; N - 4.11%. LCMS [M+1]: 653.08.

3. Results and Discussion

Their spectral data confirmed the assigned structures to the newly synthesized compounds 6a-i. IR spectra of the synthesized compounds showed characteristic signals at v 2956 cm^{-1} (Ar C-H), 1625 cm^{-1} (C=N), 1616 cm^{-1} (Ar C=C), 1090 cm^{-1} (Ether C-O). The ^1H NMR spectra exhibited peaks at δ 7.98 (d, ArH), 6.96 (d, ArH) for aromatic protons, and δ 1.81-1.19 (m, CH_2) for aliphatic protons. ^{13}C NMR exhibited a characteristic peak at δ 166.41, 164.51 attributed for 1,3,4-oxadiazole carbons, and δ 129.51, 116.44, 114.87 attributed for aromatic protons and δ 29.53- 14.04 attributed for aliphatic carbons. The synthesized compounds' LC-MS spectra exhibited a molecular ion peak at [M+1] corresponding to the molecular weight.

3.1. Photophysical characterization.

Examination of the photophysical properties involved the recording of UV and Fluorescence spectra of the final compounds, which were solid, they were dissolved in chloroform solvent (1mg/mL) and were introduced into a cuvette of 10mm path length, and the absorbance was recorded. UV-Vis absorption spectra and the emission spectra of compound **6g** are depicted in Fig.1.

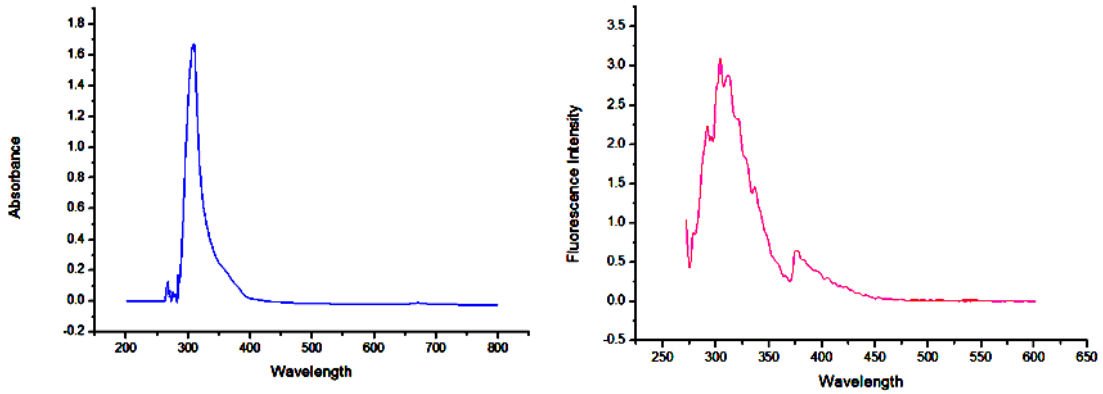


Figure 1. UV absorption spectra and fluorescence emission spectra of representative compound **6g.**

All the final compounds exhibited similar absorption and emission patterns because of the similarities in structure, and the aromatic rings present the same throughout. It was found that the maximum absorption peak obtained at 310nm; the pattern was the same irrespective of the terminal carbon chain length; the reason is uncertain. The emission spectra were recorded in the range 270-600 nm, and the excitation was found to be highest at 270nm. The maximum emission was found at 320nm.

3.2. Evaluation of thermal properties of synthesized compounds.

To study the effect of molecular shape on thermal property, 1,3,4-oxadiazole derivatives were synthesized, whose structures were unlike the typical molecular geometry, which comprises of the rigid central core attached to two phenyl aromatic rings containing terminal flexible alkyl chains. The synthesized compounds **6(a-i)** possessed a 1,3,4-oxadiazole ring linked to a phenyl ring on one side, and the other side was linked to the aliphatic group. All the synthesized molecules have the same conjugated core possessing different terminal alkyl groups. The transition temperatures of the synthesized derivatives were studied using POM and DSC. For POM studies, the compound was sandwiched between two glass plates, and the varying temperature visualized the textures at the rate of 0.5°C min^{-1}. The synthesized compounds exhibited spherulitic textures under POM. The POM images are given in Fig. 2. DSC thermograms (Fig.3) have shown only one transition from crystal to isotropic phase upon heating. Upon cooling cycle, only crystallization was observed for all compounds studied here. Transition temperatures of the synthesized compounds are reported in Table 1.

Table 1. Transition temperatures (°C) of synthesized oxadiazole derivatives.

Compound no	R	Transitions	Isotropic
6a	3	Cr-I	167
6b	5	Cr-I	154
6c	7	Cr-I	130
6d	8	Cr-I	122
6e	10	Cr-I	120
6f	12	Cr-I	116
6g	14	Cr-I	105
6h	16	Cr-I	98
6i	18	Cr-I	93

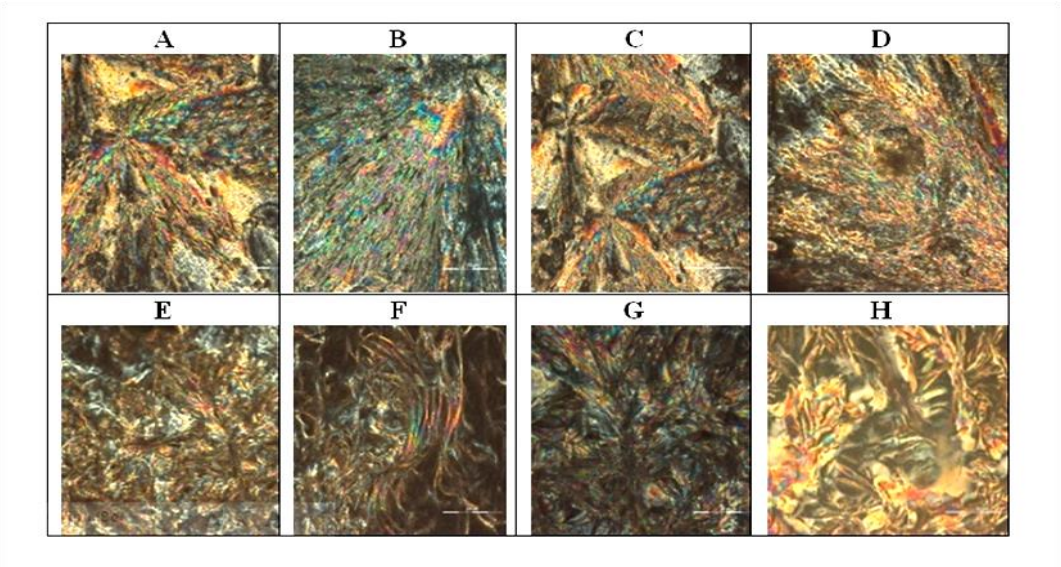


Figure 2. Spherulitic textures obtained under POM. A: **6a** at 30°C, B: **6a** at 42°C, C: **6a** at 57°C, D: **6e** at 31°C, E: **6g** at 32°C, F: **6g** at 48°C, G: **6g** at 68°C, H: **6h** at 78°C.

The present investigations showed that all the synthesized compounds on heating and cooling displayed only one transition, i.e., from crystal to isotropic state (melting point) or crystallization point upon cooling. Further, the synthesized compounds were found to exhibit spherulitic texture. POM images indicated only one transition from crystal to isotropic phase and absence of mesomorphic properties; this could probably be due to the bend which is associated with the bonds at 2 and 5-position of the oxadiazole ring, which did not favor the required packing order for the compounds to be mesomorphic or may be due to the presence of exocyclic bonds which leads to distortion in structure thereby suppressing the mesomorphic behavior.

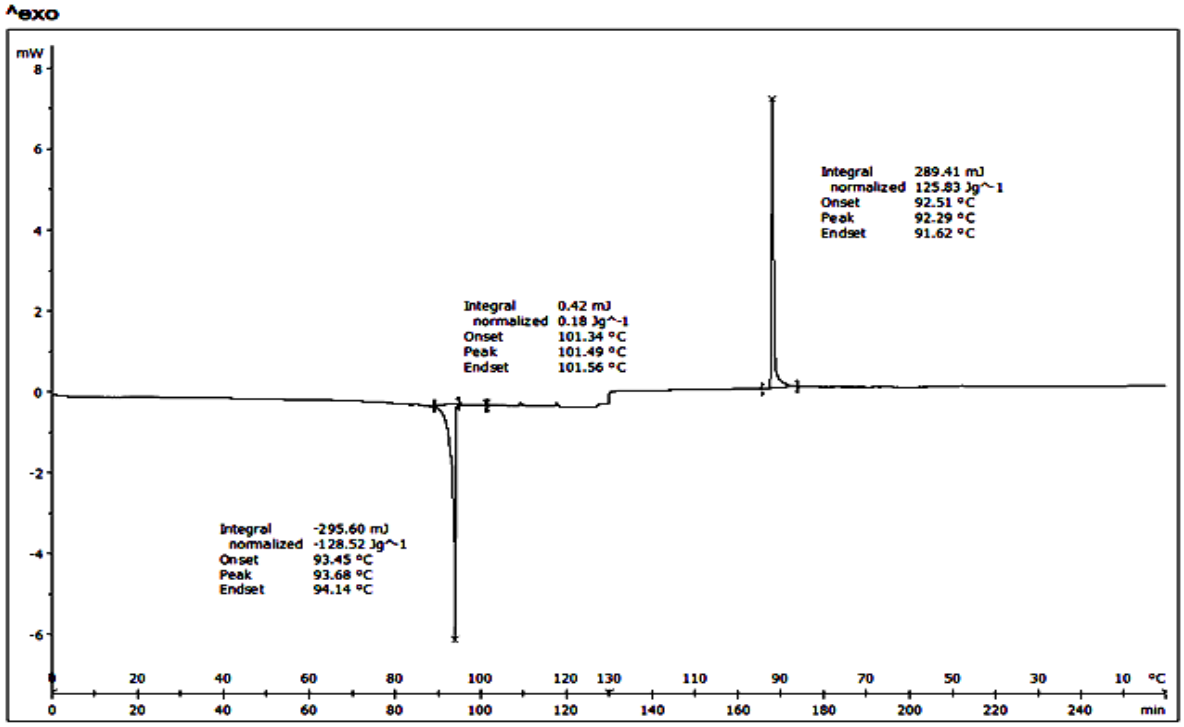


Figure 3. DSC thermogram of **6h.**

3.3. Powder X-ray diffraction study.

The synthesized compounds were studied using variable temperature PXRD. T]\he obtained diffractogram for the compound **6h** at different temperatures is shown in Fig.4. The PXRD pattern of **6h** consists of peaks at d= 30.31, 15.08 at small angle region at 2θ= 2.91, 5.85 respectively. At d = 4.24 at a wide-angle region of 2θ = 20.90 at 60ºC, all the diffractogram peaks disappeared at 63ºC, inferring the low thermal stability and appearance of the isotopic phase. Similarly, PXRD pattern of **6h** consists of peaks at d = 44.88 at a small angle region of 2θ = 1.96 and in wide-angle region d = 4.21 and 3.72 at 2θ = 21.05 and 23.86 respectively at 60ºC and the same diffractogram was observed till 89ºC, all the peaks in the diffractogram disappeared at105ºC inferring the attainment of isotropic phase.

Interpretation of the PXRD diffractogram reveals that all X-ray diffraction data did not present peaks related to the layer structure for smectic phases or broad peaks for nematic mesophase at small-angle X-ray scattering. All compounds exhibited crystalline peaks at a wide-angle area (2θ ~23 °) typically associated with crystal phase. Up to 89ºC above which crystal phase was lost (Fig.4C) and transformed into isotropic phase.

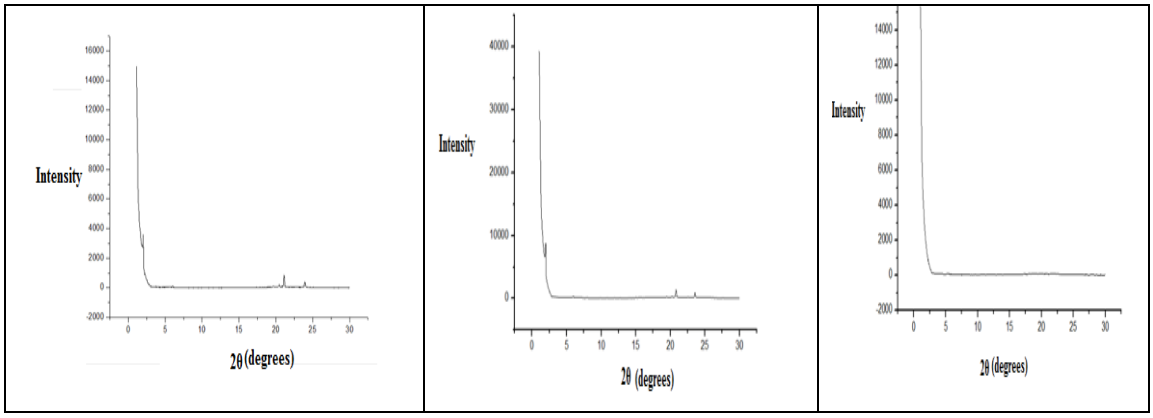


Figure 4. PXRD diffractograms were obtained at various temperatures. A: **6h** at 60ºC; B: **6h** at 89ºC; C: **6h** at 105ºC.

3.4. Biological assay.

The plates were analyzed for the zone of inhibition and the results obtained are represented in Table 2. The development of a clear zone surrounding the disc shows the antimicrobial activity of the synthesized compounds. However, the compounds' exact mechanism is not known well; it is believed that the synthesized compounds get adhered to the bacteria's cell wall, which results in the lysis of the cell, proving it to be fatal.

From the results obtained, it can be inferred that compound **6a** exhibited good inhibitory activity against both gram-negative bacterial strains. It is evident from the results that the synthesized compounds exhibited moderate to good activity against gram-positive bacteria.

Table 2. Antibacterial activity (zone of inhibition in mm)

Entry	Bacterial strains			
	Gram-negative		Gram-positive	
	E.coli	*K. pneumonia*	*B.subtilis*	*S. aureus*
6a	18	16	17	15
6b	17	14	16	13
6c	16	15	14	12
6d	11	11	-	-
6e	-	-	-	-
6f	14	16	-	-
6g	13	15	12	11
6h	11	12	-	-
6i	14	16	11	11
Std	23	22	24	21

4. Conclusions

A new series of 1,3,4-oxadiazole derivatives were synthesized using chloramine-T (CAT) as a cyclizing agent. The synthesized compounds were evaluated for their thermal properties using POM, DSC, and variable temperature PXRD. The compounds exhibited spherulitic textures. Also, the synthesized compounds showed moderate to good antibacterial activity. In conclusion, we state that the aliphatic group alone cannot contribute to good liquid crystalline property. The aromatic system is equally important for charge transportation. These synthesized compounds form a base for further studies. The introduction of more rigid groups in terminals will yield good liquid crystalline property.

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Conflicts of Interest

The authors declare no conflict of interest.

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