Article

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Synthesis and Study the monomorphic possessions of Schiff base - ester compound

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ABSTRACT

One molecule made by Schiff ester chemistry. Physicochemical methods, including 1H-NMR, mass ranges, and FT-IR spectra were used to examine the chemical's conformations. Liquid crystal behavior and transition temperatures of the produced compounds were verified with polarizing optical microscopes and differential scanning calorimeters (DSC). The chiral nematic phase: the compound synthesised showed it existed in an enantiotropic state.

Keywords: Schiff – ester , liquid crystals .

Introduction

The behavior of the liquid Crystal (LC) in organic substances can alter when there's a change in the molecular construction of the compounds, like a change in the connecting groups, terminal groups, and essential groups [1].

The presence of polar connecting groups on a molecule increases intermole cular contact and self-assembly, affecting LC behavior. The existence of polar linking groups on the molecule provides a dipole moment as well as polarizability, resulting in increased intermolecular contact and self-assembly, which can have a significant impact on liquid crystalline behavior [2-4].

In thermotropic liquid crystals, heterocyclic compounds have a particularly important structural characteristic: they can provide a lateral and / or longitudinal dipole, also will change the shape of molecules [5,6].

Furthermore, hetero aromatic rings in organic compounds' molecular structures show high hole-transporting qualities and a low ionization potential,

which makes them a viable option for use as a hole- conveying component in biological light-producing devices [7 –11].

Prajapati et al. they are doing a number of studies on compounds that contain the cinnamate group as a linking group and describe the activity of this group on the LC properties of it is. The ethylene unite is connects both ends of the molecule in calamatic mesogenic molecules. [12,13].

Solanki and colleagues studied two nonlinear compound series. The linking groups -CH=CH-COO and -CO-CH=CH are part of the first series, while group –COO- and –CO-CH=CH- are part of the second series. We contrast how these groups affect phase type, thermal stability, and liquid crystalline characteristics [14].

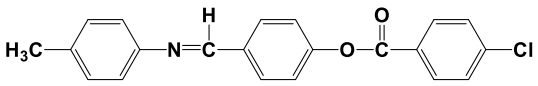
To shed light on how linking groups and terminal groups affect the compound's liquid crystalline characteristics, Thaker produced six chains with azo-ester and azo-cinnamate as connecting groups and various terminal groups [15].

Two rod-like regular groups with various kinds of connections connected to the novel misogynic benzene nucleus' central core were manufactured and described by Uhood et al.

In order to find out how different connecting groups affected the mesomorphic and current properties, researchers looked into the LC properties [16].

The current study presents a compared study of the Toluidine ring's effect on the materials' mesomorphism.

The compound's structures can be seen below:



T-S

1. Experimental

2.1 General

While the NMR spectra were captured using a Bruker spectrometer with CDCl3 as the solvent and TMS as the internal standard, the FT-IR spectra were acquired using a Buck-M500 spectrometer (Buck Scientific, USA) with potassium bromide pellets. A Perkin Elmer-Pyris DSC-8000 differential scanning calorimeter was used to estimate the transition temperatures, using a heating rate of 10°C min-1. In order to monitor the phase addition changes, a Leitz Laborlux 12 Pol Optical Microscope equipped with polarising light and a Leitz 350 stage (from Germany) supplied by Vario-Orthomat were utilised. To capture the mass spectra, a 5957C spectrometer from Agilent technologies was utilised.

2.2 Synthesis of Schiff bases

The process was modified by combining 4-Tuloudine with p-hydroxyl Benzaldehyde in a 1:1 ratio, and then adding a little amount of acetic acid [17,18]. After two hours of reflux heating, the mixture cooled, and the solid was filtered before being recrystallized twice from ethanol to get the pure chemicals.

2.3 Synthesis of 4-((p-tolylimino)methyl)phenyl 4-chlorobenzoate (T-S)

A solution was prepared by dissolving 0.01 mol of p-Chloro Benzoic acid and 4-((p-tolylimino)methyl)phenol in 25 ml of deionized water (DCM). Based on the methodology outlined in reference [19], a total of 0.002 mol of DCC and 0.002 mol of DMAP were introduced into the resulting mixture. Subsequently, the mixture was subjected to stirring at ambient infection for a duration of 6 hours. Following the extraction of the precipitated solid (byproduct), the filtrate underwent evaporation, while the residual substance underwent two rounds of crystallization using ethanol.

2.4 Schiff – ester
4-((p-tolylimino)methyl)phenyl 4-chlorobenzoate (T-S)

Chemical formula : $C_{21}H_{16}ClNO_2$; white solid; yield 69%;^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) 3.35 ppm (S , 3H), 7.20 - 8.17 ppm (m ,12H , Ar-H), 8.67 ppm (S , 1H, CH=N) ; ^{13}C-NMR ($CDCl_3$, 400 MHz): δ (ppm) 21.64 ppm, 121.64-154.46 ppm (Ar-C), 163.81 ppm, 164.23 ppm, 170.60 ppm . IR (cm^{-1}): 3061 (C-H aromatic), 2852-2929 (C-H aliphatic), 3327 (N-H) , 1681 (C=O ester), 1625 (CH=N), 1589 (C=N), MS (m/z) 349.0 [M+].

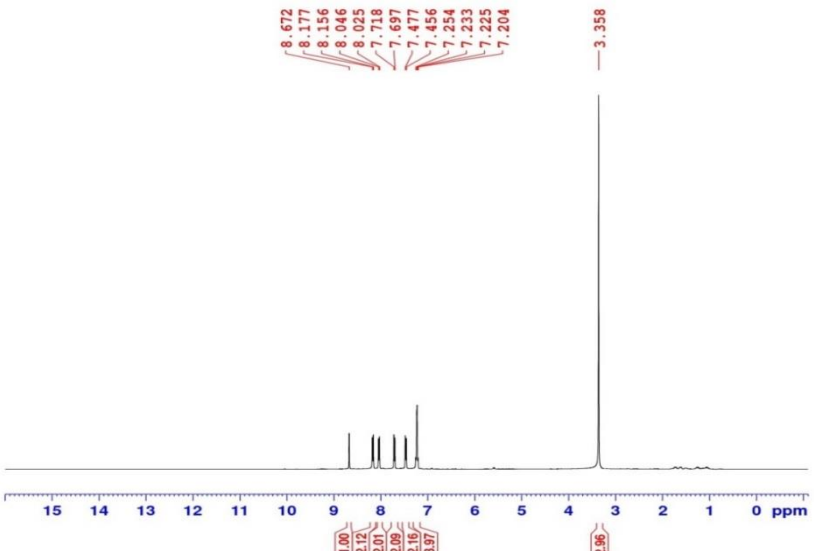


Fig. 1. ^{1}H-NMR spectrum for T-S

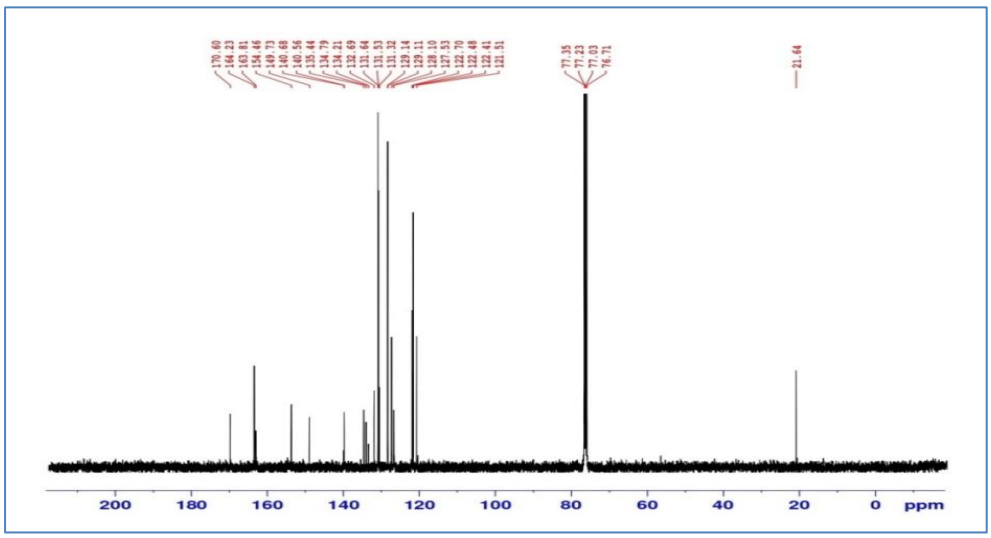


Fig.2. ^{13}C-NMR spectrum of compound T-S

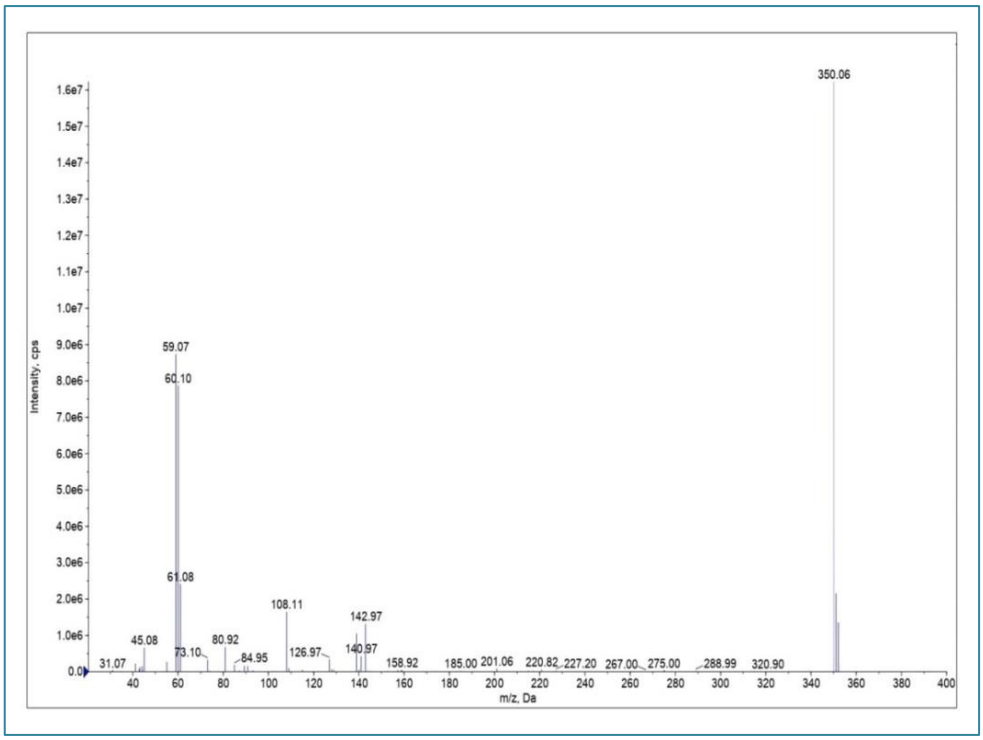


Fig.3. Mass spectrum for T-S

Discussion

To determine the LC properties of the compound in question differential skimming calorimetry (DSC) and a hot- stage microscopy equipped with polarizing filters were employed. It was found that this compound passed two major transitions, from solid to hematic and from hematic back into liquid. The enthalpy for each transition, as well as its entropy change, are given below in Table 1.

A polarised microscope analysis of the T-S compound revealed that it is a liquid crystal exhibiting just a nematic phase within a temperature range of (71.01 ℃).

Consistent with previous research, our finding validates the feasibility of developing Toluidine-based molecules having liquid crystalline properties [17, 20].

The nematic or smectic phase of a liquid crystalline substance is determined by the respective strengths of its lateral and incurable attractive militaries.

The presence of the nematic phase in the compound under investigation suggests that the lateral force of attraction surpasses the terminal attraction force:

1. The inclusion of a chlorine atom in the compound results in the generation of a dipole moment along the molecule's longitudinal axis.
2. The presence of the CH_3 group as a brief terminal chain at the molecular end results in the generation of a dipole moment that runs parallel to the particle's axis, so enhancing the terminal attraction.
3. The existence of timbre along the longitudinal axis of the particle results in an elevation of the molecule's polarity and amplifies the manifestation of a liquid crystal-like structure. [21].

Table 1.Transition infections ,corresponding enthalpy values (ΔH kJ/mol),entropy (ΔS J/mol.K) for the compounds

Compound	Transition temperatures °C	ΔH kJ.mol^{-1}	ΔS J.mol^{-1}.K^{-1}	ΔT_N
T - S	C→N 151.99 N→I 223.00	31.757 0.556	74.72 1.12	71.01

C: crystal, N: Nematic , I : Isotropic , ΔT_N :Thermal variety for nematic phase

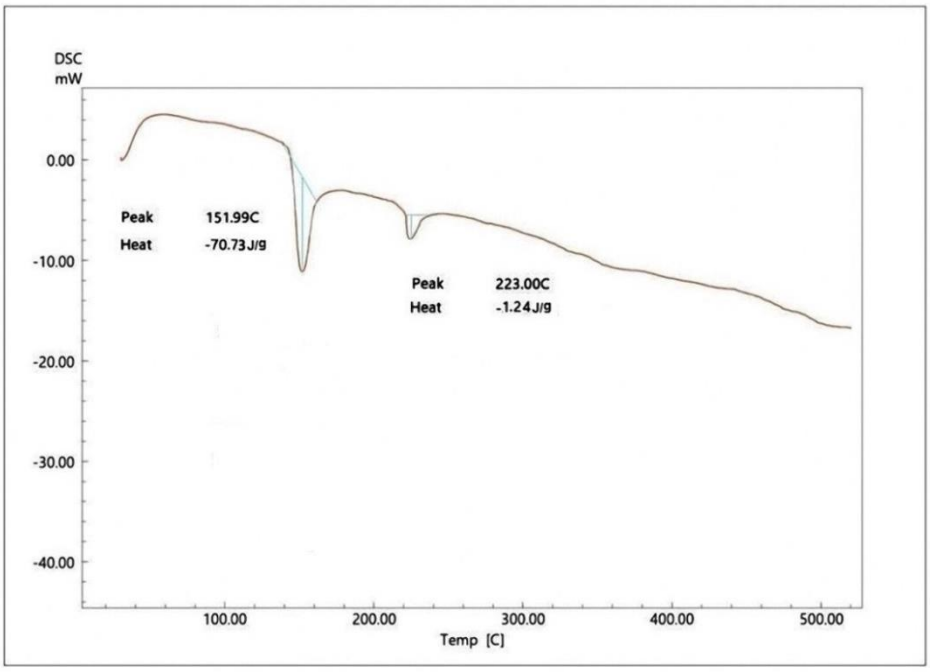
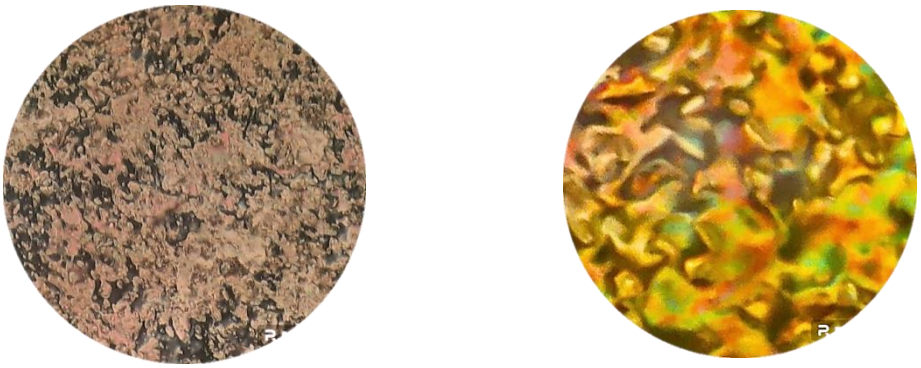


Figure 4: DSC chart for compound T-S



a **b**

Figure: 5 : a) The compound T-S exhibits a marbled texture in the Nomadic phase when heated. b) The Schlieren texture in Nomadic occurs when the compound T-S is cooled.

2. Conclusion

We have documented the synthesis and mesomorphic characteristics of a single molecule in this study. Different types of terminal groups had a significant impact on the compound's enantiotropic nematic phase, mesophase range, and thermal stability.

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