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Liquid crystalline study of new compounds and their polymers derived from 2-Propenoyl chloride

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Two types of monomers such as 2-(prop-2-enoyl)hydrazine-1-carbothioamide [I] and 5-ethenyl-4H-1,2,4-triazole-3-thiol [II], along with their derivatives such as S-(5-ethenyl-4H-1,2,4-triazol-3-yl) prop-2-enethioate [III] and polymers [P1], [P2], and [P3], have been examined in this research work. DSC and POM are used for studying the phase transitions and liquid crystallinity nature of all monomers and polymers under study. Purely nematic phase is observed in monomer [I], while dimorphism is displayed by monomers [II] and [III] with respect to smectic A (SmA) and nematic phases. Nematic phases are exhibited in polymers [P1] and [P2], while polymer [P3] shows SmA and nematic.

Keywords: Nanostructure; Liquid crystal; Phase transition; Polymers. .

1. INTRODUCTION

Materials based on liquid crystals allow the production of nanostructured products with uniform size and shape due to the combination of molecular ordering and mobility. liquid crystals have entered into the fascinating domains of nanoscience and nanotechnology. The mixing of LC with other types of soft matter systems leads to the appearance of materials with special properties. Polymer-dispersed and polymer-stabilized LC systems have drawn considerable attention for over thirty years [1]. Liquid crystal systems constitute one type of matter lying between crystalline solid materials (characterized by molecular ordering) and isotropic liquid matter (lacking long range ordering). They show different levels of orientation and/or translation in the particular space directions [2-3]. It is possible to define the liquid crystalline state as an individual state of matter existing between the fully ordered crystalline

solid-state and completely disordered isotropic liquid. Molecules in liquid crystal media demonstrate anisotropic shape and ability for self-orientation. Due to that feature, there exist different liquid crystalline mesophases showing peculiarities in their behavior. Moreover, molecular ordering in mesophase types, namely smectic, nematic, and other types of LCs, results in unique characteristics of LC systems [4-6]. Several liquid crystalline substances with heterocyclic rings and chiral centers have been synthesized over the years. Nonlinear heterocyclic liquid crystals like oxazoles, pyrazoles, triazoles, and thiophenes are said to possess intriguing properties [7]. The triazole structure is represented by a heterocyclic five-membered ring with three nitrogen atoms and two carbon atoms in its structure. Such a combination results in the formation of an electron-deficient and electron-accepting ring. In this way, triazole compounds are highly advantageous for different potential applications because of their mesogenic properties as well as biological activity and other specific properties [8–10]. However, when introducing 1,2,4-triazole into a rigid core of a thermotropic LC substance, it is possible to expect the occurrence of some changes in mesophase types and the physical properties of materials in general owing to the high polarizability of its heteroatoms. It is necessary to consider the significant impact of the nonlinear molecule shape due to a larger exocyclic angle on mesomorphism [11]. In general, molecules with more linear structures tend to have higher preference for exhibiting liquid crystalline behavior, while the latter cannot occur without bent shaped molecules [12]. Rod shaped molecules containing 1,2,4-triazole give rise to smectic and/or nematic C mesophase. Research studies on mesogenic 1,2,4-triazoles as mesogenic materials are less prevalent compared to the research done on other heterocyclic derivatives [13]. The study is devoted to the investigation of liquid crystalline properties of monomers and polymers that contain a triazole ring.

2. EXPERIMENTAL

2.1. Materials and methods

All reagents used in this study are obtained from Merck and Aldrich. The thermal analysis of all compounds is done using DSC technique on Linseis with Platinum Evaluation version 1.0.89 at the laboratory of the College of Education for Pure Science (Ibn Al-Haitham) and at the Ministry of Science and Technology in Baghdad, Iraq. The mesomorphic behavior of the compounds is studied using a MEIJI microscope with INSTEC hot stage and a central processor controller MK1000 at Al-Nahrain University, Baghdad, Iraq.

3. PREPARATION

3.1. Preparation of compounds [14,15]

2-(prop-2-enoyl)hydrazine-1-carbothioamide[I] Hydrazine carbothioamide (0.91 g, 0.01 mol) is taken in pyridine cooled in ice, and to which is added drop wise, 2-propenoyl chloride with continuous stirring. The solution is kept cold and further stirred overnight at room. Precipitated mass after adding acid and ishing with water and sodium bicarbonate solution. 5-ethenyl-4H-1,2,4-triazole-3-thiol [II]. Reaction of compound (I) (1.46 g, 0.01 mol) with 4% sodium hydroxide solution for 6 h followed by filtration and acidifying with hydrochloric acid. S-(5-ethenyl-4*H*-1,2,4-triazol-3-yl) prop-2-enethioate [III]. Compound (II) (1.27 g, 0.01 mol) is dissolved in pyridine at low temperature and treated drop wise with 2-propenoyl chloride while continuously stirred, followed by collection of the product formed after neutralization with water and sodium bicarbonate solution.

3.2. Preparation of polymers [P1,P2,P3] [16].

Polymers [P1], [P2], and [P3] are prepared by mL of dry toluene is heated in a water bath maintaining at 80 °C 10 in the presence of nitrogen gas. After that, benzoyl peroxide (0.1 g) along with 0.5 g of compound (I), compound (II), or compound (III) is added to the reaction mixture and stirred for 5 h. The resulting polymer is purified using 15 mL of toluene and acetone.

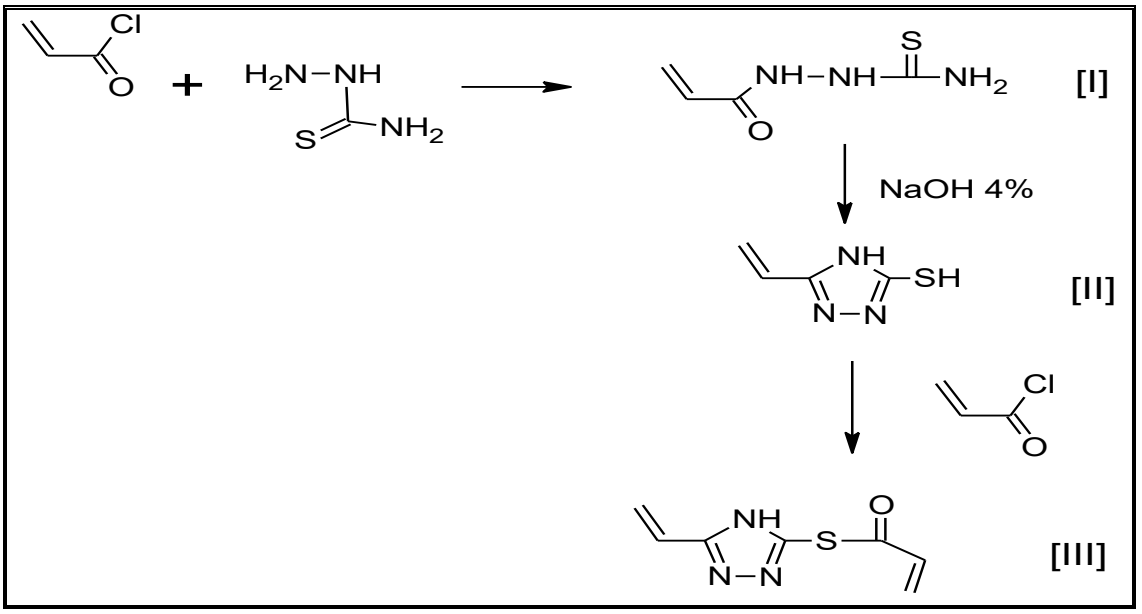


Figure 1 Synthetic procedures of compounds [I,II,III].

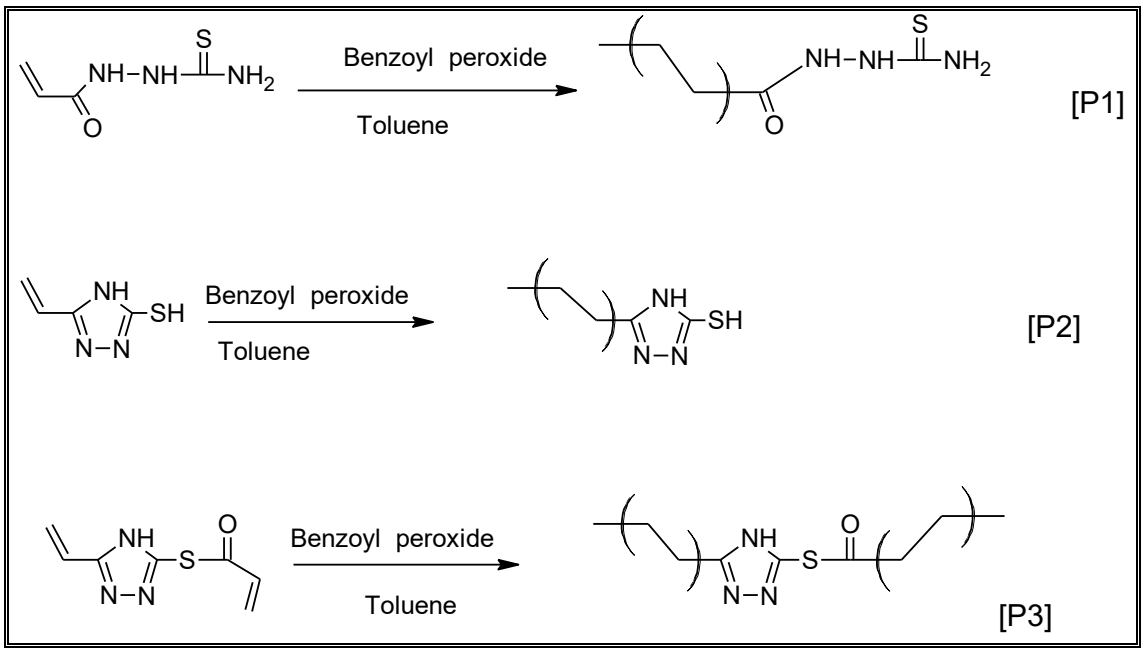
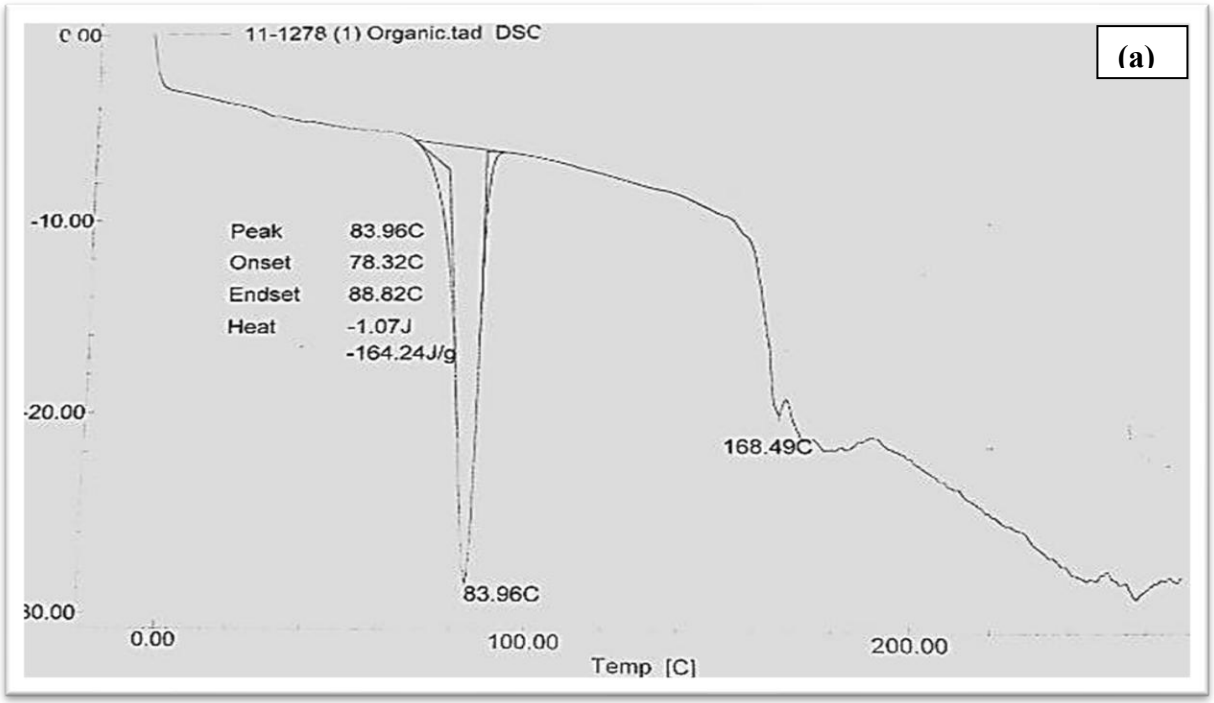


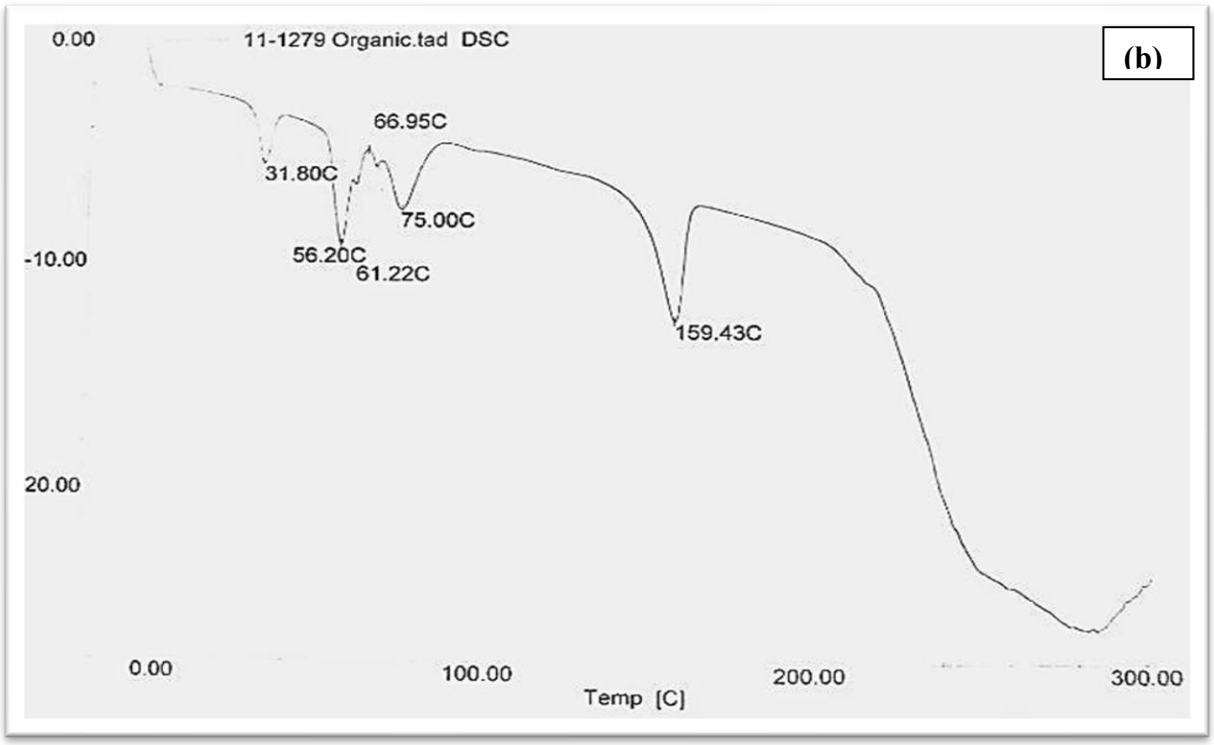
Figure 2 Synthetic procedures of Polymers [P1,P2,P3].

4. RESULTS AND DISCUSSION

4.1. Liquid crystalline properties

The liquid crystal behavior (texture analysis) of the monomers [I], [II], [III] and polymers [P1], [P2] and [P3] is investigated using polarizing optical microscopy (POM). Phase transition temperatures are evaluated using Differential Scanning Calorimetry (DSC). Measured using POM are in good agreement with those measured using DSC. These phase transition temperatures are presented below along with Table 1. The textures of the mesophases are determined using microscopic techniques described by Richter [17], Gray, and Goodby [18].





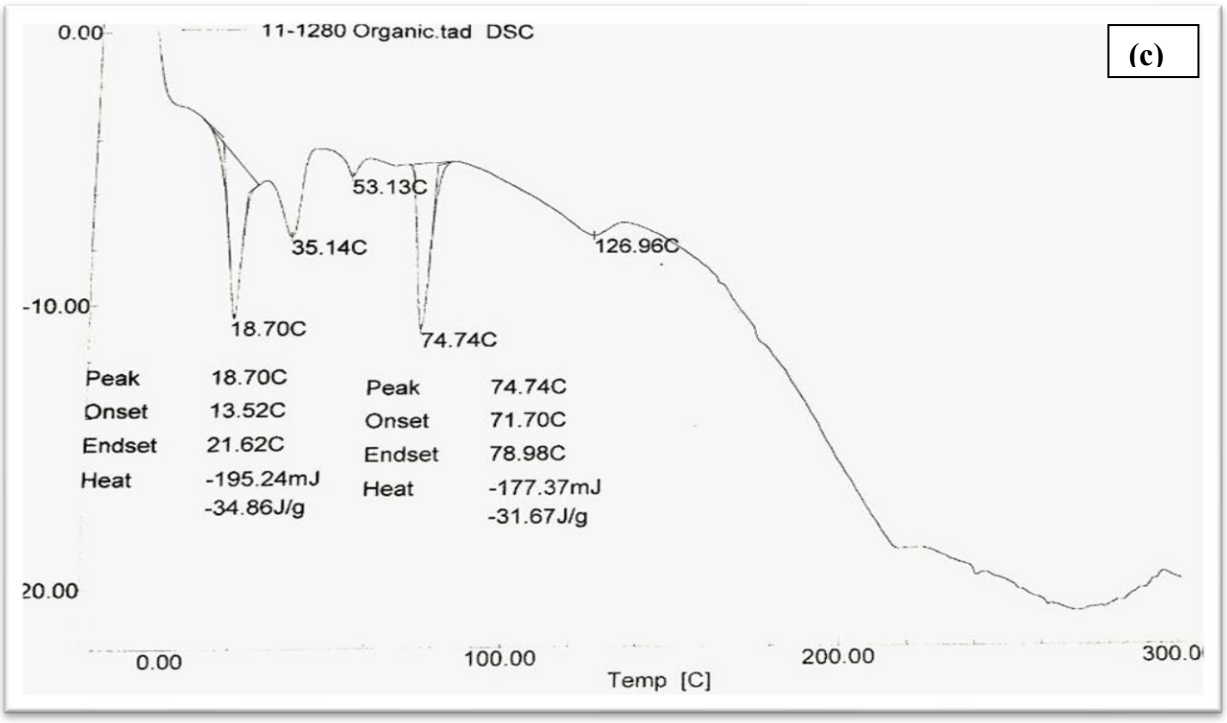
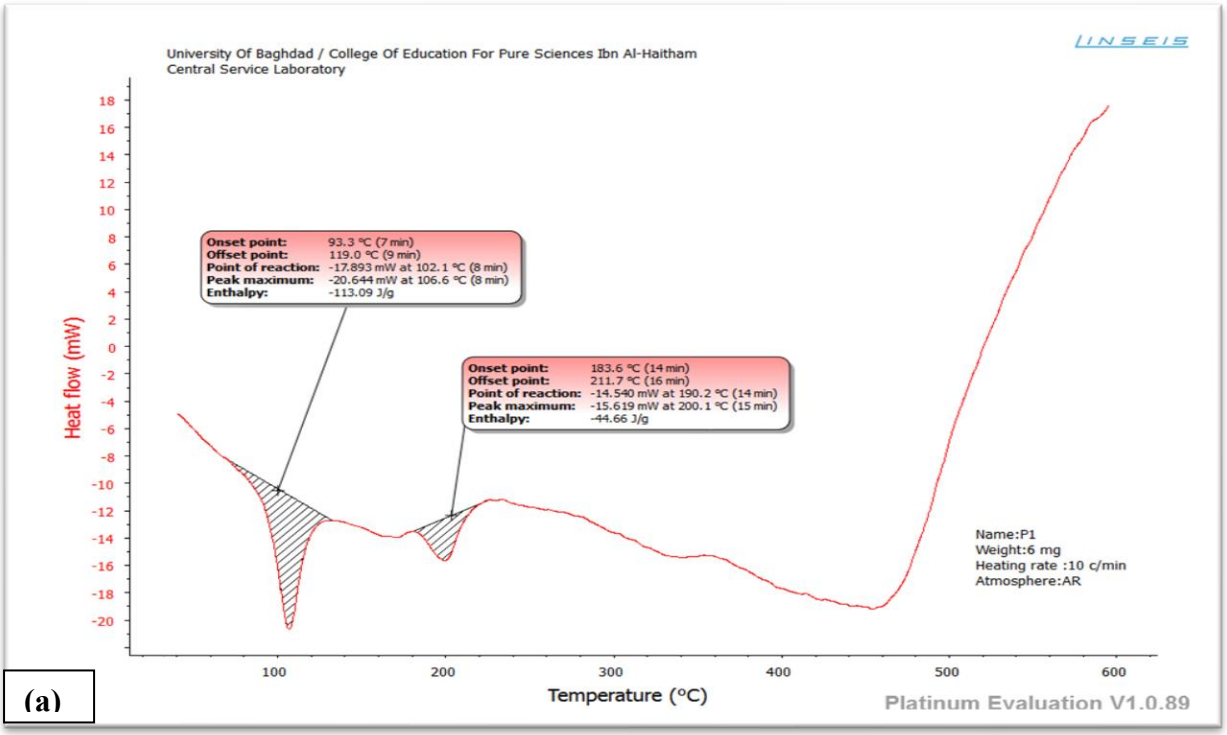
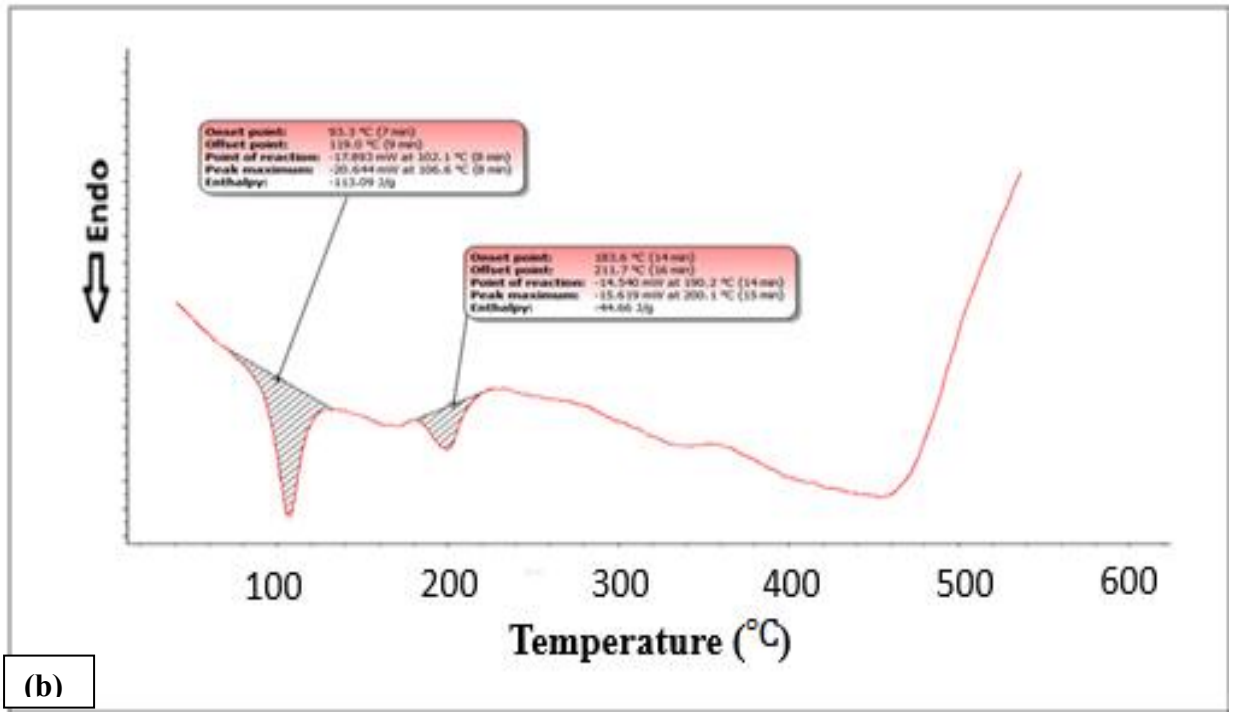


Figure 1 The DSC thermogram of a) compound [I],b) compound [II],c) compound [III].





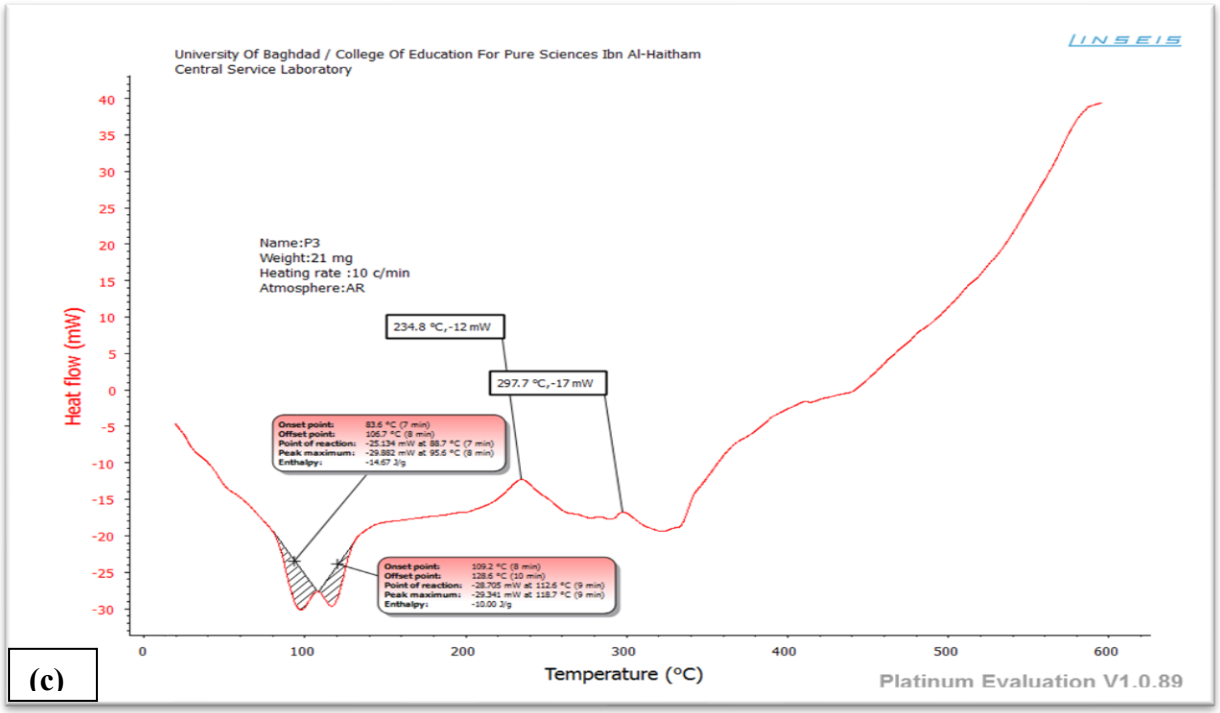


Figure 2 The DSC thermogram for a) compound [p1], b) compound [p2], c) compound [p3].

Table 1 Temperatures of phase transition (°C) of monomers [I-II-III] and polymers [p1-p2-P3] determined by DSC (10 °C/min), Cr = Crystal; SmA = smectic A ; N = Nematic ; I = Isotropic transition.

No.	Compounds	Transition temperatures (°C)
[I]	Cr 83 N 168 I	
[II]	Cr 56 SmA 75 N 159 I	
[III]	Cr 53. SmA 74 N 126 I	
[p1]	Cr 106 N 197 I	
[p2]	Cr 96 N 238 I	
[p3]	Cr 110 SmA 230 N 280 I	

Monomer [I] exhibits purely nematic liquid crystalline behavior, which can be attributed to the presence of the end group NH_2. This is because the NH_2 end group forms intermolecular hydrogen bonds, which causes an extension in the rigid-rod segment and hence the appearance of a higher number of interactions at the terminals of the molecules to become nematic [19]. Monomer [II] has the same molecular structure, only with the difference in the nature of the end group differing mainly in the nature of the core of the terminal group. Monomer [II] exhibits dimorphism, whereby it displays both smectic A (SmA) and nematic liquid crystal behavior, as is shown in Figure 2. The formation might be explained by the presence of the 1,2,4-triazole component in the monomer, since the latter forms the central moiety in thermotropic liquid crystals and can cause many variations owing to the polarizable heteroatoms present in it. Apart from the conjugation of the molecule and the strong lateral association, monomer [III] is observed to have the coexistence of the SmA and nematic mesophases. The existence of the rigid triazole framework with double bonds provides rod-shaped molecular structures, which is suitable for liquid crystal properties. The presence of the carbonyl group creates dipole-dipole interactions that make layered structure, while the sulfur group makes the molecule more polarizable. Both polymers [P1] and [P2] formed nematic mesophases, which displayed the characteristic schlieren texture with two- and four-brush singularities in [P1] and typical nematic droplets in [P2].in contrast, the polymer [P3] showed both smectic A (SmA) and nematic phases due to the rigid heterocyclic core and polar functionalities, which favor intermolecular interactions. The mesogenic compounds [I], [II], and [III] that belong to the class of low molecular weight liquid crystals formed smectic A (SmA) mesophases. However, such behavior is not noted for their corresponding polymers, appears to be due to the preference of side-chain mesogens in polymerization toward nematic over the smectic phase. The intermolecular interactions between the triazole moieties of compound [II] in [P2] polymers are constrained. Thus, leading to the formation of a nematic phase rather than the smectic A (SmA) phase shown by the model compounds [21-24]. The presence of a heterocyclic core (triazole moiety) and polar functionality (carbonyl group) promotes anisotropic interactions between the molecules in [P3]. Moreover, the relatively high temperatures of transitions, along with the existence of many mesophases, suggest high levels of cohesion between molecules and structural anisotropy in these samples, which can be considered important characteristics of modern LC polymers [25-30]. The smectic mesophase is more stable at higher temperatures than the nematic mesophase due to a higher enthalpy associated with its phase transition, visible on the DSC curve. This property might be caused by the existence of ordering both in position (layers) and orientation within the smectic phase, but not in the nematic one [31-36].

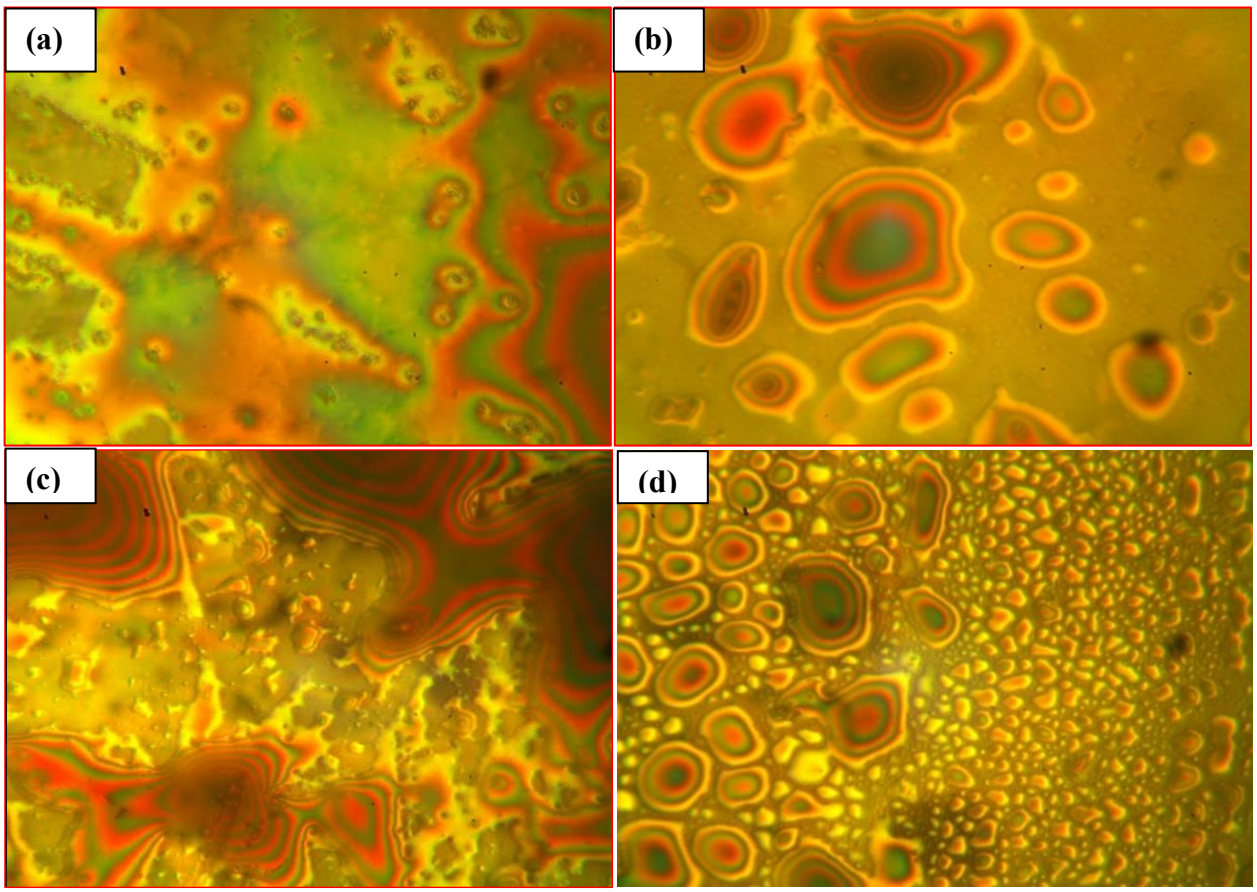


Figure 3 Polarizing microscopy images on heating: a) nematic observed at 95 °C for compound [II]; b) nematic observed at 110 °C for compound [P1]; c) nematic at 125 °C for compound [p2]; d) (Sm A) observed at 150 °C for compound [P3].

5. CONCLUSIONS

Three new monomers and their respective polymers incorporating triazole groups were examined by utilizing 2-propenoyl chloride. Liquid crystalline properties were examined via the use of POM and DSC. It has been observed that all monomers show nematic liquid crystalline behavior, along with a smectic A (SmA) phase observed for monomers [II] and [III]. In contrast, polymers [P1] and [P2] exhibited only nematic behavior whereas [P3] shows both SmA and nematic phases. Moreover, polymeric nature affects their liquid crystalline properties.

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