FTIR Analysis of Nanoparticle-Doped Polymer Dispersed Cholesteric Liquid Crystals

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Abstract: This study investigates the structural and chemical interactions in nanoparticle-doped polymer dispersed cholesteric liquid crystals using Fourier Transform Infrared (FTIR) spectroscopy. Cholesteric liquid crystals known for their helical structure and optical selectivity, were embedded in a polymer matrix, and doped with silver metal nanoparticles. Samples were fabricated using polymerization-induced phase separation and analyzed through FTIR to examine the addition of nanoparticles and their influence on functional group behavior. Shifts in characteristic absorption bands (C=O, O–H, and metal–oxygen) and appearance of new peaks in the fingerprint region suggested significant interfacial interactions among the nanoparticles and the composite matrix. The findings reveal the effectiveness of FTIR in elucidating the molecular-level effects of nanoparticle doping in liquid crystal-based hybrid systems. Such improvements underscore the significance of nanoparticle–polymer interactions in designing thermally robust functional composites, thereby expanding their potential for advanced structural, optical, and sensing applications.

Keywords: Cholesteric liquid crystal, Polymer, Nanoparticles, FTIR.

1. INTRODUCTION

Cholesteric liquid crystals (CLCs) possess a periodic helical structure that imparts unique optical characteristics such as selective reflection of circularly polarized light and temperature-tunable color changes. These properties make CLCs suitable for applications in reflective displays, sensors, lasers, and smart coatings. However, their practical implementation is limited by the inherent fluidity and mechanical instability of pure liquid crystalline phases.

To address these issues, polymer-dispersed cholesteric liquid crystals (PDCLCs) have emerged as a composite system where CLCs are dispersed within a solid polymer matrix. This configuration enhances mechanical strength, chemical resistance, and long-term durability while preserving the optical anisotropy of the cholesteric phase. The phase separation required to achieve this composite structure is typically initiated through a process known as polymerization-induced phase separation (PIPS).

Further enhancement of PDCLC performance has been accomplished through the incorporation of nanomaterials. Recent research has demonstrated that the inclusion of nanoparticles—such as ZnO, TiO_2, Ag, or quantum dots—can significantly alter the electro-optic, dielectric, and thermal behavior of PDCLCs. For instance, Mbhele *et al*. [1] investigated silver-polyvinyl alcohol nanocomposites and observed that thermal stability was improved by approximately 40°C, and the glass transition temperature was increased by up to nearly 20°C for the highest nanoparticle loading. They also noted enhancements in mechanical reinforcement of the polymer matrix. Prabhu *et al*. [2] observed notable FTIR peak shifts in ZnO and CNT-doped PDLC systems, suggesting strong interfacial bonding. Mishra *et al*. [3] reported that metal nanoparticle doping affects phase transition behavior and thermal stability in LC-polymer systems. Moreover, Zhao *et al*. [4] demonstrated how ZIF-8 nanoparticles in a cholesteric matrix broadened the reflection bandwidth and induced significant chemical interaction visible in FTIR spectra. These findings emphasize the need for a detailed spectroscopic evaluation to understand how nanoparticle doping affects molecular interactions within the PDCLC matrix.

FTIR spectroscopy is a powerful tool to probe the vibrational characteristics of functional groups and identify chemical bonding within complex systems. In the context of PDCLCs, FTIR allows for the detection of interactions between CLC molecules, polymer chains, and doped nanoparticles by observing shifts or modifications in characteristic absorption bands. Despite its relevance, comprehensive FTIR-based studies of nanoparticle-doped PDCLC systems remain limited.

In this work, we aim to bridge this gap by systematically analyzing FTIR spectra of nanoparticle-doped PDCLCs. By comparing the spectra of pure CLCs, and nanoparticle-doped PDCLCs, we reveal the molecular-level interactions that govern the structural organization of these multifunctional composites.

2. METHODOLOGY

2.1. Materials

Cholesteryl pelargonate was used as the CLC host. A Methyl methacrylate (MMA) served as the polymer

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matrix, and silver nanoparticles (AgNPs) with particle sizes of <100 nm were used as dopants. Ethanol was used as the dispersing solvent.

2.2. Sample Preparation

Cholesteryl Pelargonate and MMA are mixed to obtain PDCLC using the technique of polymerization induced phase separation method. AgNPs were ultrasonically distributed throughout the PDCLC in a water bath sonicator for 30 minutes. PDLC nanocomposite is prepared by adding 0.5%wt of AgNPs to each sample. The ultra-sonication technique produces a homogeneous dispersion of AgNPs in the CLC. The samples of NP doped PDLC are labelled as S1, S2, S3 and S4.

Sample 1: Ag NP + (2%wt CP +MMA)

Sample 2: Ag NP + (4%wt CP + MMA)

Sample 3: Ag NP + (6%wt CP + MMA)

Sample 4: Ag NP + (8%wt CP + MMA)

Sample 5: CP

2.3. Methodology

The FTIR spectra of the samples were recorded using a *Shimadzu IR Affinity-1* spectrometer. The samples were prepared by employing the potassium bromide (KBr) pellet method to ensure homogeneous dispersion. Spectral acquisition was performed in the scanning range of 4000–400 cm^{-1}, enabling the identification of characteristic functional group vibrations and possible shifts associated with nanoparticle incorporation.

2.4. FTIR Spectra

FTIR Spectra were obtained using FTIR spectrophotometer in the scanning range of 4000-400 cm^{-1}. The method used for analysis of NP doped PDCLC is potassium bromide pellet method. Samples analyzed included pure CLC and Ag-doped PDCLC. The FTIR spectra for the samples are shown in Figure **1-5**.

3. RESULTS AND DISCUSSION

A comparative summary of the FTIR absorption bands for all five samples (Pure CP, 1PDCIC+MMA+Ag, 2MMA+Ag, 3MMA+Ag, and 4MMA+Ag) is presented in Table **1**, highlighting the characteristic peak shifts, variations in intensity, and the emergence of new vibrational modes.

A comparative analysis of the spectra reveals the following features

- The C=O stretch around 1700–1740 cm^{-1} is consistent across all samples, verifying the presence of ester linkages in MMA and cholesteryl esters.
- Low-wavenumber bands (410–490 cm^{-1}) are unique markers of silver nanoparticle incorporation, absent in pure CLC systems.
- Broad O–H features (3400–3740 cm^{-1}) indicate moisture, surface hydroxyls, or polymer chain interactions—enhanced by nanoparticle dispersion.
- Variations in peak position and intensity suggest changes in molecular interactions due to

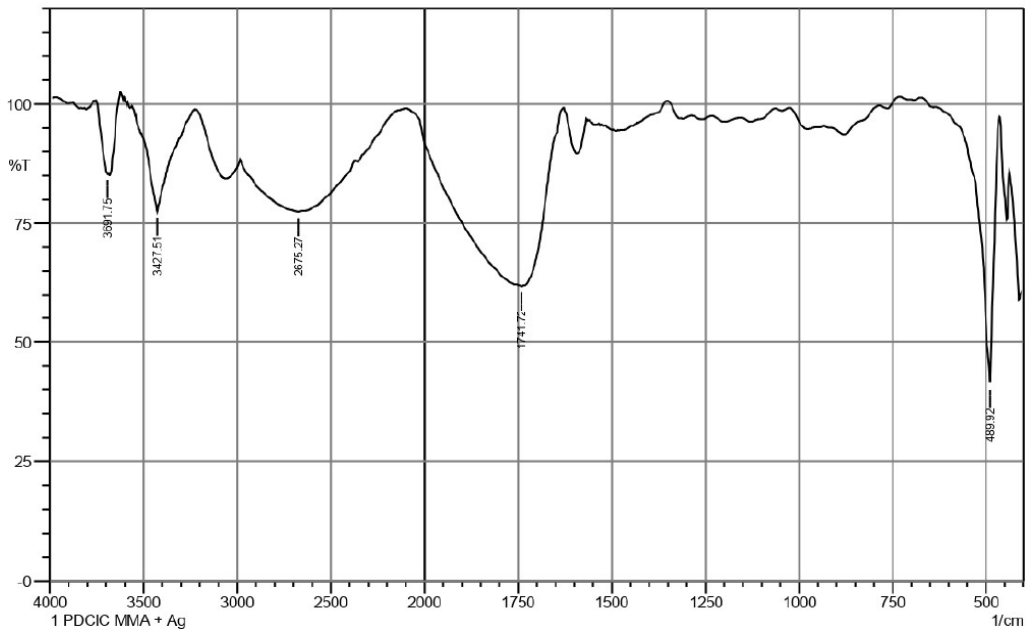

Figure 1: FTIR spectrum of Sample1 (2%wt CP + MMA + 0.5%wt Ag NP).

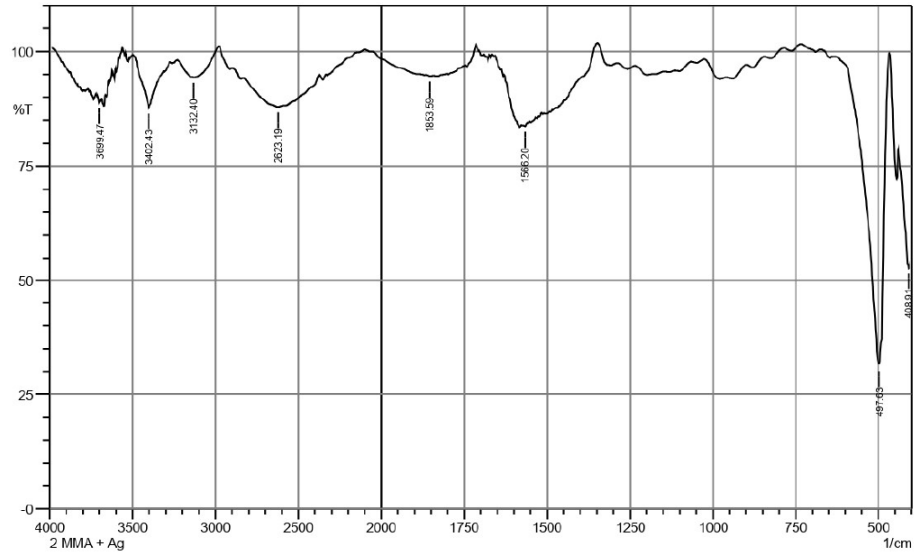

Figure 2: FTIR spectrum of Sample 2 (4%wt CP + MMA+ 0.5%wt Ag NP).

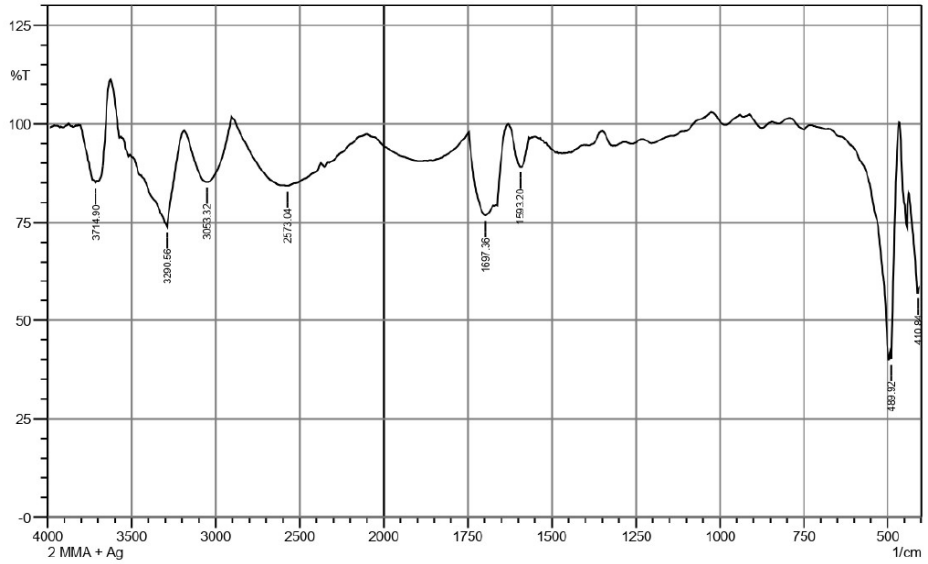

Figure 3: FTIR spectrum of Sample 3 (6%wt CP + MMA+ 0.5%wt Ag NP).

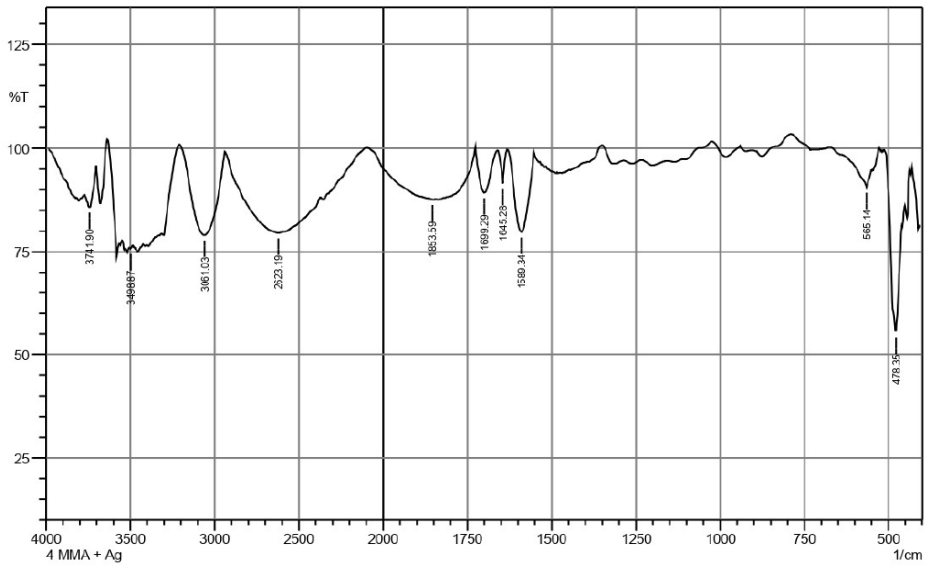

Figure 4: FTIR spectrum of Sample 4 (8%wt CP + MMA+ 0.5%wt Ag NP).

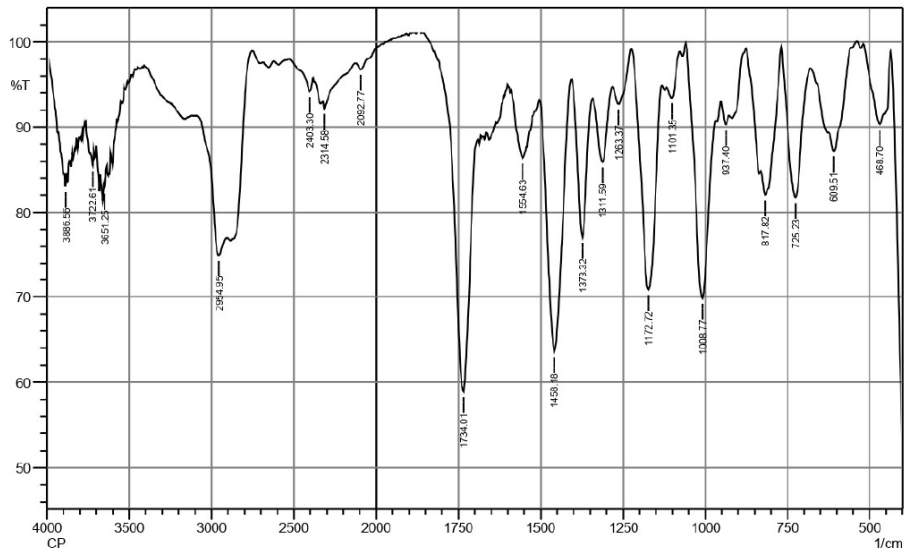

Figure 5: FTIR spectrum of Sample 5 (CP).

Table 1: A Comparative Summary of the FTIR Absorption Bands

Sample	Major Peaks (cm^{-1})	Intensity (approx.)	Tentative Assignment
Cholesteryl Pelargonate	468, 609, 725, 817, 937, 1008, 1101, 1172, 1263, 1311, 1373, 1458, 1555, 1734, 2093, 2315, 2403, 2955, 3651, 3723, 3887	Strong (multiple sharp absorptions)	- 468–817: skeletal vibrations - 937–1172: C–O stretching - 1263–1458: C–H bending - 1555: C=C stretching (aromatic/olefinic) - 1734: C=O ester stretching - 2955: aliphatic C–H stretching - 3651–3887: O–H stretching (broad)
Ag NP + (2%wt CP + MMA)	490, 1742, 2675, 3428, 3692	Medium–Strong	- 490: skeletal - 1742: ester C=O stretching (shifted vs. pure CLC) - 2675: CH_2 overtone/Ag–O related interaction - 3428: O–H stretching (broad, H-bonding) - 3692: free O–H stretching
Ag NP + (4%wt CP + MMA)	409, 498, 1566, 1854, 2623, 3132, 3402, 3699	Variable (strong at 498, 3132)	- 409–498: skeletal / Ag–O vibration - 1566: C=C aromatic/olefinic - 1854: overtone (weak) - 2623: CH_2 stretching / overtone - 3132: =C–H stretching - 3402: O–H/N–H stretching - 3699: free O–H
Ag NP + (6%wt CP + MMA)	411, 490, 1593, 1697, 2573, 3053, 3291, 3715	Moderate–Strong	- 411–490: skeletal - 1593, 1697: C=C stretching, ester C=O - 2573: CH_2 stretching - 3053, 3291: C–H / =C–H stretching - 3715: free O–H
Ag NP + (8%wt CP + MMA)	478, 565, 1589, 1645, 1699, 1854, 2623, 3061, 3499, 3742	Moderate–Strong	- 478–565: skeletal / Ag–O - 1589–1699: C=C and C=O stretching - 1854: overtone - 2623: CH_2 overtone - 3061: =C–H stretching - 3499–3742: O–H stretching (broad + free)

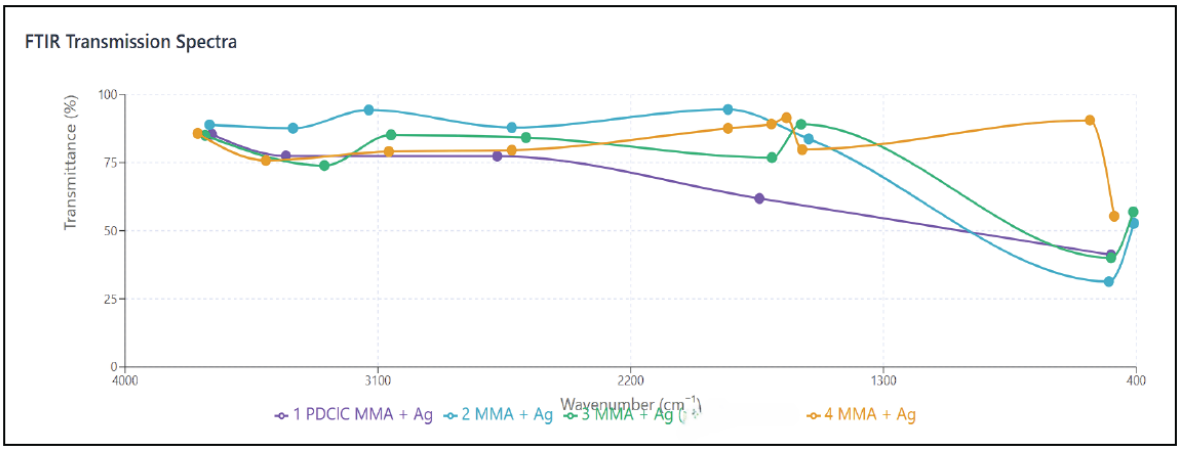

Figure 6: Analysis of FTIR transmission spectra Sample Composition.

nanoparticle presence and polymer dispersion phase.

- The FTIR transmission spectra is shown below (Figure **6**)

The spectra show characteristic peaks for MMA (methyl methacrylate) functional groups, cholesteryl pelargonate ester linkages, and silver nanoparticle interactions. The presence of C=O stretching around 1697-1741 cm^{-1} confirms ester groups from cholesteryl pelargonate. C=C stretching around 1566-1645 cm^{-1} indicates MMA vinyl groups. Low-frequency peaks (400-500 cm^{-1}) suggest Ag-O interactions [5, 6]. Variations in peak intensities and positions across samples suggest different MMA concentrations affect the molecular environment and silver nanoparticle dispersion.These spectral changes suggest successful nanoparticle integration and the presence of chemical bonding or strong physical interaction within the composite matrix.

CONCLUSION

This FTIR spectrum supports the presence of a hybrid composite of:

- MMA/PMMA polymer matrix (via carbonyl and =C–H stretches),
- Silver nanoparticles, detected through metal-oxygen bands in the fingerprint region,
- Cholesteryl Pelargonate, identified by ester carbonyls, alkene, and hydroxyl group features.

FTIR analysis confirmed successful incorporation of silver nanoparticles into the PDCLC matrix. Shifts in the carbonyl and hydroxyl stretching bands, as well as the emergence of Ag–O absorption peaks, revealed molecular-level interactions and bonding. These findings highlight the capability of FTIR in probing structural and chemical modifications in nanoparticle-doped liquid crystal systems, aiding the design of advanced functional composites for optical and sensing application.

Application and Future Scope

The strong interfacial interactions between silver nanoparticles and the PDCLC matrix significantly enhance the composite's thermal stability by restricting polymer chain mobility and delaying degradation. This improvement broadens the material's applicability across industrial and research domains, including flexible electronics, coatings, and sensing devices. Building on this molecular-level understanding, future work can focus on designing composites with tailored interfacial strength and specific optical or electro-optic properties for advanced functional materials [7, 8].

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