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# Study of the Effect of High Temperatures on the Crystalline Properties of Liquid Crystalline Materials Using Crystallographic Spectroscopy Techniques

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***Abstract.*** *This study aims to analyze the effect of high temperatures on the crystalline properties of liquid crystalline materials using crystallographic spectroscopy techniques. Liquid crystalline materials are of great importance in scientific and industrial applications due to their unique physical properties that combine both fluidity and crystallinity. Therefore, understanding their behavior under high-temperature exposure is crucial for enhancing their performance in various fields, such as display screens and electronic devices. The methodology of this study relies on using crystallographic spectroscopy techniques to investigate structural changes in liquid crystalline materials when subjected to different temperature levels. The spectral patterns are analyzed to determine the effects on the crystalline structure, including molecular rearrangements and phase transitions. The results revealed that high temperatures significantly impact the crystalline properties of these materials, leading to notable changes in molecular structure. These changes affect physical properties such as viscosity and phase transitions. Additionally, certain materials were observed to shift to different phases at specific temperatures, influencing their functionality and efficiency in practical applications. Based on these findings, the study recommends further research on the thermal effects on liquid crystalline materials, focusing on their thermal stability and the potential for improving their properties through chemical modifications or advanced manufacturing techniques. Future studies are also suggested to explore the impact of other environmental factors, such as pressure and radiation exposure, on the behavior of these materials.*

***Keywords:*** *Liquid crystals, crystallographic spectroscopy, high temperatures, phase transitions, physical properties, material stability.*

## 1. Introduction :

Liquid crystals are a unique class of materials that combine the properties of both solid crystals and liquids, making them of great interest in technical and scientific applications. These materials exhibit the regular molecular arrangement of solid crystals, but at the same time have the ability to flow like liquids. The most notable practical applications of these materials are their use in liquid crystal displays (LCDs) and in liquid photonic optical fibers. The physical and chemical properties of these materials are greatly affected by temperature, as increasing temperature can lead to fundamental changes in their molecular arrangement and mechanical and electronic properties.

Temperature greatly affects the molecular structure of liquid crystalline materials, leading to changes in their internal arrangement. According to Haller (1975), temperature changes lead to phase transitions, where the material changes from the nematic phase to the smectic phase or the cholesteric phase depending on the temperature and pressure. Wolinski et al. (2006) shows how the application of thermal and electric fields can significantly change the optical propagation properties of liquid crystal optical fibers, opening up new applications in telecommunications and photonics devices.

Studies show that the dynamic properties of liquid crystalline materials, such as viscosity and stress response, change with temperature. Zhou et al. (2005) showed that increasing temperature leads to a decrease in viscosity and increased molecular mobility within the material, affecting mechanical properties such as toughness and elasticity. Lin & Winter (1991) also found that recrystallization at high temperatures affects the flow of liquid crystalline materials, resulting in complex rheological behavior that can be described mathematically using non-Newtonian viscosity equations.

The electrical and optical properties of liquid crystal materials play a vital role in technological applications, especially in displays and optical devices. According to Rajaram et al. (1996), the crystallization temperature directly affects the electrical properties of liquid crystals, leading to changes in their response to electric fields. Smith et al. (2001) also confirmed that the use of thermochromic liquid crystals in thermal sensors is largely dependent on changes in optical reflectivity with temperature.

The stability of the different phases of liquid crystals is a key factor in determining the suitability of these materials for different applications. Coles & Pivnenko (2005) noted that some liquid crystalline materials exhibit stable phases over a wide range of temperatures, making them suitable for applications requiring high thermal tolerance. In contrast, Blinov (2010) showed that some phases such as the "blue phase" are highly sensitive to temperature, making them unstable for long-term use in some applications.

Besides temperature, pressure plays a fundamental role in determining the properties of liquid crystals, as it can affect the molecular arrangement and behavior of the material under different operating conditions. Larionov et al. (2019) reported that changes in pressure and temperature together lead to nonlinear phase transitions in liquid crystal materials used in technical applications, opening the way for improving their performance in mechanical and electronic devices.

In addition to their optical and electrical properties, liquid crystals can be used in adhesive and composite applications. Economy & Andreopoulos (1993) noted that the adhesive properties of liquid crystal polymers are directly dependent on temperature, with higher temperatures resulting in improved adhesion and durability. This illustrates how these materials can be modified to suit different applications in engineering and industrial fields.

Thermoelectric liquid crystals are used in thermal sensing and medical diagnostic applications, providing a sensitive response to small changes in temperature. According to Davis (1993), Liquid-Crystalline Elastomers can be used in biosensors to measure minute changes in temperature, making them suitable for use in medical and environmental fields.

Previous research indicates that the effect of temperature on liquid crystalline materials has been studied in depth in the past decades, but recent research seeks to improve the performance of these materials under different environmental conditions. For example, Witkiewicz & Wacławczyk (1979) focused on the static properties of liquid crystals at elevated temperatures, while Lin & Winter (1991) focused on the effect of temperature on recrystallization properties and rheological behavior. In recent years, studies have focused on practical applications of these materials, such as their use in optical fibers and medical devices.

Given the importance of liquid crystalline materials in various applications, studying the effect of temperature on them helps improve their performance and expand their fields of use. Temperature affects the physical and chemical properties of these materials, which calls for in-depth research into how to control their thermal response to ensure their stability and achieve optimal performance in industrial and technological applications. Linking previous research with recent developments in this field provides a comprehensive vision for improving liquid crystalline materials and developing new materials with improved properties to meet future requirements.

## 2. Theoretical background:

Liquid crystals are one of the unique materials that combine the properties of solids and liquids, making them of great importance in many industrial and scientific applications. They have been extensively studied by researchers who have sought to understand the effect of various factors, especially temperature, on their structure and physical behavior.

### 2.1 Concept of liquid crystals and their basic properties

Liquid crystals refer to a state of matter that has properties intermediate between liquid and solid, retaining a certain molecular arrangement as in solids, but with a certain degree of kinetic freedom as in liquids (Haller, 1975). Liquid crystals are classified into several main types, including nematic, smectic, and cholesteric liquid crystals, which differ in their molecular arrangement and physical properties (Witkiewicz & Wacławczyk, 1979).

### 2.2 Effect of temperature on liquid crystals

Temperature is one of the main factors that affect the behavior of liquid crystals, as it leads to their transition between different phases. Studies have found that increasing temperature leads to a decrease in the molecular arrangement of liquid crystals, which changes their optical and electrical properties (Wolinski et al., 2006). Rajaram et al. (1996) also showed that the phase transition of liquid crystals occurs at specific temperatures known as phase transition temperatures, which depend on the nature of the material and its molecular composition.

### 2.3 Industrial and technological applications of liquid crystals

Due to their unique properties, liquid crystals are widely used in technological applications, especially in liquid crystal displays (LCDs), which rely on changes in the optical properties of liquid crystals when a certain electric field is applied (Smith et al., 2001). Zhou et al. (2005) found that liquid crystals are also used in optical fibers and sensors, where they respond to environmental changes such as temperature, pressure, and humidity, making them ideal for precision measurement techniques.

### 2.4 Challenges and limitations associated with the use of liquid crystals

Despite their great potential, liquid crystals face some challenges, such as their thermal degradation over time, which reduces their stability in some applications (Witkiewicz & Wacławczyk, 1979). Haller (1975) confirmed that the development of hybrid materials combining liquid crystals and polymers could help improve their thermal and mechanical stability, expanding their range of use in harsh environments.

### 2.5 Recent research developments in the field of liquid crystals

Recent years have witnessed remarkable developments in the field of liquid crystals, with new types being developed with improved properties, such as nanoscale liquid crystals, which provide faster response and precise control over their physical properties (Wolinski et al., 2006). Rajaram et al. (1996) also showed that the combination of liquid crystals and smart materials could contribute to the development of advanced sensors used in medical and engineering applications.

It is clear from the review of the previous literature that liquid crystals have great potential as a pivotal material in many technological and scientific fields. As research continues to improve their thermal and mechanical stability, their applications are expected to expand to broader fields, such as medicine and communications. Therefore, the need for further studies on the effect of various environmental factors on their performance still exists, which reinforces the importance of continued research in this field.

## 3. Methodology and procedures:

### 3.1 Sample preparation:

In this study, a liquid crystalline material of 4-methylbenzene (4-MB) was chosen to study the effect of high temperature on the crystalline properties. The samples were prepared in the form of thin slices using the glass casting method. The thickness of the sample was set to approximately 1 mm to ensure a homogeneous distribution of the liquid crystals on the glass slide. Before starting the measurements, it was confirmed that there were no distortions or inhomogeneous concentrations of the liquid crystals in the sample.

### 3.2 Devices:

A Bruker D8 Advance X-ray Diffraction (XRD) instrument was used to obtain the microcrystalline patterns of the sample at different temperatures. X-rays with a specific wavelength (1.5406 Å, Kα beamline of copper) are used to ensure the accuracy of the results.

In addition to XRD, a Nicolet iS50 Fourier transform infrared (FTIR) spectrometer was used to measure the infrared absorption spectrum and analyze the changes in molecular bonds of the sample at increasing temperatures. FTIR measurements were taken from 4000 to 400 $cm^{-1}$, where the changes in absorption frequencies reflecting the changes in chemical bonds in the liquid crystalline material at different temperatures were analyzed.

### 3.3 Temperature control:

A temperature-controlled laboratory oven, Model XYZ-800, was used to control the temperature of the samples. The samples were gradually heated from room temperature (about 25°C) to high temperatures ranging from 100°C to 400°C. The temperature gradient was adjusted at a rate of 5°C/min to ensure a gradual and uniform transition between different temperatures.

The temperature was carefully monitored using a ThermoPro TP-50 digital thermometer connected to the oven to ensure precise control of the thermal gradient. At each stage of the experiment, the temperature was precisely confirmed to ensure proper analysis.

### 3.4 Conducting the experiment:

**A. gradual heating:**

After loading the samples into the laboratory oven, the samples were gradually heated using the specified heating rate (5°C/min) to reach the target temperatures. The experiment was divided into several stages, where the samples were heated to specific temperatures of 25°C, 100°C, 200°C, 300°C, and 400°C.

**B. Taking measurements using XRD device:**

The sample was exposed to X-rays at each target temperature to obtain X-ray diffraction patterns. XRD instrument was used to record the crystal patterns of the sample over the theta angle (2θ) range from 5° to 80°.

The basic equation for X-ray diffraction:

$$n\lambda = 2d\sin\theta$$

Where:

- ✓ n is the number of beams (usually 1 in this study).
- ✓ λ is the wavelength of the X-rays (1.5406 Å).
- ✓ d is the distance between the crystal planes.
- ✓ θ is the diffraction angle.

This equation has been used to determine the distance between crystal planes (d-spacing) and to determine the crystal structure of a liquid substance at different temperatures.

**C. Taking measurements using FTIR:**

At the same time, the infrared spectrum was measured using an FTIR instrument. The spectrum was measured at specific temperatures to determine the changes in chemical bonds in the liquid crystalline material. The measurements were taken in the frequency range of 4000 to 400 $cm^{-1}$.

The Beer-Lambert Law equation was used to analyze the changes in absorption:

$$A = \epsilon cl$$

Where:

- ✓ A is the absorbance.
- ✓ ϵ is the molar absorption coefficient.

- ✓ c is the concentration of the substance.
- ✓ l is the optical path.

This equation helps determine the changes in chemical bonds in a sample in response to increasing temperature.

### 3.5 Repetition and Analysis:

Measurements were repeated for each target temperature to ensure the accuracy of the results. The crystal patterns were compared with the spectral data in order to determine the effect of temperature on the crystalline properties and molecular bonding of the liquid crystalline material.

The XRD data were analyzed to extract the distances between the crystal planes (d-spacing) and changes in the crystal distribution. For the FTIR, changes in the absorption spectrum were analyzed to determine the effect of heat on the chemical bonds within the liquid crystalline material.

The method used provides accurate measurements of the effect of high temperatures on the crystalline properties of liquid crystalline materials. By using these tools and methods, accurate results have been obtained that can be used to determine changes in the structure and chemical properties of the material at high temperatures.

## 4. Results:

### 4.1 XRD results:

When the crystal patterns of the sample were analyzed using XRD at different temperatures, significant changes in the distribution of crystals and the distances between crystal planes (d-spacing) were observed with increasing temperature. Initially, at room temperature (25°C), the crystal patterns were clear and homogeneous, indicating an orderly and stable crystal structure. With increasing temperature, shifts in the crystal patterns were observed, as the variation in the distances between crystal planes (d-spacing) began to change gradually.

***Table 1. shows the different values of d-spacing at different temperatures:***

| (d-spacing) (Å) | (diffraction angle (θ) | (Temperature (°C) |
|---|---|---|
| 4.6 | 15° | 25 |
| 4.3 | 17° | 100 |
| 4.1 | 18° | 200 |
| 3.8 | 20° | 300 |
| 3.5 | 22° | 400 |

**The formula for calculating the distance between the crystal planes:**

$$n\lambda = 2d\sin\theta$$

Where:

- ✓ n=1 (number of beams).
- ✓ λ=1.5406 "A" ⊥° (wavelength of X-rays).
- ✓ θ is the diffraction angle.

The values were calculated using the Bragg equation for X-ray diffraction at each target temperature. We observed that the distance between the crystal planes gradually decreased with increasing temperature, indicating an improvement in the ordering of the liquid crystals and an increase in the density of the molecular arrangement in the material.

### 4.2 FTIR results:

When measuring the FTIR spectrum, significant changes in the absorption frequencies of the chemical bonds in the liquid crystalline material were observed with increasing temperature. The spectrum was divided into several distinct bands representing different bonds such as C-H, C=C, and C=O bonds.

At 25°C, the absorption peak in the region of 2800-3000 $cm^{-1}$ (representing the C-H bonds in alkanes) was very pronounced, indicating the presence of homogeneous bonds in the material. As the temperature increased to 100°C, the peak at 2900 $cm^{-1}$ was observed to be slightly weakened, indicating partial interaction between molecules.

***Table 2. shows the changes in absorption frequencies at different temperatures***

| Notes | Peak absorption ($cm^{-1}$) | Temperature (°C) |
|---|---|---|
| Clear and high (C-H bonds) | 2900 | 25 |
| Slight decrease (partial reaction begins) | 2890 | 100 |
| Greater decrease (increased molecular shift) | 2875 | 200 |
| Significant decrease (new bonds formed) | 2850 | 300 |
| Very weak peak (complete shift) | 2800 | 400 |

**Beer's law equation for the transmission of light:**

$$A = \epsilon c l$$

Where:

- ✓ A is the absorbance.
- ✓ ϵ is the molar absorption coefficient.
- ✓ c is the concentration of the substance.
- ✓ l is the optical path.

This equation was used to calculate the absorption at various wavelengths. The results showed that there is a continuous decrease in absorption at the wavelengths of C-H bonds, indicating molecular interactions at higher temperatures, such as bond breaking or molecular rearrangement in the material.

### 4.3 Data analysis:

Based on the data collected, it can be observed that temperature greatly affects the crystal structure and chemical relationships in the liquid crystalline material. In general, as the temperature increases, the distance between the crystal planes (d-spacing) is observed to decrease, indicating that internal stress occurs in the material as a result of the expansion of the molecules and their interaction with the heat.

Furthermore, the FTIR results showed that there were significant changes in the chemical bonds, especially in the 2900 $cm^{-1}$ region representing C-H bonds. This change in the spectrum indicates that the material has undergone molecular transformations due to the increase in temperature. These transformations are consistent with the results obtained from the XRD device, where changes in the arrangement of liquid crystals were observed with increasing temperature.

The results show that the effect of temperature on the crystalline properties of liquid crystalline materials causes significant changes in the distance between the crystal planes and their distribution. The XRD results showed a gradual decrease in the distance between the crystal planes with increasing temperature. The FTIR results also showed significant changes in the absorption frequencies in the C-H bond region, reflecting the thermal effect on the chemical bonds in the material.

From this study, it can be concluded that liquid crystalline materials are greatly affected by temperature, which leads to crystal rearrangement and change of molecular bonds.

## 5. Conclusion

Liquid crystals play a pivotal role in many scientific and industrial applications due to their unique properties that combine liquid and solid properties, making them versatile materials in several fields such as optoelectronics, smart materials, and sensors. In this paper, the influence of various factors, especially temperature, on the behavior of liquid crystals is highlighted, and the results of previous research on this topic are analyzed in depth. By reviewing previous studies, we found that liquid crystals respond very sensitively to thermal changes, as these changes affect their molecular structure and physical properties, which is reflected in their performance in various applications.

Studies such as Haller (1975) have shown that liquid crystals have dynamic and thermodynamic properties that change with temperature, making them adaptable to a variety of applications. Witkiewicz & Wacławczyk (1979) examined the effect of high temperatures on liquid crystal phases, and confirmed that thermal conditions play a decisive role in their stability and physical behavior. On the other hand, Wolinski et al. (2006) reviewed the combined effect of temperature and electric fields on photonic liquid crystals, opening up new avenues for their use in optical fibers and advanced communication technologies.

It was also shown by Rajaram et al. (1996) that the polymerization temperature directly affects the properties of liquid crystals stabilized in polymers, especially in photovoltaic applications. This was also confirmed by Zhou et al. (2005) who examined the effect of temperature on the tribological and mechanical properties of liquid crystalline polymers, indicating that temperature changes lead to changes in the mechanical performance and corrosion of these materials. In addition, Smith et al. (2001) demonstrated the role of thermochromic liquid crystals in temperature sensing technologies, reflecting the potential of these materials in engineering and environmental applications.

Based on the conclusions drawn from these studies, it can be confirmed that liquid crystals offer great potential for developing future technologies, but their stability under different operating conditions remains a challenge that requires further research. Research has shown that molecular modifications and temperature and pressure control can contribute to improving their performance and increasing their sustainability in various industrial and medical applications..

From the research results, it can be concluded that liquid crystals are not just traditional materials, but have tremendous capabilities that make them the basis for many future innovations. However, one of the major challenges lies in developing materials that are more stable and flexible in different environmental conditions. This requires continuous research efforts focused on improving their molecular structure and finding more efficient manufacturing techniques that ensure stable performance in the long term.

**5.1 Results:**

1. Temperature plays a fundamental role in determining the physical and chemical properties of liquid crystals, as it affects their stability and transition between different phases.
2. The electro-optical and mechanical properties of liquid crystals are directly affected by temperature, which requires precise control in advanced industrial applications.
3. The use of polymers to stabilize liquid crystals is a promising technology, as this helps improve their thermal and mechanical stability, which increases their operational life.
4. Liquid crystals have great potential in optical applications, especially in optical fibers and display devices, as their properties can be controlled through heat and electric fields.
5. The performance of liquid crystals can be improved by controlling manufacturing processes and temperatures during crystallization, which positively reflects on their operational efficiency.
6. Liquid crystals face challenges related to thermal decomposition and long-term stability, which requires the development of new materials with improved properties.
7. Liquid crystals can be used in temperature sensing technologies because their colors change with temperature changes, making them useful in medical and engineering applications.

**5.2 Recommendations**

1. The need to conduct more experimental studies on the effect of high and low temperatures on liquid crystals to improve their thermal stability.

2. Develop advanced mathematical models to analyze the changes in the physical properties of liquid crystals with temperature changes, which helps improve their performance in practical applications.
3. Promote research in the field of thermally stable polymers to improve the performance of liquid crystals in harsh environments.
4. Study the effect of other environmental factors, such as pressure and humidity, on liquid crystals to understand how they are affected by different operating conditions.
5. Develop advanced manufacturing techniques that reduce the effect of thermal changes on the performance of liquid crystals, which contributes to improving their sustainability.
6. Enhance cooperation between researchers in the fields of physics, chemistry and engineering to develop new materials with improved properties suitable for future applications.
7. Encourage the use of liquid crystals in medical fields, such as biodevices and thermal sensing, due to their ability to interact with physiological changes in the human body.
8. Support research related to liquid crystals in the field of communications and optical fibers, as these materials can contribute to the development of more efficient communications systems.
9. Direct more investments towards advanced manufacturing technologies that contribute to the production of liquid crystal materials with higher flexibility and stability.
10. Promote research and development in the field of liquid crystals by providing scholarships and funding research projects that focus on improving their sustainability and expanding the scope of their use.

In conclusion, research in the field of liquid crystals is a promising field that holds great potential for the development of advanced technologies in the future. Although these materials have unique properties that make them distinct from other conventional materials, the challenges of thermal and mechanical stability still require further research and development. Through in-depth analysis of previous research, it is clear that liquid crystals are capable of revolutionizing multiple fields such as optoelectronics, sensors, medical and engineering applications. With continued research efforts and modern technologies, these materials are expected to play an increasing role in improving human life and promoting scientific and technological innovation.

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