Original Article

Presenting Percent Crystallinity and Crystallization Order of 80CB Liquid Crystal

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Received: 20 March 2025

Revised: 28 April 2025

Accepted: 16 May 2025

Published: 03 June 2025

Abstract - This paper reports the details of percent crystallization, degree of crystallization, and order parameters of 4-oxo-4'-cyano-biphenyl (80CB) Liquid Crystal (LC) during crystallization transitions that occur when heated and cooled at various ramp rates. It is found that 80CB exhibits dynamic behavior during its crystallization transition. The Differential Scanning Calorimetry (DSC) technique was used to determine the heat flow of 80CB as a function of temperature at three ramp rates: 5 °C/min, 10 °C/min, and 20°C/min. Heating was performed from -40 °C to 100 °C, followed by cooling from 100 °C to -40 °C. LoggerPro was then used for further data analysis of the DSC data to identify dynamics in its crystallization. As 80CB was heated and cooled, the crystallization phase, both in heating and cooling, showed changes in its degree of crystallization, order parameters, and percent crystallinity. There were also noticeable movements and degradation of the crystallization phase transitions as the ramp rate increased. It was found that the number of sub-peaks that appeared during crystallization changed for both heating and cooling. The degree of crystallization decreased with heating and increased during cooling for increased ramp rates. Furthermore, the study of order parameters supports the dynamic behavior of crystallization, with a lower-order parameter for heating crystallization and a higher-order parameter for cooling crystallization. This further complicates cooling crystallization. This further supports the phenomenon where LC molecules do not completely return to a completely ordered state when cooled and retain some energy within the molecules before reheating. However, the stability of nOCB during these temperature changes retains a high degree of crystallinity throughout, providing valuable insight into the practical application of 80CB in the Liquid Crystal (LC) world.

Keywords - Liquid Crystal (LC), 80CB, Heat Capacity, Temperature, Ramp Rate, Reheating/Re-cooling, Percent crystallinity, enthalpy, Fractured Integration, Order Parameters, Models, Pure and Applied Research.

1. Introduction

Typically, three states of matter exist in the world: solid, liquid, and gas. Matter transitions between these states of matter due to a change in energy. [1] Liquid Crystals (LC) are the material of interest for research as they show more than three states of matter. The molecules of LC undergo multiple states that can be named as solid (crystalline) to liquid (isotropic) and more in detail as crystalline, Smectic C, Smectic A, Nematic, and isotropic. LCs are also categorized into thermotropic, lyotropic, or metallotropic. [2] Lyotropic LCs are affected by temperature and the concentration of water solvents.

Metallotropics are Liquid Crystals (LCs) that involve both inorganic and organic materials, whose behavior is heavily dependent on the concentration of the inorganic material. Finally, thermotropic LCs are a type of liquid crystal highly affected by temperature changes and are most relevant in technological applications, such as Liquid Crystal Displays (LCDs). [3] The properties of LC molecules and their application in LCDs can be analyzed using Differential Scanning Calorimetry (DSC). A DSC was used in this study to analyze the thermodynamic behavior of Liquid Crystal (LC) molecules, specifically during the heating and cooling phases of the crystallization process. The DSC tracks the phase change of LC molecules by measuring heat flow relative to the material's temperature for various ramp rates.[4]

More specifically, an LCD is a type of display that utilizes the polymorphic characteristic. An important phenomenon that enables LCDs to function is the 90° orientation of a bilayer of Liquid Crystals (LCs), which allows polarized light to be twisted and pass through the polarizers to the pixel, creating the intended image.

[5] This technique revolutionized technology from its predecessor, the cathode ray tube monitors, especially in making technology more streamlined. [6] The n(O)CB family of LCs has become a significant discovery in LCD research.

However, LC molecules were discovered long before contemporary electronics by Austrian botanist Friedrich Reinitzer in 1888.[7] The most important for LCDs is the nematic phase of the subphases integral to LC molecules. Nematic is a phase from crystalline to isotropic.

Specifically, in terms of technology, LCD utilizes the nematic phase of liquid crystals when an electric field is applied for light polarization. [8-9] This current research study is important as it shows some hidden facts about 80CB as a member of nOCB that can bring significant change in the LCD research area.

80CB is an organic molecule with a biphenyl structure and cyano group at the "head" of the LC and octyloxy groups connecting to the "tail" (4-oxy-4'-cyano-biphenyls). See Figure 1 for a 2D rendering of 80CB. The molecular formula is $C_{21}H_{25}ON$. 80CB differs from the nCB family due to adding an oxygen atom before the hydrocarbon tail.[10] Both 80CB and 8CB have similar phase transitions.

However, the added oxygen increases the stability of the dipole moment induced by a stronger hydrogen bond network through the CN group, thereby stabilizing the LC phases at higher temperatures compared to 8CB. [11] The characteristics of 8OCB's phase transitions can be explored using the LoggerPro program.

LoggerPro by Vernier is graph-based software used in many academic institutions to collect data from various devices for real-world applications in undergraduate research settings. [12]

This paper focuses on the thermodynamic properties of 8OCB and how its structure affects various phenomena, particularly in heating and cooling crystallization. This type of study is absent from 8OCB in the research and brings more interest towards revealing new facts about 8OCB that may be useful in LCDs. [13, 14] This research will explore the integrity of the crystalline phase of 8OCB to further its candidacy in LCD manufacturing, particularly in environments without constant temperature control, which require affordable and reliable technology.

2. Materials and Methods

For this experiment, 4-oxy-4'-cyano-biphenyls (8OCB) LC was the molecule of interest. 8OCB is an organic molecule with a biphenyl structure, a cyano group at the head, and an octyloxy group at the tail. The molecule contains 21 carbons, 25 hydrogens, one nitrogen, and one oxygen, which are characteristic of the nOCB family.

A multitude of other molecules have been explored in other research. Figure 1 shows the linking of the octyl-oxy and biphenyl characteristics of the nOCB family. The molecular weight of 8OCB is 307.43 g/mol.



Fig. 1 2D rendering of 8OCB.

The instrument used for this study was Differential Scanning Calorimetry (DSC). Five milligrams of 80CB were sealed within a DSC apparatus model 214 from the NETZSCH company at the WPI Chemistry and Biochemistry Department in Worcester, MA. This sample of 80CB was heated from -40 °C to 100 °C and then cooled from 100 °C to -40 °C at three different heating and cooling ramp rates: 5 °C/min, 10 °C/min, and 20 °C/min. All experimental and environmental conditions were kept identical. The sample was heated and cooled for three consecutive cycles at increasing ramp rates. The data collected from the DSC showed the heat flow within the sample over time and temperature. This data was taken to Logger Pro for further analysis. The isothermal data were then computationally manipulated to explore heat capacity (Cp), enthalpy (ΔH), and the Johnson-Mehl-Avrami Law model, which was also found in a similar study for 5OCB [15]. Further research on the non-isothermal effects of 8OCB can be found in other studies. [16]

3. Theory

Liquid crystals can form lattice structures characteristic of various phase transitions. The data were analysed as outlined to analyze crystal nucleation, crystallinity, and other information about 80CB data collected from a DSC. The DSC measured the heat flow through the liquid crystal molecules over time and at increased ramp rates. Heat flow can be represented as dQ/dt in Equation 1, which is derived from the material's specific heat capacity. By manipulating Equation 1, the heat capacity can be solved to describe the change in energy when Liquid Crystal (LC) molecules are heated and cooled. This is representative of Equation 2 and is used to visually illustrate the relationship between Cp and temperature.

$$\frac{dQ}{dT} = m * Cp * \frac{dT}{dt} \tag{1}$$

$$Cp = \frac{1}{m} * \frac{dT}{dt} * \frac{dQdt}{dTdt}$$
(2)

In understanding the heat capacity of LCs, enthalpy can be calculated by manipulating Equation 2 to derive Equation 3, which demonstrates the connection between how LC molecules under constant pressure conditions exhibit increasing heat capacity and enthalpy changes.

$$\Delta H = \int C_p * dT \tag{3}$$

Equations 1-3 have the following units: dQ/dt or Heat Flow is in Watts or J/s. After establishing the HF in W/g, specific heat capacity units could be concluded as J/g°C. Mass was measured in grams, time in seconds, and temperature in °C.

Another way to examine how effective LC molecules are at handling the stress of changing energy is through the previously discussed crystal growth. The "Johnson-Mehl-Avrami Law" [17] mathematical representations of nucleation and their growth in terms of the degree of crystallization (alpha) and order parameter (n) can be seen as follows:

$$\alpha = 1 - \exp\left(-Kt^n\right) \tag{4}$$

K is a function of temperature and can be given as:

$$\mathbf{K} = \mathbf{K}_{0} \exp\left(-\Delta \operatorname{Ec}\left(\mathbf{RT}\right)^{-1}\right)$$
(5)

 K_o is a constant, Ec is the activation energy of crystallization, R is the gas constant, and T is the absolute temperature. Matusita and Sakka [18] showed a model for the degree of crystallization depending on temperature, ramp rates, and order parameters by inserting equation 4 into 5 to produce equation 6:

$$-\ln(1 - \alpha) = B(\beta n)^{-1} (\exp) - [(n\Delta E_c)(RT)^{-1}]$$
(6)

With beta as ramp rate and B as a constant, equation 6 can be rearranged to resemble the equation of a line: y=mx+b to extrapolate a graphical relationship between the $ln(\beta)$ and ln $(ln (1-\alpha)^{-1})$ where the slope of the line is the order parameter of crystallization at different temperatures for different ramp rates:

$$\ln (\ln (1-\alpha)^{-1}) = -n * \ln \beta + (\ln B) - [(n\Delta E_c)(RT)^{-1}]$$
(7)

Alpha can also be represented by Equation 8, which relates the entire area under the curve of a heat capacity graph to different fractions of the curve's area. These predetermined fractionated areas are outlined in Tables 2 and 3. The respective enthalpies were calculated using Equation 3.

$$\alpha_{\rm T} = A(A_{\rm T})^{-1} \tag{8}$$

To determine the percentage of crystallinity, equation 9 was derived, where H_H is the enthalpy of the heating crystalline phase, H_c is the enthalpy of the cooling crystalline phase, and H_{m^*} is the pure enthalpy of the entire sample, respectively:

% crystallinity =
$$|(H_H - H_c)[(H_m^*)^{-1}]| \approx 100$$
 (9)

4. Results

In this section, detailed results obtained from DSC are shown. The data was first shown as a heat flow versus temperature plot for heating and cooling and then changed to a Heat capacity versus temperature plot for both heating and cooling.

The detailed graphs for 8OCB, showing heating and cooling as a function of Heat Flow versus Temperature, are plotted below in Figures 2 and 3 for three ramp rates: 5 °C/min, 10 °C/min, and 20°C/min, represented by red, green, and blue lines, respectively.

The graph shows three different phase transitions for 8OC during heating and cooling, including crystallization, the Smectic A phase, and the Nematic phase. More detailed Smectic A and Nematic transition results can be seen in our previous publication and research materials. [16] In this paper, more focus is given to the Crystallization transition.

For various ramp rates, the size, shape, appearance, and number of peaks appear in Crystallization in 8OCB changes. The first giant peak in heating and the last significant peak in cooling is the crystallization peaks for three different ramp rates.

The size, shape, and position of the Crystallization peak also change. As the ramp rate increases, the heat flow peaks shift to the right, broadening into a single peak and a small peak at the beginning of the run, present in the ramp rate of 20 but not in 5 or 10 °C/min.



Fig. 2 Heat Flow of 8OCB at various temperatures for heating rates of 5, 10, and 20°C/min.

Figure 3 shows a similar phenomenon, where the peak occurrence does not occur at the same temperature for increased ramp rates. For the cooling of 8OCB, the peaks occur at increasingly lower temperatures or sooner in the ramp rate. Similarly, the peaks become broader and lose specificity.



Fig. 3 Heat Flow of 80CB at various temperatures for cooling rates of 5, 10, and 20°C/min.

Figures 4-5 represent the heat capacity of 80CB as a function of temperature for the three different ramp rates: 5 °C/min (pink), 10 °C/min (orange), and 20 °C/min (black). The heat capacity of the samples was calculated by manipulating Equation 1 to solve for Cp, which resulted in Equation 2. The heat capacity represents the energy needed to cause a unit temperature difference in a particular sample. As the ramp rate increases during heating, there is a subsequent shift in the temperature peak of the heat capacity and a decrease in overall heat capacity for the sample as the peak becomes broader and shallower. In Figure 5, there is also a change in peak placement as the phase transition peaks shift to lower temperatures, accompanied by a decrease in the heat capacity of the phase transitions. There is also a similar loss of peak specificity in the increased ramp rates during cooling.



Fig. 4 Full range heat capacity of 8OCB during heating of 5, 10, and 20°C/min.



Fig. 5 Full range heat capacity of 8OCB during cooling of 5, 1,0 and 20° C/min.

Detailed attention is given in this paper to the crystallization peak of 8OCB to determine what dynamics are occurring during heating and cooling with different ramp rates. Zoomed-in data details are presented as graphs in Figures 6 and 7, illustrating crystallization during heating and cooling for all three ramp rates.

As seen in the previous figure, peak shift, broadening, and lowering are still observed in the crystalline phase, along with an additional heating crystallization peak at a ramp rate of 20°C/min. A further small peak also appears at the highest ramp rate in the crystallisation.



Fig. 6 Heat Capacity for heat crystallization phase of 8OCB during 5, 10 and 20°C/min



5, 10 and 20°C/min

Interestingly, there is also a shift in the cooling crystallization peak, with a broadening and decreasing heat capacity for the phase transition.

Still, the crystallization of 8OCB cooling has three peaks, beginning with the first ramp rate, which transitions into a larger, single, and undefined peak for the last ramp rate, as shown in Figure 7.

To further explore the actual alignment of the crystals during these phase transitions, the heat capacity data were manipulated to determine the enthalpy of these phase transitions by integrating Cp, as shown in Figures 8 and 9.



Fig. 8 Full integration of 8OCB for heating 5, 1,0, and 20°C/min



Using Logger Pro, the Zoomed-in images of the Crystallization peak of 8OCB are further analyzed. The shaded colors indicate the peak area as measured by Logger Pro. From the values of these areas, the enthalpy values are calculated using the equations shown in the theory section and presented in Table 1.

Table1. Enthalpy of crystallization peak for heating and cooling for
various ramp rates. The enthalpies for the heating and cooling
crystallization peaks are denoted as H _H and H _C , respectively. The
enthalow for the first crystallization is $H_{M}^{*} = 154.20 \text{ J/g}$.

 FJ								
Rate (°C/min)	$H_{\rm H}$ (J/g)	$H_{C}(J/g)$						
5	154.20	83.04						
10	128.60	87.70						
20	119.30	94.78						

Table 1 shows a noticeable decrease in enthalpy during heating phase transitions and, conversely, an increase in enthalpy during cooling phase transitions when the ramp rates are increased.

The enthalpies of the three-phase transitions for heating and cooling of 8OCB were then divided into seven segments to analyze the enthalpies and crystallization of the LC molecules before and after significant changes in the phase transitions, such as rapid increases in heat capacity and peak transitions. The temperatures for each fragment are shown in Tables 2 and 3, along with their corresponding enthalpies, which consecutively incorporate the previous pieces. These enthalpies are graphically represented in Figures 10-16 below.



Fig. 10 Integration of heating crystallization at T_1 for 5, 10, and 20° C/min



Fig. 11 Integration of heating crystallization at T_2 for 5, 10, and 20° C/min



Fig. 12 Integration of heating crystallization at T_3 for 5, 10, and $20^\circ C/min$



5



Fig. 14 Integration of heating crystallization at T_5 for 5, 10, and 20° C/min



T6 Integration of Crystallization to Smectic A 5, 10 and 20°C/min Heating

20°C/min



Fig. 16 Integration of heating crystallization at T₇ for 5, 10, and 20°C/min

 Table 2. The enthalpy of heating crystallization peaks at temperatures T1 through T7. The temperatures for each fragment and their corresponding enthalpies are recorded. This data is graphically represented in Figures 10-16.

Rate	T ₁ =58.22°C	T ₂ =59.30°C	T ₃ =59.68°C	T ₄ =60.33°C	T5=61.00°C	T ₆ =61.86°C	T7=64.06°C
(°C/min)	J/g	J/g	J/g	J/g	J/g	J/g	J/g
5	37.18	72.47	89.07	114.7	129.50	136.60	144.50
10	48.17	70.85	79.56	93.69	104.40	112.00	120.80
20	32.99	44.89	50.03	59.75	70.28	83.35	106.20

 Table 3. The enthalpy of cooling crystallization peaks at temperatures T1 through T7. The temperatures for each fragment are recorded, along with their corresponding enthalpies. The figures for this data are not shown.

Rate	T ₁ =20.01°C	T ₂ =21.90	T ₃ =22.79°C	T ₄ =24.50°C	T5=25.18°C	T ₆ =27.20°C	T ₇ =28.42°C
(°C/min)	J/g	°C J/g	J/g	J/g	J/g	J/g	J/g
5	0.49	0.97	1.30	2.65	3.40	37.88	67.41
10	3.98	8.90	15.40	52.90	69.71	83.98	84.81
20	40.07	64.30	74.91	85.76	87.41	89.81	91.08

Table 4. Degree of crystallization for heating 8OCB for ramp rates 5, 10, and 20°C/	min at temperatures T_1 - T_7 .
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Rate (°C/min)	$T_1 \alpha$	Τ2 α	Τ3 α	Τ4 α	Τ5 α	Τ6 α	Τ7 α
5	0.289	0.469	0.577	0.743	0.839	0.885	0.937
10	0.374	0.550	0.618	0.728	0.811	0.870	0.939
20	0.276	0.376	0.419	0.500	0.589	0.698	0.890

Tables 2-3 above illustrate the enthalpies of each fragment at increasing ramp rates, allowing comparison of the internal energy of the peak transition at the given ramp rate. For the heating of 80CB, as the ramp rate increases, there is a general decrease in the system's energy. Conversely, the system's energy increases when the ramp rate increases during the cooling crystallization phase. There is

also a decrease in the energy change in the system when horizontally following the enthalpies for the ramp rate. The ramp rate of 5°C/min changes by about 67 J/g, while 20°C/min has a difference of about 50 J/g in the overall enthalpies, equating to a 17 J/g decrease in the overall shift in energy in the system when the ramp rate is increased. Similarly, in the heating of 80CB, there is a 107 J/g difference between the beginning and end of the phase transition at a ramp rate of 5°C/min, while there is only a 74 J/g difference at a ramp rate of 20°C/min. Overall, a 28 J/g decrease in energy difference in the system occurs when the ramp rate increases.

Tables 4-5 illustrate the Johnson-Mehl-Avrami Law, where the alpha value represents the fragmented enthalpy divided by the total enthalpy for rates of 5, 10, and 20°C/min. Comparing the fragments, as the temperature increases, there is a general increase in the alpha value. Similar patterns are

observed in alpha values when comparing the beginning and end alpha rates at 5 and 20°C/min and rearranging the equation solving for alpha to then solve for the value of K, Matusita and Sakka derived order parameter due to the linear relationship between the ln(B) and ln (ln $(1-\alpha)^{-1}$) where the corresponding slope is "n" order parameter. Figures 17-20 below follow this equation model, where the x coordinates are the values of ln(B), where B is the ramp rate, and the y coordinates are the values of ln (ln $(1-\alpha)^{-1}$). The slope values for the various temperature fragments at the three increasing ramp rates are shown in Tables 6 and 7 below.

Table 5. Degree of crystallization for cooling of 8OCB for ramp rates 5, 10, and 20°C/min at temperatures T1-T7.

Rate (°C/min)	Τι α	Τ2 α	Τ3 α	Τ4 α	Τ5 α	Τ6 α	Τ7 α
5	0.005	0.011	0.015	0.031	0.040	0.456	0.811
10	0.045	0.101	0.175	0.603	0.794	0.957	0.967
20	0.422	0.678	0.790	0.904	0.922	0.947	0.960



Fig. 17 Finding the order parameters of heating crystallization at T₁.



Fig. 18 Finding the order parameters of cooling crystallization at T₁.



Fig. 19 Linear relationship of ramp rate and degree of crystallization for T1-T7 during heating



Fig. 20 Linear relationship of ramp rate and degree of crystallization for T₁-T₇ during cooling

Figures 17-20 are the graphical analysis of ln(B) and $ln (ln (1-\alpha)-1)$ to demonstrate how the slope was calculated. Figures 17 and 18 are singular temperature fragments from heating and cooling, while Figures 19 and 20 are all the temperature fragments from heating and cooling, respectively. The order parameter for the heating and cooling the 80CB crystallization phase change can be found in Tables 6 and 7. Values of "n" above one indicate significant disorder, and over two indicate extremely complex disorganization. Values of "n" less than one indicate a lack of disorder, and the closer to zero, the more ordered the alignment of the LC.

Table 6. Order parameters (absolute values) of T_1 - T_7 during heating crystallization.							
T(°C)	T ₁ =58.22°C	T ₂ =59.30°C	T ₃ =59.68°C	T4=60.33°C	T5=61.00°C	T ₆ =61.86°C	T7=64.06°C
n	0.0381	0.2137	0.3324	0.4855	0.5210	0.4277	0.1622

Table 7. Order parameters of T_1 - T_7 during cooling crystallization.							
T(°C)	T ₁ =20.01°C	T ₂ =21.90	T ₃ =22.79°C	T ₄ =24.50°C	T5=25.18°C	T ₆ =27.20°C	T7=28.42°C
n	3.274	3.296	3.315	3.090	2.966	1.138	0.4787

Figures 21 and 22 best articulate the changes in order parameters. As seen in Figure 21, there is a relatively steep decline in order parameters and a more gradual increase in temperature fragments. Compared to Figure 22, which shows the overall decrease in order parameters for the temperature fragments of the cooling phase transition and crystallization.





Fig. 22 Variation of order parameters during cooling crystallization for T_1 - T_7 .

As seen in Figures 21-22, dynamic differences in the order parameter can be observed, which help mathematically quantify the orientation and organization of the liquid crystals. As 8OCB is continuously heated, the order parameter first becomes closer to zero, indicating increased order, and then sharply increases away from zero, indicating increased disorder in orientation. There is a consistent downward trend for the cooling transition to zero for the order parameter, but it starts above 3 initially, indicating an extreme amount of misorientation.

5. Discussion

As can be seen from Figures 2-5, looking at Hf and Cp vs. temperature for 80CB at increasing ramp rates, there is an apparent shift in the overall phase transitions for the crystalline, smectic A, nematic, and isotropic phases. This phenomenon can also be observed in other members of the nOCB family and the nCB family to varying extents due to the distinct properties of these families of LC molecules [19-20]. The focus was narrowed to examining the crystalline phase transitions of 80CB when heated and cooled at increasing ramp rates. This was explored by first reviewing their heat capacities, as shown in Figures 8 and 9. Table 1

lists the enthalpies extracted from Figures 8 and 9, and Equation 3 outlines the relationship between heat capacity and enthalpy. When the ramp rate increases, the heating crystallization peaks decrease in their specific heat capacities and enthalpies, resulting in an equal area under their curves. Conversely, as the ramp rates increase, the areas for the cooling crystallization increase.

Figures 10-16 show the fragmented areas of the heating and cooling phases to understand better the acceleration of the phase transition peaks in specific increments. This allows for comparing the three different ramp rates and the phase transition at the same temperatures for each ramp rate. Tables 2-3 catalogue the heating and cooling crystallization temperature fractions and the subsequent enthalpies collected. For the ramp rate of 5°C/min heating crystallization, there was a noticeable difference of 107 J/g. In contrast, at 20°C/min, the difference was only 74 J/g. This is because the reaction retains heat from previous ramp rate cycles; therefore, the LC molecules do not need to absorb as much energy to continue moving through their various phase transitions. For cooling crystallization, there was also a minor change in enthalpy seen for the higher ramp rates, indicating that the exothermic nature of the liquid crystals is decreasing, and the reaction is not releasing all the energy it is taking in when the samples are initially heated up; corroborating the previous findings of energy retention found in 5OCB.

This phenomenon was then further explored mathematically through Johnson-Mehl-Avrami Law that explored crystallization (alpha) and, from the continued work of Matusita and Sakka, exploited a linear relationship to extract order parameter (n) to demonstrate that as 80CB is consecutively cooled and reheated, the crystalline phase transition is not completely returning to its original crystalline form when cooled. This causes the subsequent heating crystalline phase to retain some of the energy from the previous cycle, shifting the entire course of phase transitions. The order parameters found in Tables 6-7 demonstrate the complex nature of the LC through its various phase transitions. However, they also highlight that the cooling crystallization phase has increased complexity, with most of its order parameters being greater than one and even greater than two, which shows its dynamic nature.

Another way the crystalline phase transition was analyzed was by examining the percent crystallinity and the percent amorphous states of 80CB at increasing ramp rates. As the ramp rates rise, a greater amount of the LC material falls into the amorphous state, where it is no longer in its ordered rows and columns due to the already evident phenomenon of energy being retained by the crystals as the ramp rate increases. This data is presented below in Table 8 and graphically represented in Figure 23, where the amorphous state data is shown in red, and the crystalline state data is shown in blue.

using Equation 9, which are presented in Table 1.						
Rate (°C/min)	% Crystallinity	% Amorphicity				
5	46.15	53.85				
10	26.52	73.48				
20	15.90	84.10				

Table 8. Shows percent crystallinity in the Crystallization of 8OCB for all ramp rates. The values for percent crystallinity were calculated using Equation 9, which are presented in Table 1.



Fig. 23 Percent crystallinity and amorphous states of 8OCB.

All findings shown in this paper so far demonstrate the dynamic behavior of the crystallization transition of 80CB. To explain the dynamic behavior of 80CB, a Model is predicted, and its visualization is shown in the form of a cartoon of the LC molecular arrangement in Figure 24.



Fig. 24 Model prediction to explain dynamics of crystallization of 8OCB, (a) 100% crystallized state for the 1st run of heating, (b) partially crystalline at second run of heating, (c)least crystalline and more disordered molecules for 3rd heating run, showing the presence of more amorphous state.

A model was constructed to represent the LC molecules as their alignment changes with increasing ramp rates, as shown in Figure 24. The crystals outlined in blue indicate organized alignment; for simplicity, they are aligned on a simple 2-dimensional plane. Liquid crystals typically exist in multidimensional spaces with stacks of rows and columns where order variation can occur in three dimensions. The red crystals indicate disorganization and variation in their original horizontal and vertical positions, as seen in images a, b, and c, which correspond to the increasing ramp rates.

Figure 24 again demonstrates the various ways in which 80CB is dynamic. With increasing ramp rates, changes in enthalpy, heat capacity, order parameter, and percent crystallinity show that the LC molecules do not completely return to their ordered state during the crystalline phase transition upon heating and cooling. For comparison, 80CB has lower order parameters for the heating crystallization phase than 5OCB, but higher order parameters and greater complexity in crystal alignment upon cooling. This demonstrates how the added oxygen of the nOCB family consistently helps stabilize the LC. However, the larger the molecules, the issue of the tangling phenomenon arises, demonstrating the intricate balance between the stability and simplicity of LC molecules, depending on the intended application. Based on previous research on 80CB, this member of the nOCB family can stabilize during increased ramp rates as it retains its crystalline phase transitions throughout, adjusting to the energy stored within its crystal structure. [21] This makes it a reasonable candidate for applied use, such as in LCDs and shows some hidden facts about 8OCB LC that are absent from the literature.

6. Conclusion

The details of percent crystallization, degree of crystallization, and order parameters for the crystallization transition of 4-oxy-4'-cyano-biphenyl (80CB) Liquid Crystal (LC) are reported at various ramp rates in this paper to investigate the dynamics of the crystallization peak of 8OCB. Differential Scanning Calorimetry (DSC) is used to collect data for the heating and cooling of 8OCB at various ramp rates of 5, 10, and 20°C/min. LoggerPro is then used for further analysis to explore the details of the 8OCB crystallization peak. As ramp rates increase, the shape and size of the crystallization peak change, becoming broader and containing additional sub-peaks within the original peak. The size of the crystallization peak also changes. It visually attempts to demonstrate this occurrence at the molecular level, accounting for the increasing order parameters, the increased amorphous state of 84% of 8OCB, and the decreased percent crystallinity of 15% of 8OCB after a ramp rate 20. The presence of multiple peaks or subpeaks in crystallization and changes in their shape and size indicate that one crystallization peak changes into numerous peaks.

Furthermore, on the molecular level, 8OCB molecules retain some energy when cooled after heating and do not return to a completely ordered state. Whenever 8OCB molecules are heated and cooled, they revert to a less ordered state because they retain some thermal energy each time they are heated or cooled. That is why 8OCB exhibits dynamic behavior in its crystallization, which is explained in terms of percent crystallinity and order parameters. Although it seems like pure research in 8OCB, these results can be helpful in the applied research world of Liquid Crystals (LCS), such as Liquid Crystal Displays (LCDs), by providing an in-depth understanding of 8OCB's behavior when thermal energy is introduced under various conditions and exploiting its stabilizing abilities as an nOCB LC.

Acknowledgments

The authors gratefully acknowledge Professor John C. MacDonald of the Department of Chemistry and Biochemistry and the Life Sciences and Bioengineering

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Center at Worcester Polytechnic Institute (WPI), Worcester, MA, for providing access to the NETZSCH 214 Differential Scanning Calorimetry (DSC) instruments. Appreciation is also extended to the NETZSCH company for supplying the DSC 214 pans and lids. The student author wishes to sincerely thank Dr. Dipti Sharma for her supervision during the research internship and Emmanuel College for offering and supporting internship opportunities.