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Crystal Growth, Percent Crystallinity and Degree of Crystallization of 5OCB Liquid Crystal (Analyzing using Logger Pro)

Juliana Mello 1, Dipti Sharma (PhD) 2*
1 Undergraduate student, Emmanuel College, Boston, MA, 02115 USA
2 Supervisor, Emmanuel College, Boston, MA 02115 USA and *Corresponding Author

Abstract:
In this paper, we are reporting the details of the crystal growth, percent crystallization and degree of crystallization that appeared in pentyl-oxy-cyanobiphenyl (5OCB) Liquid Crystal (LC) during heating and cooling. This LC shows two types of crystallization when it was heated and cooled multiple times using Differential Scanning Calorimetry (DSC) at different ramp rates. The typical crystallization shown by LC is in its cooling usually appears as a sharp exothermic peak, but 5OCB shows a broad and double peak in cooling for cool crystallization. The second crystallization peaks shown by 5OCB are in heating and referred to as 'Krystallization' which is an additional crystallization in 5OCB. As 5OCB is heated and cooled multiple times, the crystal shows its growth is ramp rate dependent. The data details of crystal growth, percent crystallinity and degree of crystallization of 5OCB at different temperatures are shown with their graphical plots. It is observed that 5OCB crystallizes partially after cooling and then crystallizes more when heated after cooling. Both crystallizations show the presence of an order parameter where Krystallization has a higher order parameter than crystallization. Krystallization shows higher percent crystallinity than crystallization whereas crystallization shows higher growth in crystallization as ramp rates increase. These results can be useful in the crystal industry where people make types of crystals.

Keywords:
Crystallization in heat and cool, crystal growth, percent crystallinity, degree of crystallization, Exothermic, Endothermic peaks, DSC, Liquid Crystal, 5OCB, Heating and Cooling, LoggerPo.

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I. Introduction:

A crystal is a type of solid material; it gets its name from the crystalline structure its atoms or molecules adopt when they are arranged. A crystal is usually a solid that is very hard and shiny. On an atomic or molecular level, the constituents that make up the substance are neatly packed together in their structure. There is little to no room for the molecules or atoms to move past each other and the components will display a long-ranged order in the form of lattice. A long-range order of molecules means that no matter where they are in the solid (front, back, side, middle) they show the same structured order as the other molecules in the substance.[1]

A solid can be either amorphous or crystalline; the difference between these two classifications is in how the atoms are arranged and how they break apart. An amorphous solid does not have any distinct pattern or orientation of atoms; there is hardly consistency between the arrangement. Breaking an amorphous solid would lead to the solid splitting into irregular pieces because of the disordered arrangement. A crystalline solid, as mentioned, is extremely ordered and usually contains a pattern of geometric shapes. For example, salt is arranged into small cubes of alternating sodium and chlorine as a crystal. When breaking a piece of salt or a crystalline solid into smaller pieces, it would lead to the solid splitting into its geometric patterns. Crushing a big cube of salt would result in a bunch of smaller cubes of salt. [2-3]

Typically, there can be four known types of solids of matter in the world: molecular solids, covalent bonded solids, ionic bonded solids, and metallic solids. The first one, molecular solids, have molecules or atoms that are held together and interact with one another through intermolecular forces. This is in direct contrast to the covalently bonded solid which has its molecules or atoms held together by covalent bonds (sharing of electrons) and the ionic bonded solid which has its atoms or molecules held together by ionic bonds (the transfer of electrons). Finally, a metallic solid contains atoms of a metal, and it is held together by metallic bonds. [4]

Crystals are organized, long ranged ordered solids. Often, a crystal is referred to as ‘growing’ which makes it sound like a living organism. Although crystals are not living organisms, they do have the ability to get bigger and acquire new mass under some circumstances. The growth of a crystal occurs in two steps, with the first step being called nucleation. This is the stage where a nucleus with the new crystal is formed and ready to begin taking on minerals and atoms. The actual ‘growing’ stage of a crystal happens because this nucleus of the crystal begins absorbing free atoms and minerals in the air or surroundings. The free atoms and minerals are distributed outward and add to the ordered structure of the crystal. [5-6]

Crystallinity is an important aspect of crystalline solids. The crystallinity of a solid is the amount or, in this paper’s case, the percentage of the solid that is arranged in a crystalline structure. The crystallinity of a solid will affect how hard, dense, or transparent a solid is; solids with a higher crystallinity will tend to be denser and harder. For example, a solid with 100% crystallinity means that all molecules or atoms in that solid are arranged into a crystalline ordered structure. [7-8]

Our interest is to find some hidden facts of crystallization of 5OCB liquid crystal; our goal is showing how its crystalline state shows growth in crystalline structure, increase in crystallinity, and how the state of crystallinity depends on temperature and rates, and show the process of nucleation and growth in terms of the order parameter. Some studies on such types of research can be seen in these publications. [9-11] Some other types of liquid crystals are analyzed using DSC in these publications, like 4CB, 5CB and 8CB. [12-14]

II. Experimental and Theoretical Details:

To study details of crystallizations appeared in pentyl-oxy-cyanobiphenyl (5OCB) Liquid Crystal (LC), the 5OCB was run in Differential Scanning Calorimetry (DSC) instrument in the department of Chemistry and Biochemistry at WPI using TA DSC Model MDSC 2920. The sample was run at four different ramp rates at 10 °C/min, 15 °C/min, 20 °C/min and 25 °C/min. The sample showed two types of crystallization in heat and cool, we call heat crystallization (Krystallization) and cool crystallization (Crystallization). The size, shape, appearance, and position of both crystallization peaks have changed as ramp rates have changed or multiple times heating and cooling is done. The detailed study of both crystallization is being reported in this paper. We are going to report, crystal growth, percent crystallinity, degree of crystallization and order parameter of both crystallizations appeared in 5OCB in heat and cool. All data analysis is performed using the Logger Pro Data analysis tool.Some details reported recently by us can be seen in our two recent papers on 5OCB. [15-16]

A crystalline material is made of the molecules that are long ranged ordered and show lattice or highest organization within their structure. That structure makes a crystal hard, brittle, shiny, sharp and transparent. An example can be salt, sugar, honey crystals or a diamond. The crystals show a nucleation and growth process that helps crystal molecules to form lattices, maintain their crystal structure, and show growth. The size of a crystal may grow or shrink based on the environment and conditions where they are kept or used. The conditions can be physical or chemical, can be permanent or temporary based on types of material.

To understand the nucleation and growth process of crystals, several scientists and authors studied phenomena of how crystals are formed and then they gave their theories and models. We are going to use “Johnson-Mehr-Avarami Law” [17-20] reported in several publications in types of crystalline and amorphous material where one can be seen here. [17] According to this theory, there are some equations that can be written to explain the nucleation and growth process of a crystal in terms of degree of crystallization (alpha) and order parameter (n). The following equations highlight the same laws:

$$\alpha = 1 - exp\ (-Kt^{\ n}) \qquad (1)$$

Where Alpha is degree of crystallization, K is function of temperature, t is time, n is order parameter. The K can be given as:

$$K = K_o\ exp\ \left(\frac{-\Delta E_c}{RT}\right) \qquad (2)$$

Where Ko is a constant, Ec is activation energy of crystallization, R is gas constant and T is absolute temperature.

Later, another group of scientists called Matusita and Sakka [18-20] showed their model where they mentioned that the degree of crystallization depends on temperature and ramp rates and order parameters. Matusita and Sakka, then used their model in the equation # 1 by plugging equation # 2 and got following equation:

$$-ln\ (1 - \alpha) = \frac{B}{\beta^n}\ exp\ \left[-\frac{n\Delta E_c}{RT}\right] \qquad (3)$$

Where beta is ramp rate and B is a constant. If some math is applied and equation # 3 is solved to simple terms, we can get a rearranged equation from equation # 3 as:

$$\ln \left(\ln (1-\alpha)^{-1} \right) = -n * \ln \beta + \ln B - \left(\frac{n\Delta E_c}{RT} \right) \qquad (4)$$

If we compare this equation # 4 with an equation of a line and plot a graph between ln ln(1-alpha)^-1 vs ln beta, we can find out the order parameter of each crystallization at different temperatures that indicates the order of reaction of nucleation and growth process of both crystallizations in 5OCB.

The degree of crystallization, alpha, can be found at different temperatures from the graph that is plotted between specific heat capacity vs temperature plot for different ramp rates for crystallization peak. The value of alpha at a particular temperature can be given by equation # 5. The process of how alpha is calculated at a given T, can be seen in the model shown in **Figure 1**.

$$\alpha_T = \frac{A_T}{A} \qquad (5)$$

Where alpha at T means degree of crystallization at temperature T and A_T means area of the peak at T and A means full area of the peak.

The percent crystallinity of both crystallization of 5OCB can be found using the following equation # 6 that has been used by multiple authors in the past and published by them. [18-20]

$$\% \text{ crystallinity} = \left| \frac{H_m - H_c}{H_{m*}} \right| * 100 \qquad (6)$$

Where Hm, Hc, Hm* are enthalpies of melting, crystallization, and enthalpy of melting of the pure sample of 5OCB respectively.

Percent crystallinity represents how much material is crystalline after cooling and heating.

Crystal growth of each crystal is ramp dependent and can be found by finding how much energy is released by the molecules of 5OCB when it is moving to its crystallized state. This can be shown by equation # 7.

$$\Delta H = \int C_p * \Delta T \qquad (7)$$

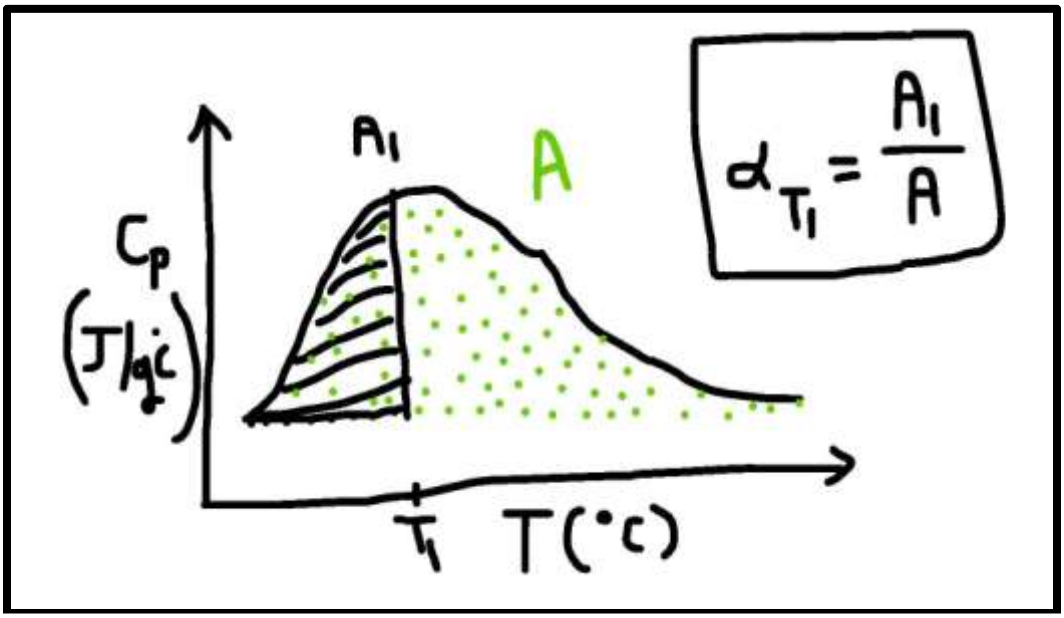

Figure 1: The model of how alpha at T1 is calculated from the exothermic peak of crystallization.

The schematic in Figure 1 explains the theory analysis of what is going to be performed on the Krystallization and crystallization peaks of 5OCB after being heated and cooled multiple times. Alpha can be found by finding the entire area of the peak (A) and then finding the partial area of the peak (A1) up until a certain temperature point (T1). Dividing this partial area by the full area yields alpha, which was then used to make a linear trend graph with the natural log of the rate.

III. Results:

The sample of 5OCB was heated and cooled in DSC four times without taking it out from DSC. It is observed that 5OCB shows melting and nematic phase transitions, for its 1st heating, as endothermic peaks and then nematic and crystallization phase transitions during cooling as exothermic peaks. These are typical expected phase transitions of liquid crystals, that is why the DSC graph for the 1st heat and cool is not shown here. The DSC graph for the 1st heat and cool can be seen in our other publications. [15-16] When 5OCB is heated 2nd time, an additional crystallization (heat krystallization) appears as an exothermic peak during heating and then a double peak in cool crystallization during cooling for the 2nd run in DSC. This DSC graph is shown as a specific heat capacity vs temperature plot in Figure 2.

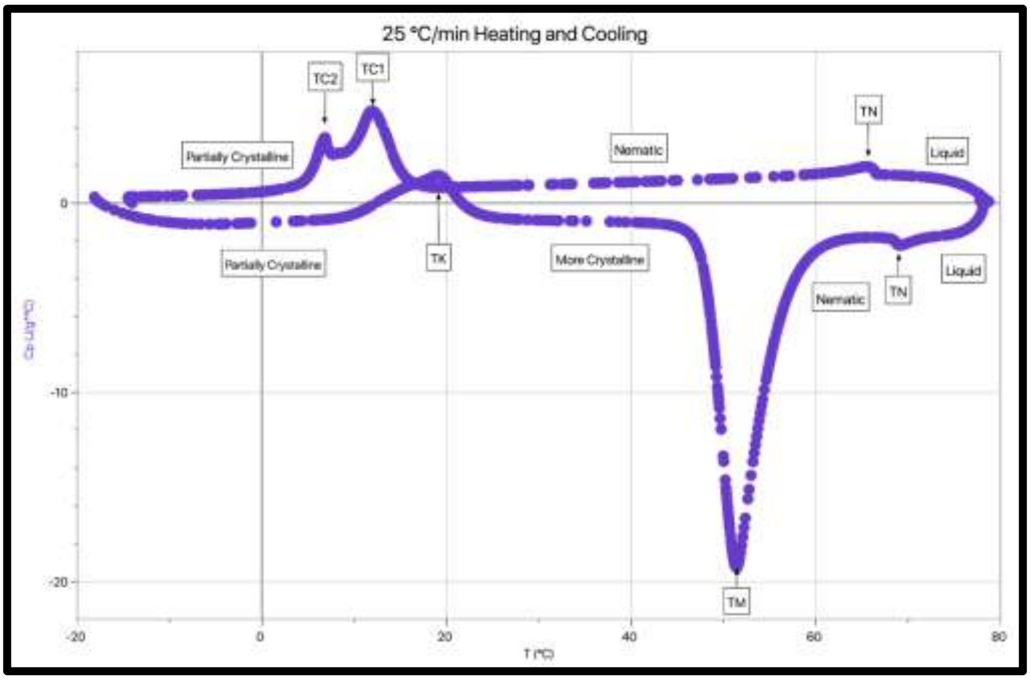

Figure 2: DSC thermogram of 5OCB's liquid crystal for its 2nd run of heating and cooling.

Usually, LC should be fully crystalline after cooling once it is heated to fully melting. However, in this case, 5OCB is fully melted after heating it to 80 ℃. When it is cooled back to - 20 °C, Figure 2 shows a double exothermic peak in cooling and an extra exothermic peak in heating. Thus, indicating that 5OCB is not fully crystalline after cooling and some part is left to be crystalline. When it is heated the 2nd time, it shows that it releases some thermal energy to be more crystalline. Hence, we prefer calling the stage after nematic in cooling as partially crystalline because 5OCB is not fully crystalline at this state, and it takes two steps to get that stage TC1 and TC2. We also prefer calling the stage that comes after Krystalline in heating as more crystalline. After releasing some thermal energy, 5OCB molecules get more aligned and organized and show a higher crystalline stage.

The most exciting part of this research is to see Heat Krystallization (Krystallization) that starts appearing from the 2nd heating as an exothermic peak during only heating, whereas the typical trend of peaks appearing in LCs in heating is endothermic only. To see a clear appearance of the Krystalline peak in heat, the zoomed in plot is shown in Figure 3 for Krystallization.

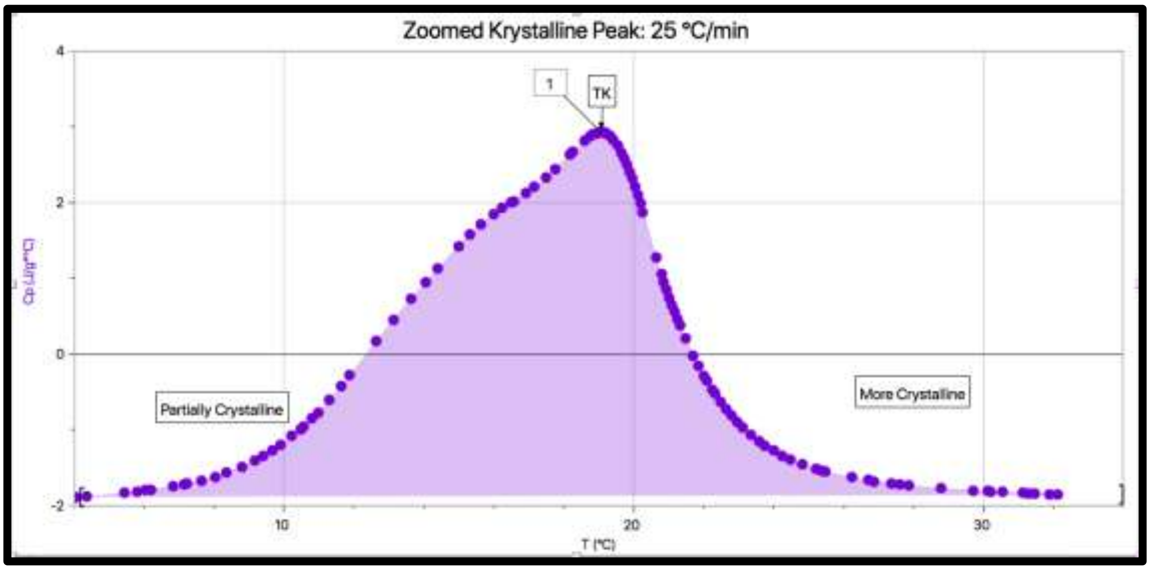

Figure 3: Run 2’s Krystalline peak during heating of 5OCB.

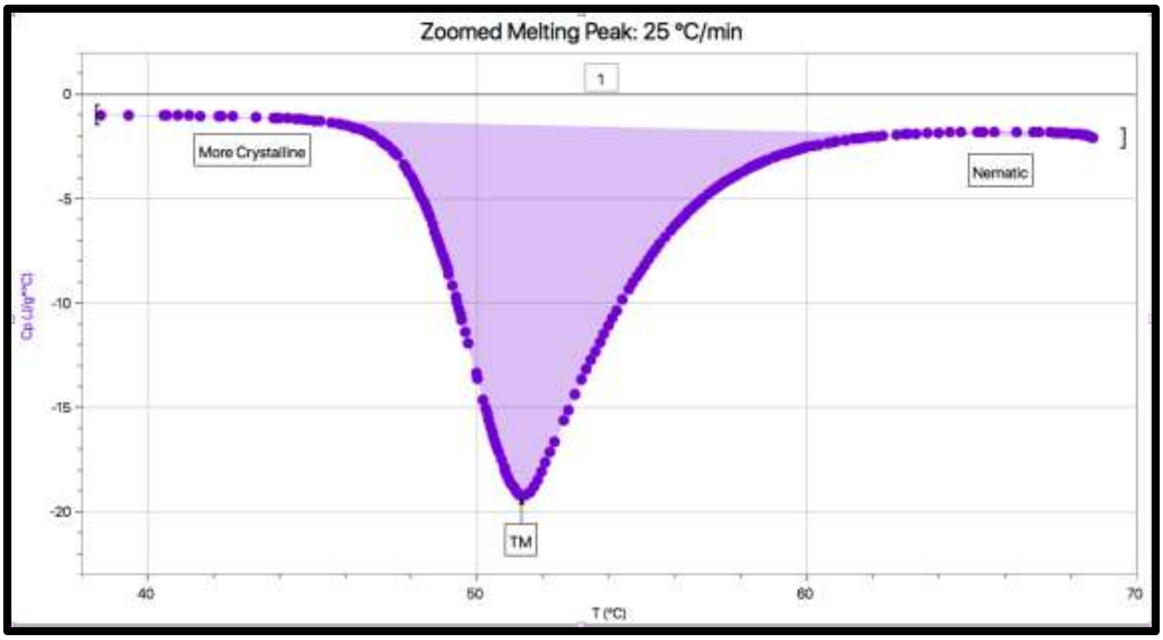

Figure 4: Run 2’s melting peak for the reheating of 5OCB.

The zoomed in peak for melting transition for 5OCB for the 2nd run can be seen in Figure 4. The highlighted purple area shows the amount of thermal energy absorbed to make 5OCB molecules to go from more crystalline state to nematic state.

The zoomed in graph for Crystallization is shown in Figure 5 for the Cool Crystallization (Crystallization) peak for 5OCB’s 2nd cooling. It can be seen that it shows double peaks, not a single peak. It was run with a ramp rate of 25 ℃/min in DSC. It is broader than the Krystalline peak shown in Figure 3.

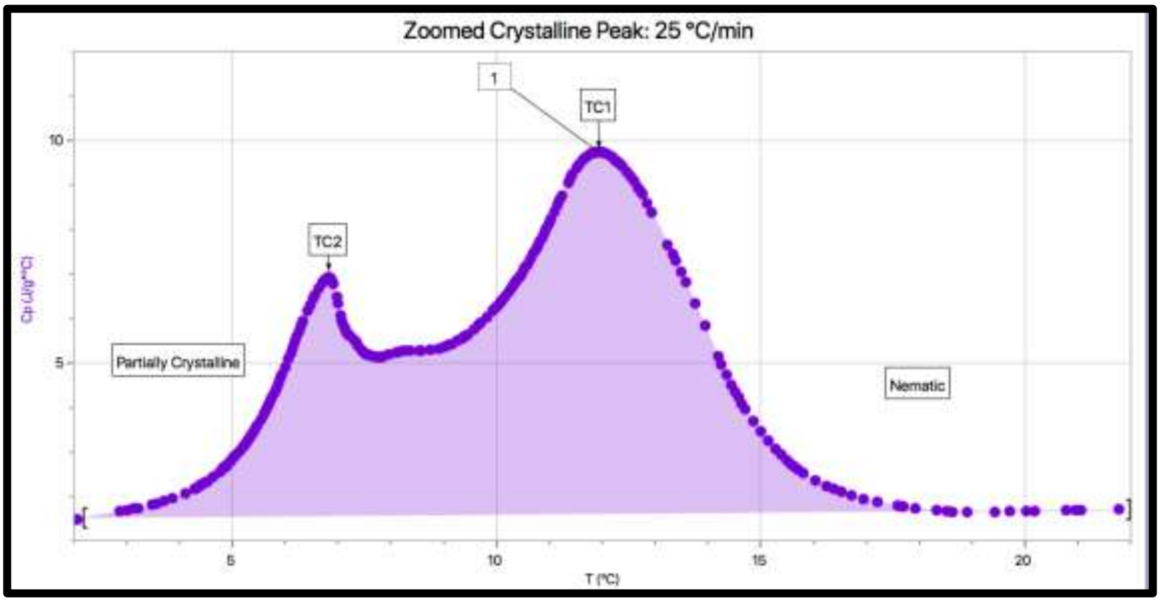

Figure 5: The Crystalline peak of the cooling for Run 2 of 5OCB using DSC.

The similar zoomed in plots are plotted for the cool Crystallization peaks of 5OCB for its 1st, 3rd and 4th cool runs; those are with ramp rates of 20 ℃/min, 15 ℃/min and 10 ℃/min, respectively.

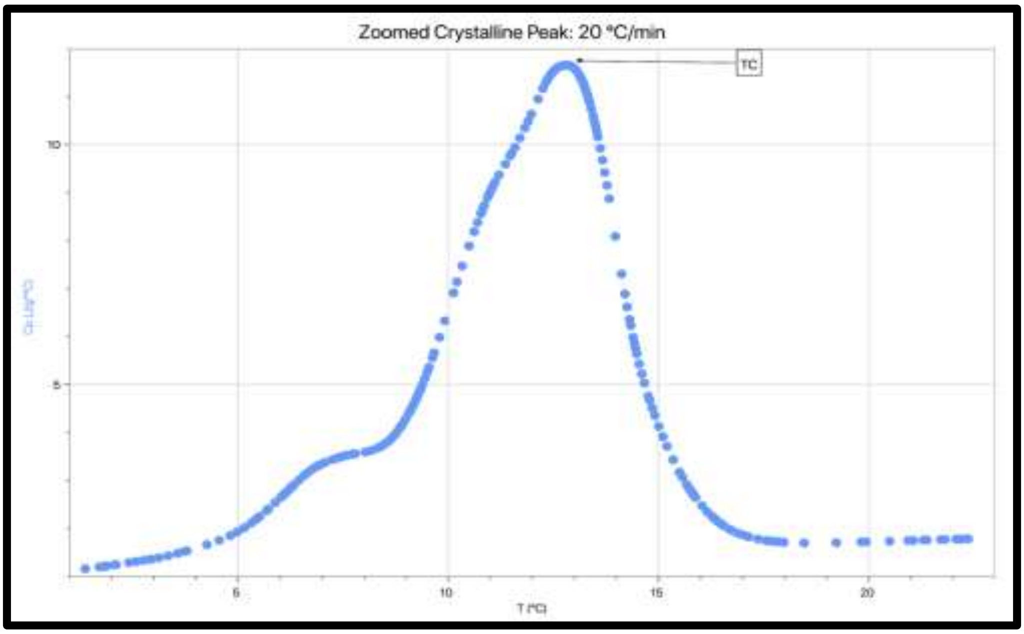

Figure 6: The zoomed in peak showing a single peak of cool crystalline for the first cool run in DSC.

It can be seen clearly in Figure 6 that the 1st run of cooling shows a single peak, but from the 2nd cooling runs, the Crystallization is showing double peaks, showing a two-step process taking place in its cool crystallization. These plots can be seen in Figure 5, 7, and 8 respectively.

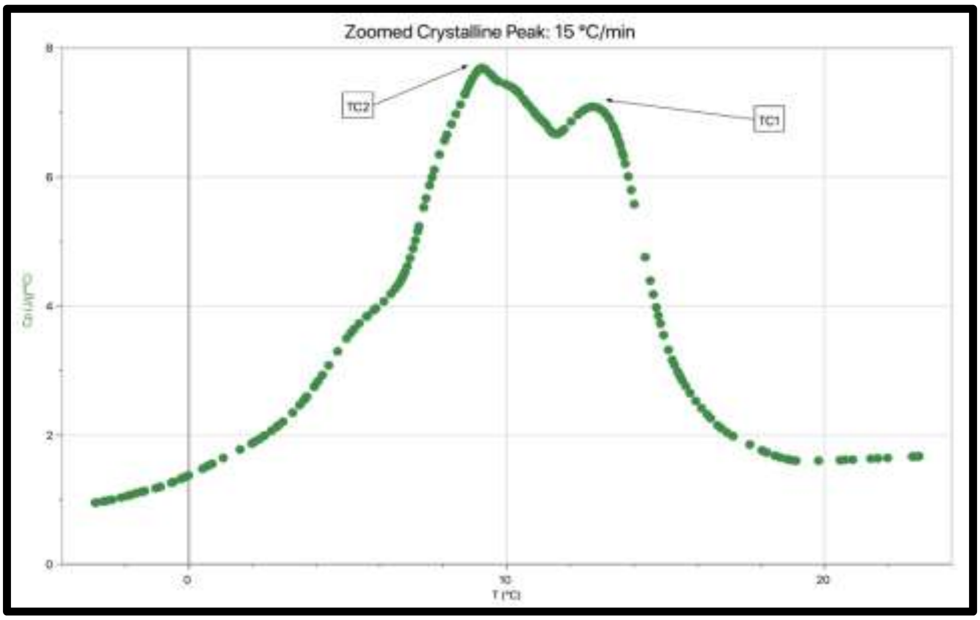

Figure 7 : Zoomed in peak for Crystalline showing double peak for 3rd run in DSC.

The transition of 5OCB from nematic to crystalline state in cooling is shown in Figure 7 in green. Like in run 2, the crystalline peak is a doublet. These doublet peaks started to occur once the liquid crystal had already been reheated and then cooled down. This can be seen in Figure 8 as well.

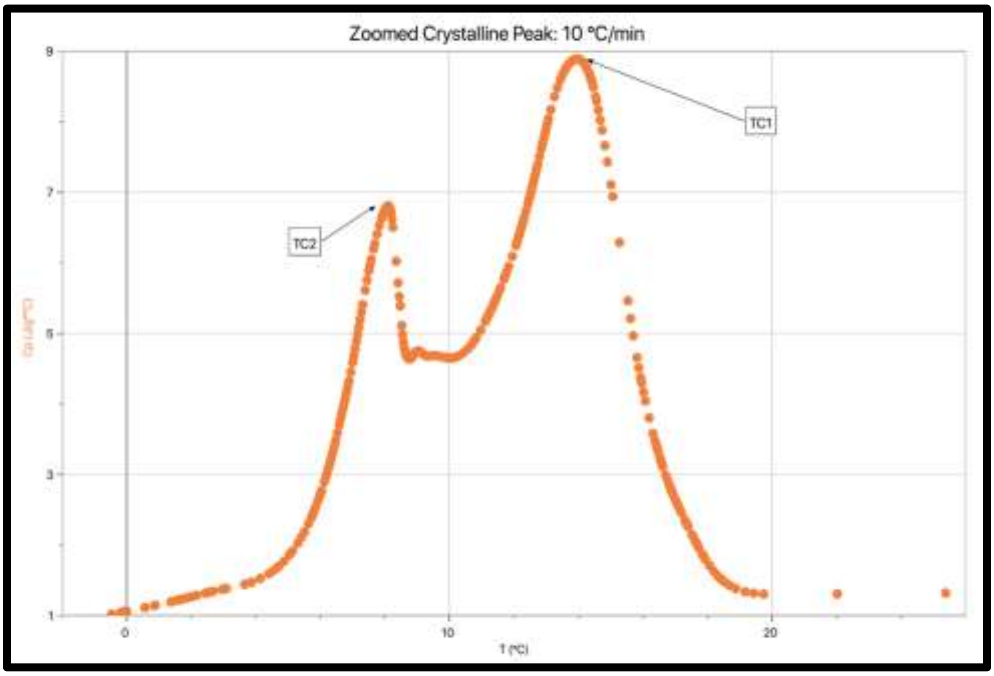

Figure 8: Zoomed in peak of Crystalline showing double peak for 4th run in DSC.

The zoomed in graphs are also plotted for the Krystallization phase transition that appears during heating for both the 3rd and 4th runs; those were done at the ramp rates of 15 ℃/min for run 3 and 10 ℃/min for run 4. Figures 9 (run 3) and 10 (run 4) show these fascinating peaks that only resulted after reheating the liquid crystal.

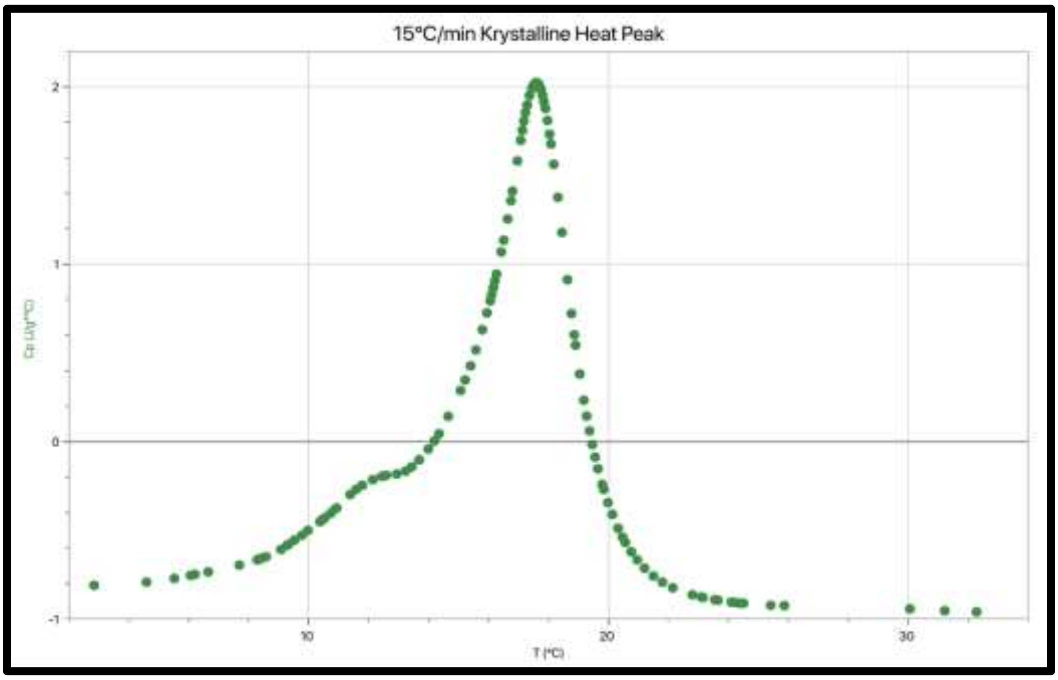

Figure 9: Zoomed in Krystallization peak of 5OCB being heated at 15 ℃/min.

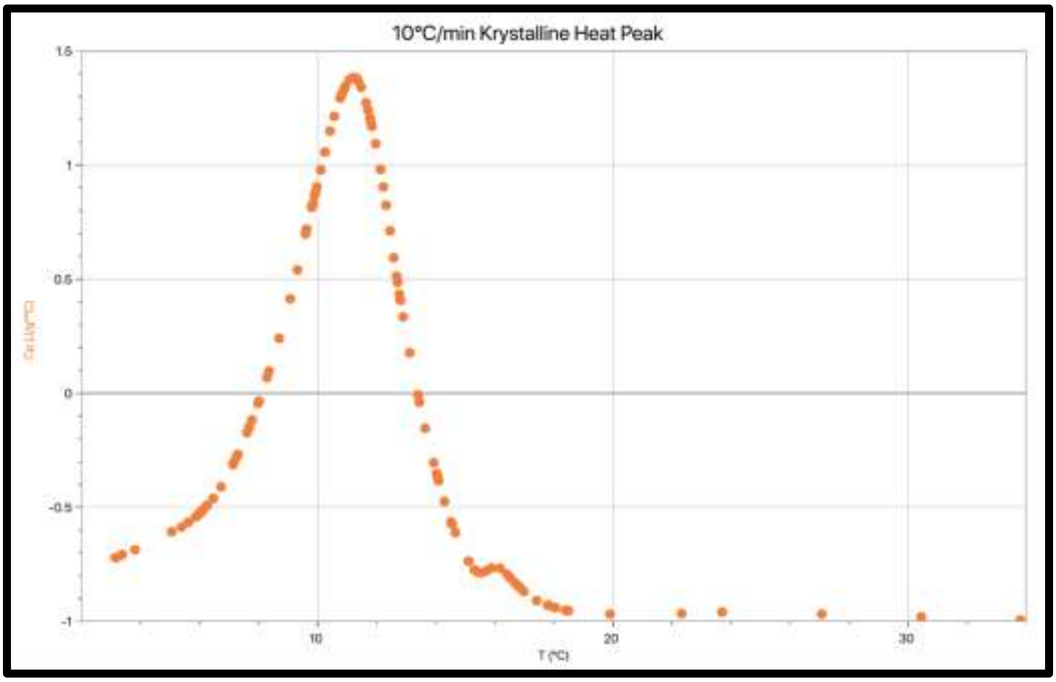

Figure 10: Zoomed in Krystallization peak for 10 ℃/min ramp rate.

It can be seen that Krystallization peak is changing in its size, shape and position as ramp rates are changed. The detailed comparative graphs for Crystallization and Krystallization can be seen in Figure 11 and Figure 12 showing all ramp rates and all runs for cooling and heating to see how these Crystallization and Krystallization peaks shift and differ from each other.

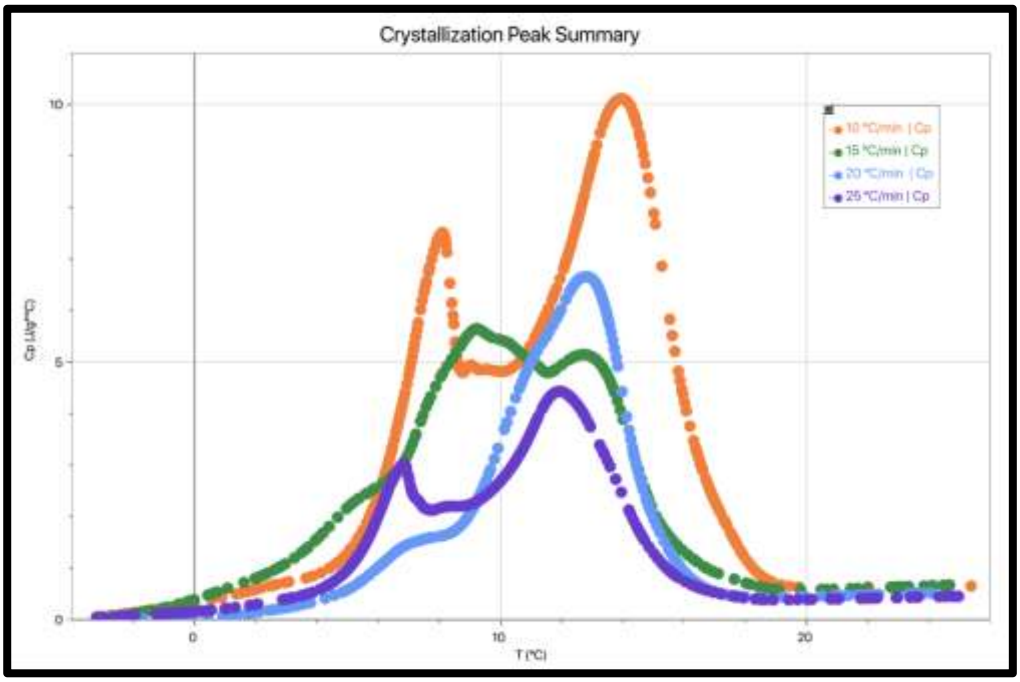

Figure 11: Comparing Crystalline peak for all ramp rates for four cooling runs.

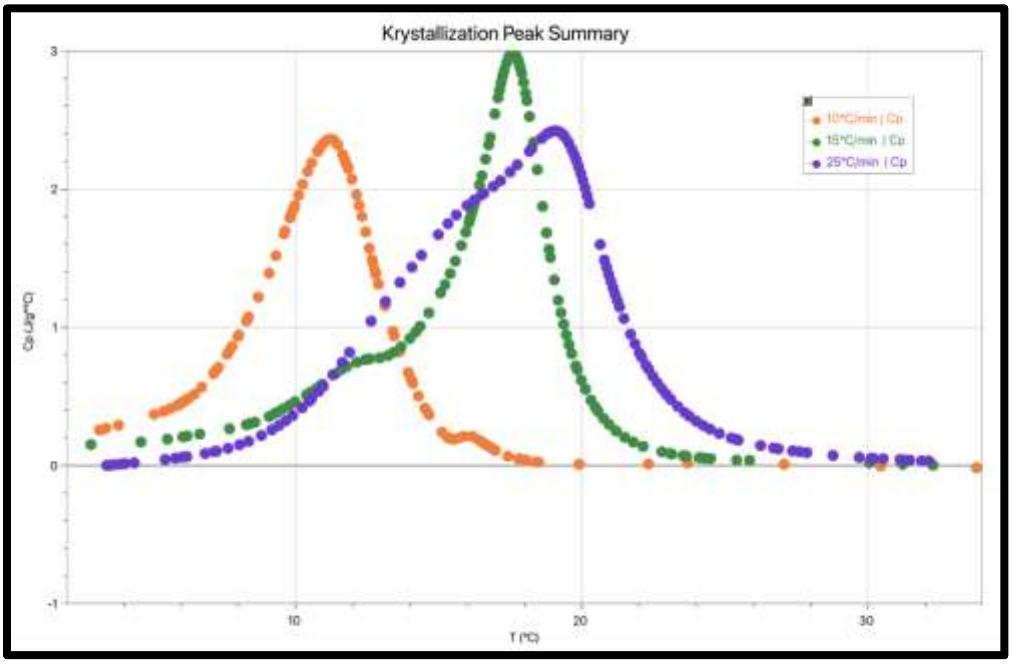

Figure 12: Comparing all Krystalline Peaks at all ramp rates for all three heating runs.

Now, the model shown in Figure 1 is applied to all Crystallization and Krystallization peaks following theories shown from equations # 1, 3, 4 and 5 to get the degree of crystallization of each peak at four different temperatures: T1, T2, T3, T4 and then for the full area of each peak as T. These plots are shown for Crystallization as Figure 13, 14, 15, 16 and 17 respectively. Similar plots are shown for Krystallization peaks as Figure 18, 19, 20, 21 and 22 respectively.

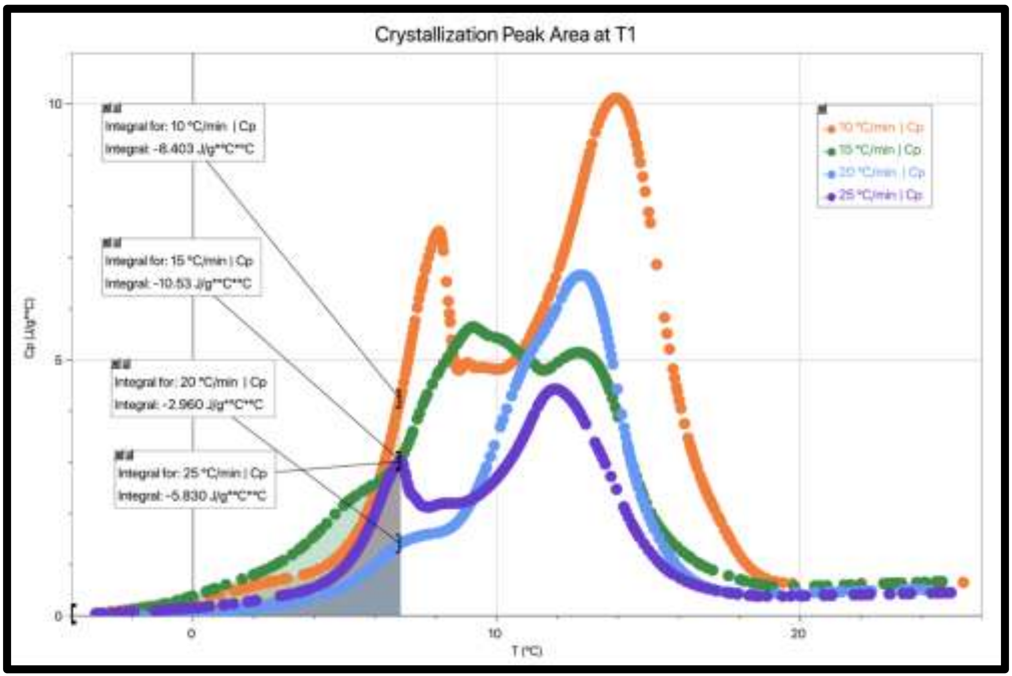

Figure 13: Zoomed in peaks of all Crystalline peaks at all ramp rates showing peak area at T1.

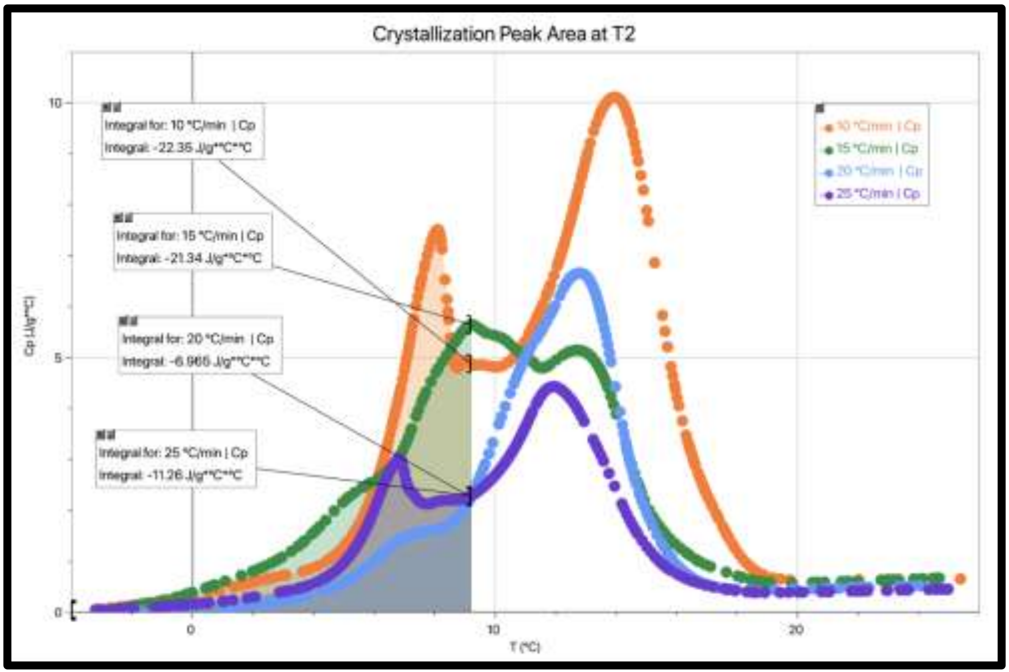

Figure 14: Zoomed in peaks of all Crystalline peaks at all ramp rates showing peak area at T2.

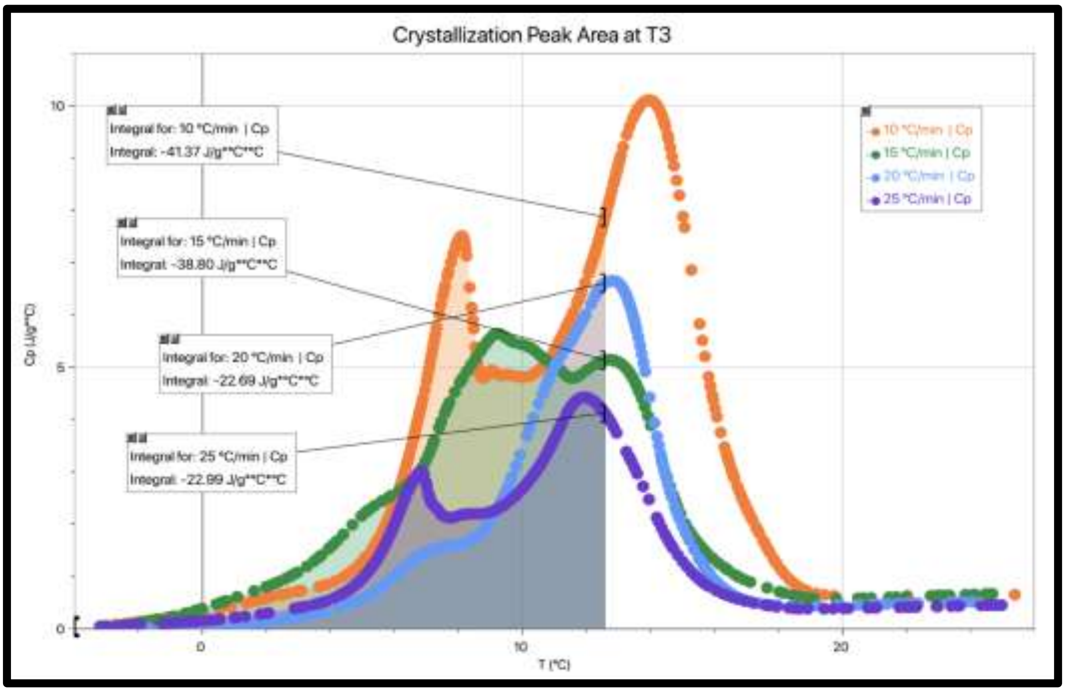

Figure 15: Zoomed in peaks of all Crystalline peaks at all ramp rates showing peak area at T3.

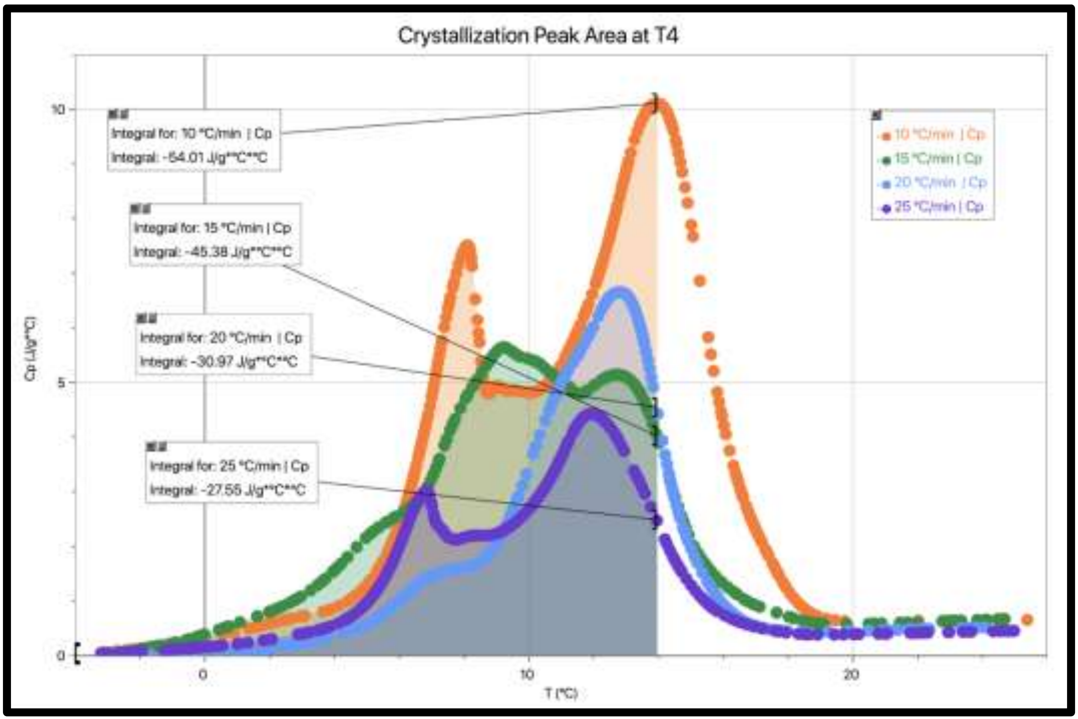

Figure 16: Zoomed in peaks of all Crystalline peaks at all ramp rates showing peak area at T4.

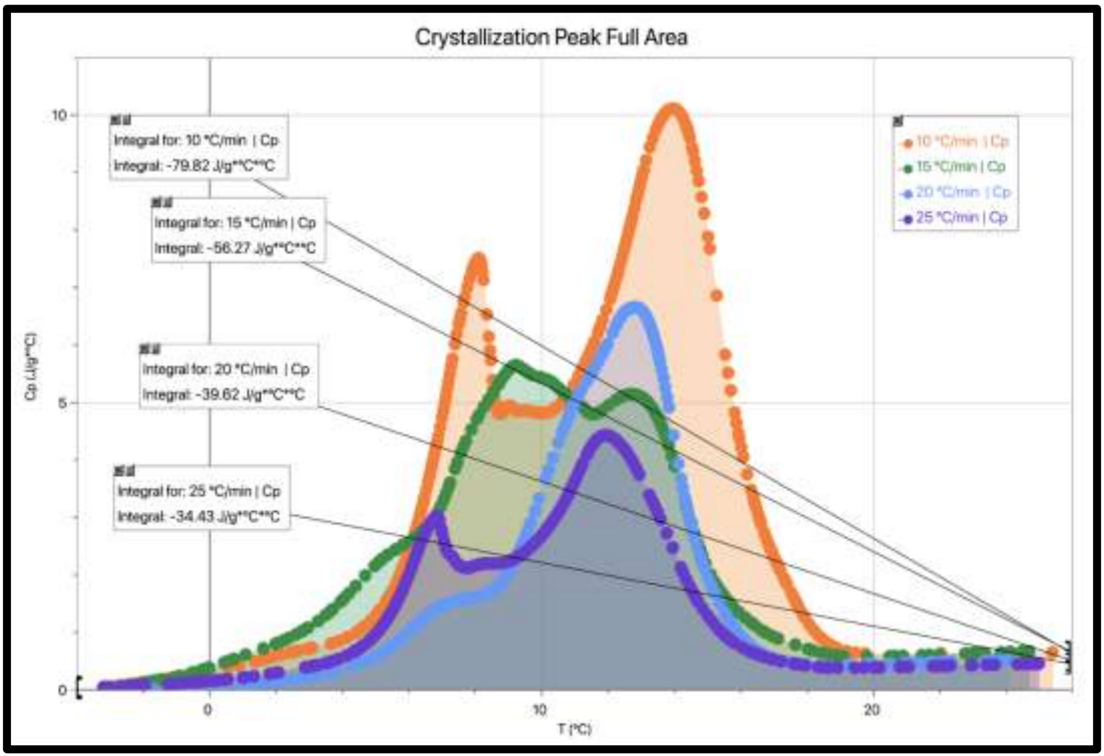

Figure 17: Zoomed in peaks of all Crystalline peaks at all ramp rates for showing full peak area.

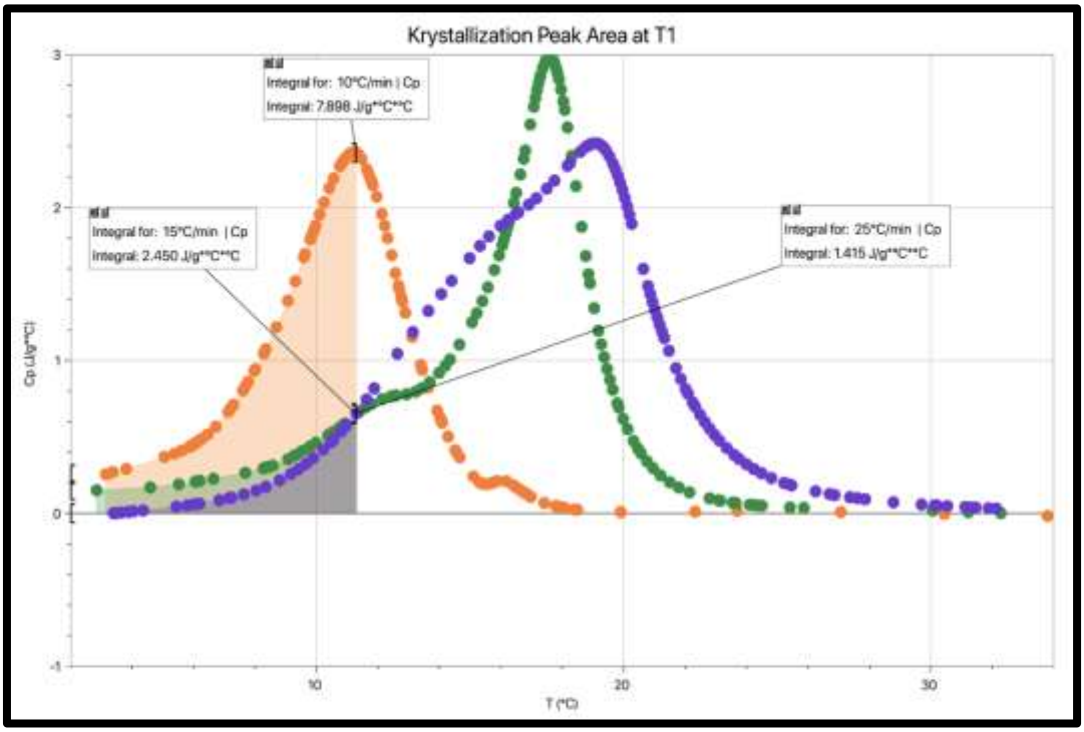

Figure 18: Zoomed in graph of mixed solid-state peak with area taken at T1.

The same process was applied to the Krystallization phase transition peak that occurred during heating for runs 2, 3, and 4. As mentioned before, run 1 did not have a heat Krystallization peak and is therefore the reason the ramp rate skips from 15 to 25. The partial areas were taken first and then the full area was found at the end, shown in Figure 18, 19, 20, 21 and 22 respectively.

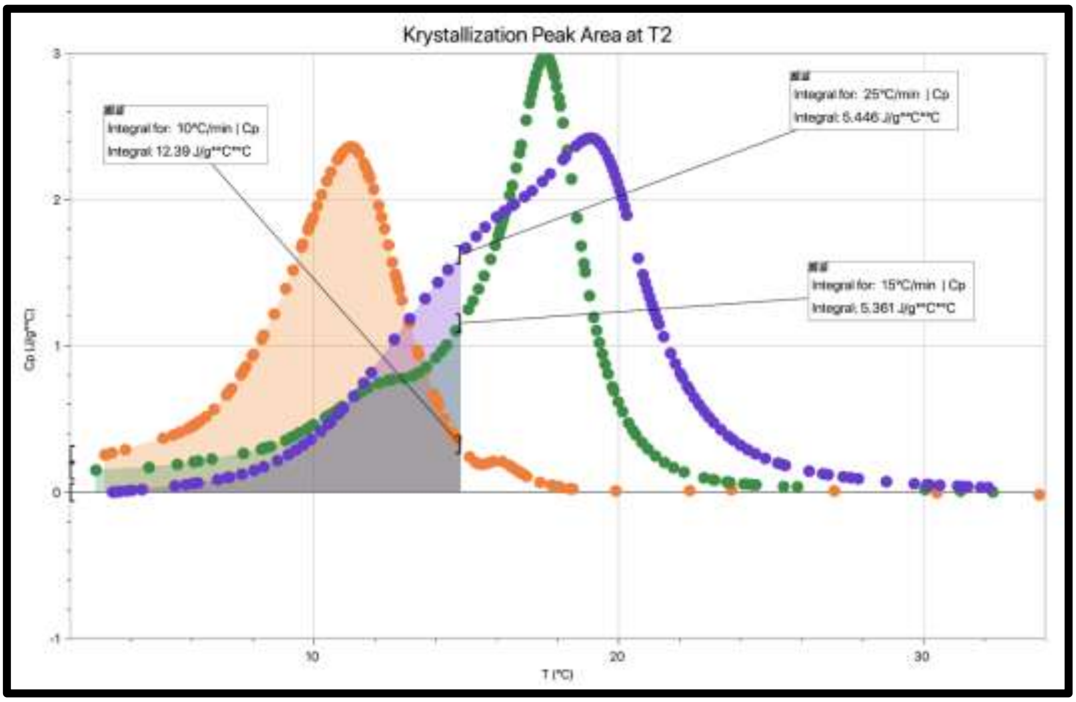

Figure 19: Zoomed in graph of Krystalline peak for all runs with area found under the curve until T2.

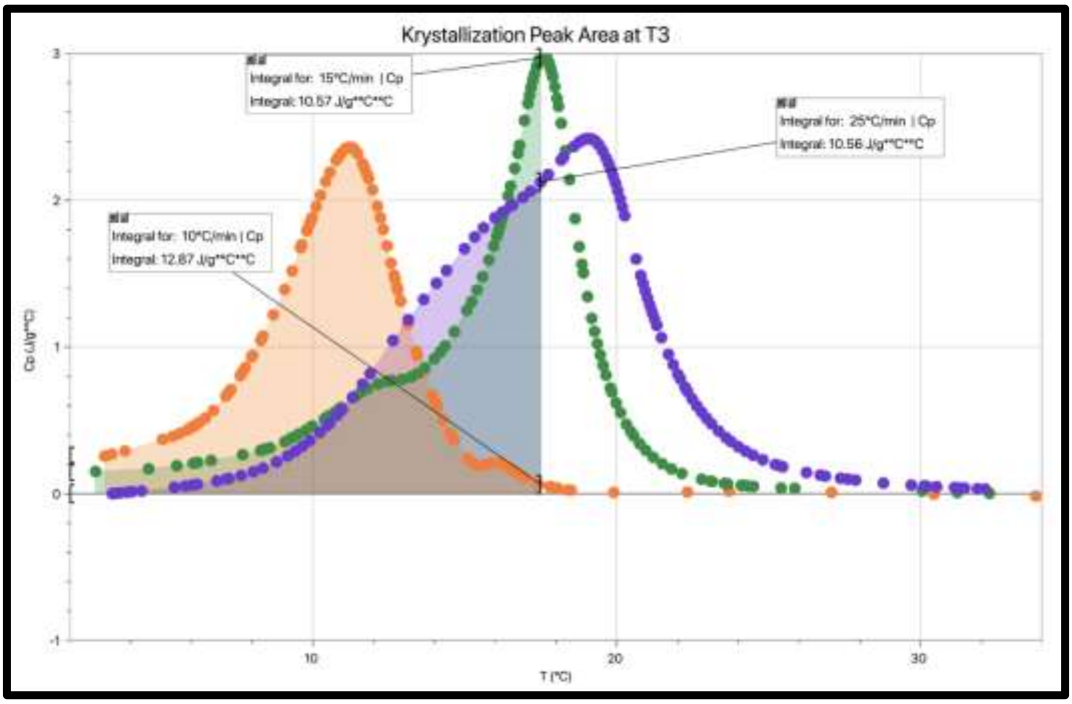

Figure 20: Mixed solid-state peak of all rates with integration until T3.

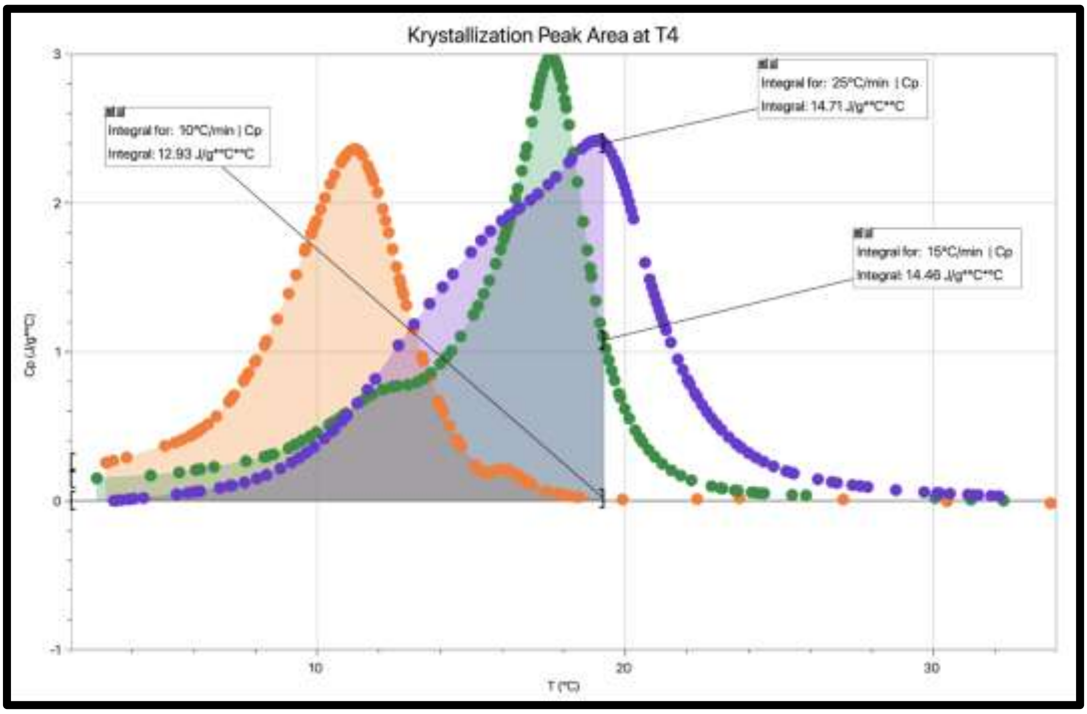

Figure 21: Mixed solid state or Krystalline heat peak of each rate with area found up until T4.

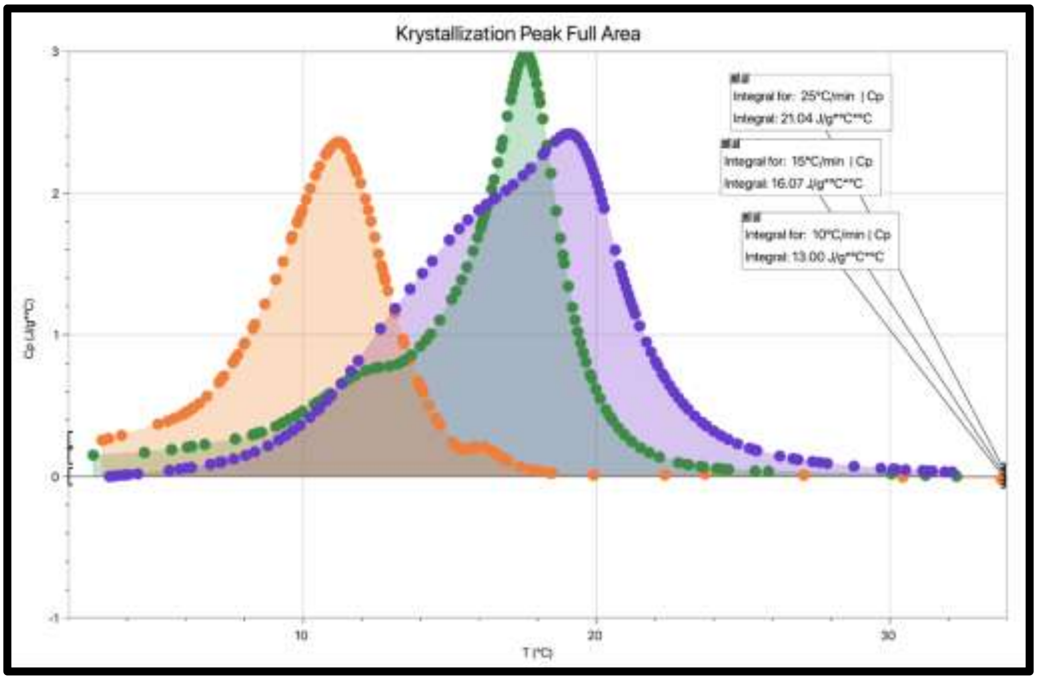

Figure 22: Krystalline or mixed solid-state peak of each rate with full integrated area.

IV. Data Tables:

The area under the peak was found using LoggerPro and the ‘peak integration’ action under the analysis tab. The area under the curve is equal to the enthalpy of the transition. The enthalpies have been split into whether they occurred during heating or cooling. For example, HK denotes the enthalpy for the Krystallinepeak that occurred during heating and HC is enthalpy occurring in cooling for Crystallization whereas HM is the enthalpy for Melting. These data details can be seen in the Table # 1.

Table 1: The details of Enthalpy of Krystallization, Melting and Crystallization of 5OCB as function of ramp rates.

Rate (℃/min)	HK (J/g)	HM (J/g)	HC (J/g)
10	13.00	146.37	79.82
15	16.07	150.87	56.27
20	N/A	158.05	39.62
25	21.04	158.24	34.43

The enthalpy of the Krystallization peak, melting peak, and crystallization peak are recorded in Table 1. The enthalpy has a unit of Joules/gram, and the rate remains as °C/min. Organizing the enthalpies based on rate allows for any trend in behavior to be observed. The melting transition and the Krystallization transition had enthalpies that increased with the rate; the crystallization transition during cooling had enthalpies that decreased as the rate increased.

Table 2: Crystal growth and percent crystallinity of both types of crystallization of 5OCB for all ramp rates.

Rate (℃/min)	Crystal Growth GK (J/g)	Crystal Growth GC (J/g)	% Crystallinity for K	% Crystallinity for C	% in Amorphous State after Heating	% in Amorphous State after Cooling	Increase in % Crystallinity from cool to heat
10	13.0	79.8	91.2	29.7	8.8	70.3	61.5
15	16.1	56.3	89.3	51.1	10.7	48.9	38.2
20	N/A	39.6	-	66.1	-	33.9	-
25	21.0	34.4	86.7	72.0	13.3	28.0	14.7

Table 2 analyzes the Krystallization peak from heating and the crystallization peak from cooling and how this affects crystal growth and percent crystallinity as the rate increases. The percent crystallinity between the crystallization cool peak and the Krystallization heat peak is compared in the last column by displaying the percent change in crystallinity from heat to cool. Crystal growth increases with rate during the heat Krystallization but decreases during the cool crystallization. The opposite is true for percent crystallinity, in which this value increases for crystallization but decreases during Krystallization.

Since 5OCB is not fully crystallized after each cool and heat, there is some part of the material left as non-crystalline or partially crystalline. The partially crystalline 5OCB gets more crystalline when heated 2nd or for further heating. This indicates that 5OCB molecules get more organized by releasing heat from 2nd heat after cooling. Hence the percent of material that is not crystalline can be compared with amorphous material or non-crystalline material that is also shown in the Table 2. The percent difference in percent crystallinity from heat to cool is also shown in the same table as how much percent crystallinity increased from cool to heat and from Table 2 that percent crystallinity in 5OCB has increased from cool to heat but it decreases as ramp rate increases.

Table 3: The degree of crystallization of the cool crystallization peak (C) that appeared in cooling of 5OCB at four different temperatures from T1 to T4.

Rate (℃/min)	T1 = 6.8 ℃ *alpha*$_{T1}$	T2 = 9.2 ℃ *alpha*$_{T2}$	T3 = 12.5 ℃ *alpha*$_{T3}$	T4 = 14.0 ℃ *alpha*$_{T4}$
10	0.175	0.337	0.583	0.698
15	0.241	0.418	0.704	0.795
20	0.153	0.260	0.619	0.768
25	0.226	0.379	0.697	0.796

The degree of crystallization for the cool crystalline transition is recorded in Table 3, along with the ramp rate and temperature at which the area under the curve was found. Each crystallization peak from each run had a partial area found at the temperature points shown in the table. This partial area was then divided by the full area of the peak.

Table 4: The degree of crystallization of the heat Krystallization peak (K) that appeared in heating of 5OCB at four different temperatures from T1 to T4.

Rate (℃/min)	T1 = 11.3 ℃ *alpha*$_{T1}$	T2 = 14.8 ℃ *alpha*$_{T2}$	T3 = 17.5 ℃ *alpha*$_{T3}$	T4 = 19.3 ℃ *alpha*$_{T4}$
10	0.608	0.953	0.990	0.995
15	0.153	0.334	0.658	0.899
20	-	-	-	-
25	0.067	0.259	0.502	0.699

The calculated alphas for the heat Krystallization phase transition are recorded and shown in Table 4, with the corresponding ramp rates in the first column. Run 1, or the run with a ramp rate of 20 ℃/min, did not have this peak in heating so it could not be analyzed. The data that relates to this table are Figures 18-22.

Table 5: The presence of the order parameter (n) of cool Crystallization peak (C) that appeared in cooling of 5OCB at four different temperatures.

T (℃)	11.3 ℃	14.8 ℃	17.5 ℃	19.3 ℃
n	0.1715	0.1269	0.3256	0.3532

Table 5 uses the temperatures at which the partial areas of the cool crystallization phase transition were taken and compares them with the slope of the resulting graph plotted in Figure 23. The n parameter is the slope of the graph between the natural log of the rate and ln ln (1-alpha)^-1, the alphas found in Table 3.

Table 6: The presence of the order parameter (n) of heat Krystallization peak (K) that appeared in heating of 5OCB at four different temperatures.

T (℃)	6.8 ℃	9.2 ℃	12.5 ℃	14.0 ℃
n	2.793	2.452	2.009	1.605

Table 6 uses the temperatures at which the partial areas of the heat crystallization phase transition were taken and compares them with the slope of the resulting graph plotted in Figure 24. The n parameter is the slope of the graph between the natural log of the rate and ln ln (1-alpha)^-1, the alphas found in Table 4.

V. Discussion:

To understand the results of 5OCB liquid crystal shown in the result section, the data obtained in Table 3 and Table 4 are used to follow equation # 4 and "Johnson-Mehr-Avarami Law" [17-20] to plot Figure 23 and Figure 24 to find order parameters of Krysllization and Crystallization peaks using values of degree of crystallization as function of ramp rates at different temperatures. These figures are compared to the equation of a line to find slope of the lines that gives the value of n for both types of crystallization of 5OCB. The values of order parameter (n) are reported in Table 5 and Table 6. Figure 23 and Figure 24 can be seen below.

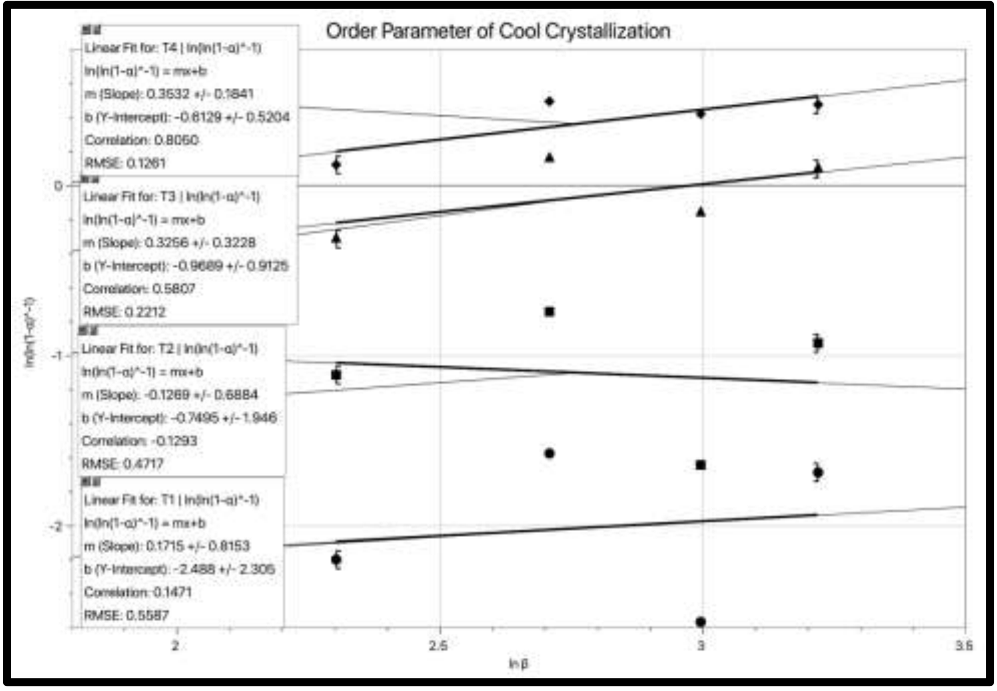

Figure 23: Finding order parameter (n) for Crystallization using equation # 4 and data table 3.

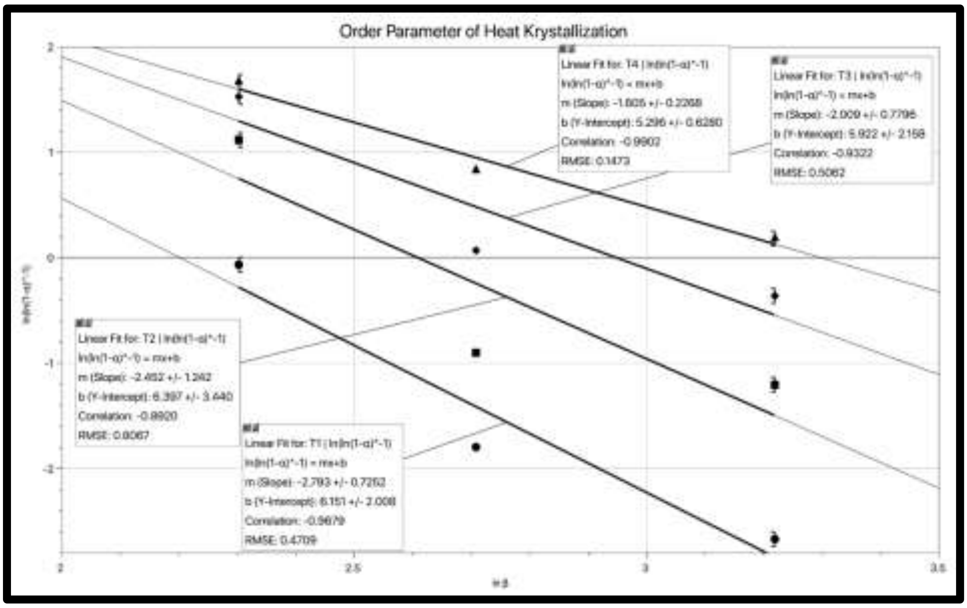

Figure 24: Finding Order parameter (n) for Krystallization using equation # 4 and data table 4.

The order parameters for the Crystallization and Krystallization plotted in Figures 23 and 24 are the natural log of the ramp rate on the x-axis while the alphas, found in Table 3 and 4, have been transformed for the y-axis. The alpha value was subtracted from 1 and then raised to the -1st power. The natural log of this product was then taken twice and used for the y-axis. The linearized data has a trendline fit to it and the slope of these trendlines is the order parameter for that temperature.

The values of order parameters (n) for both types of crystallizations of 5OCB as reported in Table 5 and Table 6 are then plotted as summary graphs in Figure 25 and Figure 26.

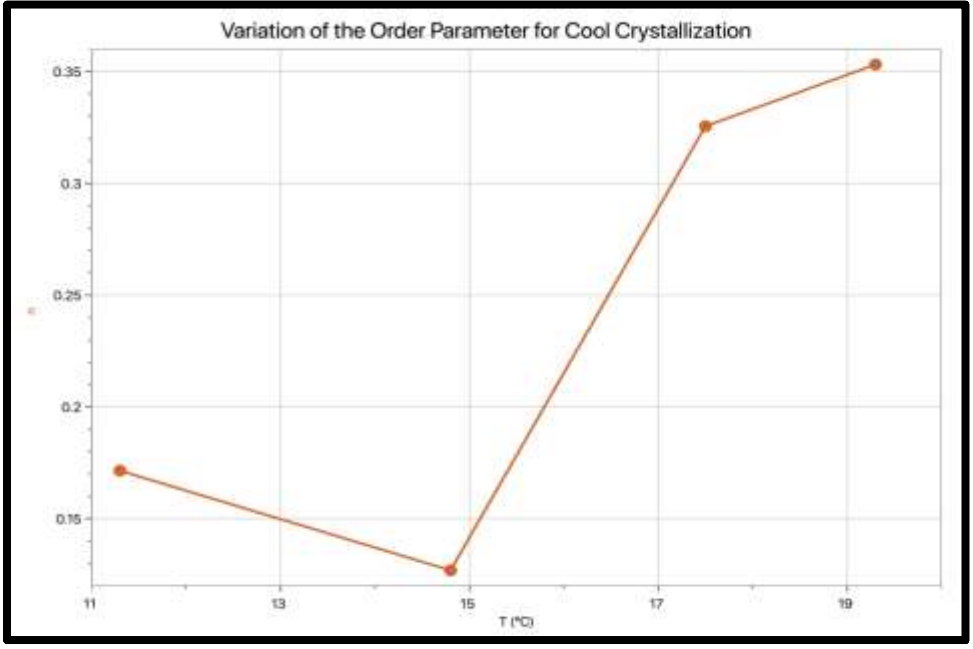

Figure 25: The order parameter (n) of the cool crystallization as a function of temperature (T).

The order parameter of the cool crystallization phase transition as a function of temperature shown in Figure 25. The value of n increases on average as a function of temperature but stays within the numerical value of 1. It indicates that cool Crystallization is more linear than dynamic and stays almost constant as a function of temperature.

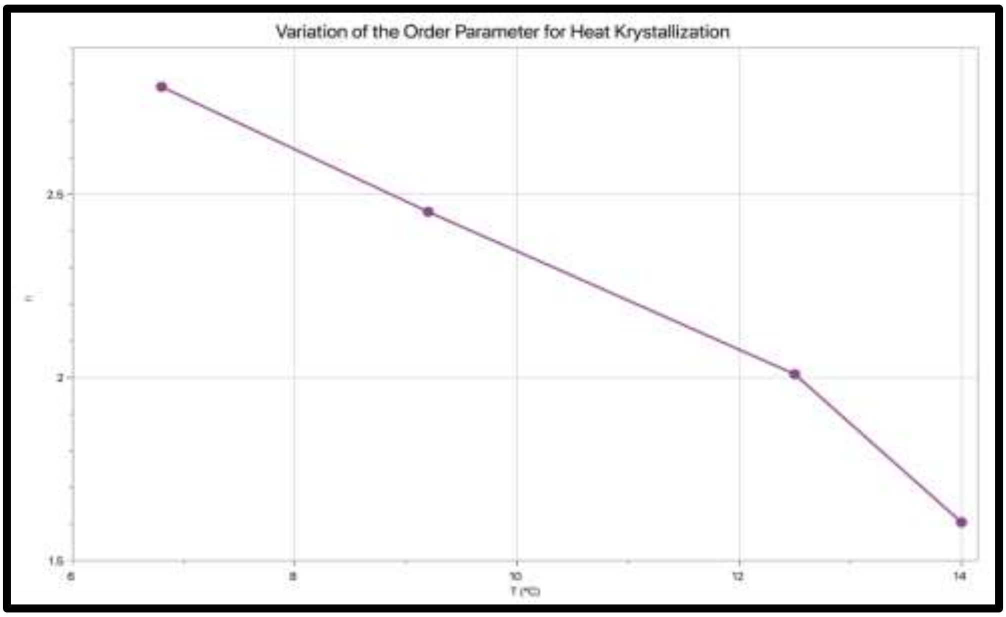

Figure 26: The order parameter (n) of the heat Krystallization as a function of temperature (T).

Figure 26 is a result of the data displayed in Table 6; it shows how n varies as a function of temperature for Krystallization. As temperature increases the value of n goes down but stays above 2. This indicates that the order of reaction of Krystallization is dynamic and changes with temperature and reheating.

The crystalline nature of 5OCB liquid crystal can be explained by its molecular behavior of orientation, alignment, and arrangement. When 5OCB is in 100 percent crystalline ordered state before it is heated and then when it is heated, it gets thermal energy, absorb energy in terms of endothermic peaks of DSC and then go to melt state which makes them into a completely disorganized state - isotropic state. Then when they are cooled from their melting state to a solid state, the molecules start releasing thermal energy and go back to an organized state,but they cannot reach their 100% ordered state after their first heat and cool. They get a partially crystalline state where some molecules are in an ordered state, but some are in a disordered state. This happens because of the high cooling rate that makes them go to a mixed solid state where they have some percent crystalline and some percent amorphous. Now, when 5OCB is heated the 2nd time, some molecules that were under amorphous state, form an unorganized structure, not ordered structure as shown in our model by Figure 27. They release some thermal energy, and the unorganized molecules get organized. Now 5OCB is in a more crystalline state than what it was before post-cooling. When 5OCB is continually heated and cooled multiple times, the process of molecular arrangement changes frequently from organized to unorganized, more crystalline to less crystalline, and hence 5OCB starts showing double peak in cooling when it goes to partial crystalline state. It is an indication of having two energy levels in its molecules as a semi-crystalline or partially crystalline state. The 5OCB also shows that Krystallization is more dynamic than Crystallization as it shows a highly organized molecular state of 5OCB with higher percent crystallinity.

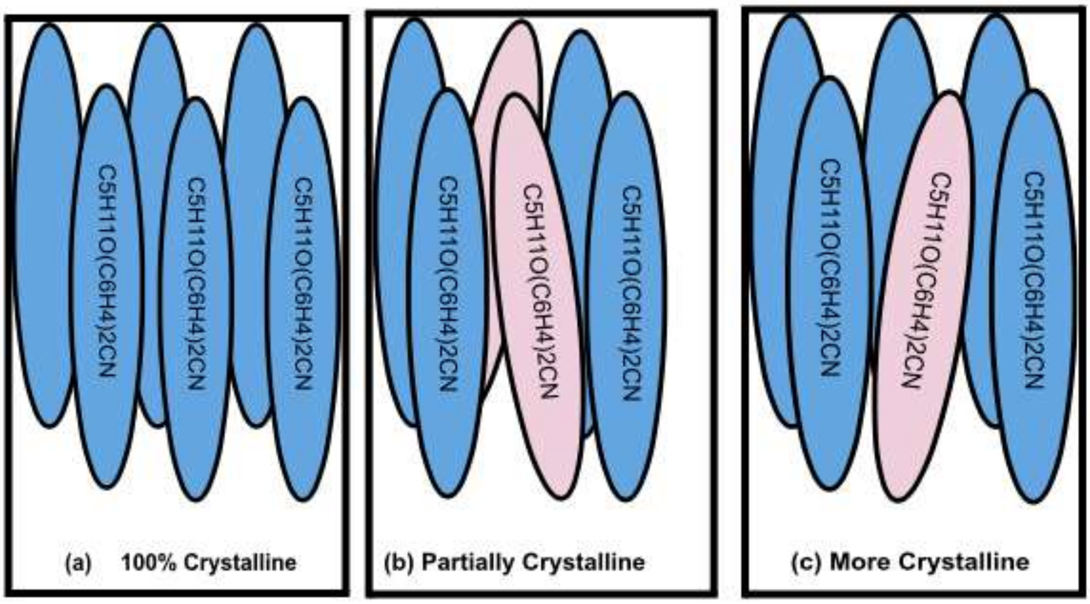

Figure 27: Drawing of molecular arrangement of 5OCB when they are partially crystalline, more crystalline, and fully crystalline.

Figure 27 attempts to explain the different stages of crystallization in the 5OCB molecule, while also showing its chemical formula and the rod-like shape of the liquid crystal. A perfect crystal, like a clear and hard diamond, is 100% crystalline; all the molecules of this substance are organized and neatly packed together. Once the molecules gain energy, one of the molecules may become excited and start to move, losing its orientation and structure. Even though one of the molecules is excited, the substance is in a more crystalline state. As more energy is gained further, more molecules may join the excited molecule and lose its rigidity. Most of the molecules are still neat and organized, however, a few are not. This state would be partially crystalline and most resembles the state of 5OCB before the heat Krystallization peak.

It is seen from data that were analyzed from the graphs plotted in the result section that 5OCB has higher percent crystallinity after heat crystallization than cool crystallization. It is also seen that the presence of non-crystalline 5OCB decreases as it is heated again and again. As ramp rate increases, fast heating and cooling takes place and hence 5OCB molecules show crystal growth in cooling and crystal shrink in heating. The degree of crystallization at different temperatures shows the order parameter and order of nucleation and growth process of 5OCB molecules. It is found that Krystallization show higher order parameter than Crystallization and indicates the presence of crystal dynamics in 5OCB. These types of results may make 5OCB significant in the crystal industry where 5OCB can be used for heating and cooling types of crystals or making jewelry.

VI. Conclusion:

Crystallization is a process that shows how molecules of crystals get organized and follow a long range ordered pattern when they get cooled and go back to crystal form. Since Liquid Crystals show multiple phase transitions between crystalline and liquid, our interest is to study detailed behavior of crystallization of pentyl-oxy-cyanobiphenyl (5OCB) Liquid Crystal. The 5OCB shows two types of crystallization when it is heated and cooled. It shows an exothermic peak in cooling for a cool crystallization, and one heat crystallization that appears from 2nd heat and onwards as an exothermic peak on heating. We call the heat crystallization as Krystallization(K) and Crystallization (C) to cool crystallization. It is observed that as ramp rates increase, the C grows and K shrinks. The 5OCB becomes partially crystallized after each cooling run and gets more crystalline after every heat run when it gets K from the 2nd heat. The percent crystallinity is higher for K than C. The degree of crystallization of each K and C crystallization changes with temperatures. The K has higher order parameters than C. The range of order parameters for K is above 2 whereas for C is less than 1. This can be explained in terms of molecular arrangement and molecular behavior of 5OCB. The 5OCB has an oxygen that gives more weight and makes it stable. As 5OCB is heated multiple times, it releases thermal energy and gets more organized with higher percent crystallinity and higher order parameters whereas 5OCB shows partially crystalline state after it is cooled to lower temperatures with increase in crystal growth when ramp rates are increased. These types of study can make 5OCB useful in the crystal industry to be used in the form of temperature dependent crystalline material.

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