International Journal of Research in Engineering and Science (IJRES)
ISSN (Online): 2320-9364, ISSN (Print): 2320-9356
www.ijres.org Volume 10 Issue 9 ǁ September 2022 ǁ PP. 197-217

Details of Nematic Phase Transition and Nematic Range of 5OCB Liquid Crystal 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:
Liquid crystals (LCs) have been implemented in recent technology in order to increase the efficiency of a device. These LCs are used in their nematic states in Liquid Crystal Display (LCD) screens to display high resolution images. Mostly the 8CB liquid crystal is used in LCDs. The 5OCB liquid crystal is rarely seen in LCDs today. The n-alkoxy-cyanobiphenyl (nOCB) is a family of LCs that contain oxygen, two biphenyl rings, and a cyano group. The pentyl-oxy-cyanobiphenyl (5OCB) is the youngest member of this family with the shortest carbon chain. In this research, we are reporting detailed significant results of nematic phase transitions and nematic range for heating and cooling of 5OCB. The data for heating and cooling of 5OCB is obtained from Differential Scanning Calorimetry (DSC). The sample of 5OCB was heated from -40 ℃ to 80 °C and then cooled from 80 °C to -40 °C four times. Our interest is to see how multiple heating and cooling of the same sample of 5OCB can change its phase transitions and the effects on its nematic phase transition and nematic range. The nematic phase transition and nematic range are the important parts of LCD where LCD specifically works. It is found that the nematic range increases in cooling when compared with its nematic range in heating.
Keywords:*Liquid Crystals, Nematic, Isotropic, Phases, Nematic Range, Differential Scanning Calorimetry, LCD, Heat Flow, Specific Heat Capacity, Endothermic, Exothermic, Thermodynamics, Enthalpy, Peak Integration, 1st Derivative, 2nd Derivative, Temperature, LoggerPo.*

Date of Submission: 02-09-2022 Date of acceptance: 15-09-2022

I. Introduction:

Liquid crystals (LCs) are unique materials to study due to the fact that they exist between solid and liquid, two common states of matter. They share some aspects of the liquid state and some aspects of the solid state. At cooler temperatures, an LC will present itself in a more solid/crystalline structure with long range ordered organization. At high temperatures, the LC will be in a liquid or 'isotropic' state with no organizational structure of molecules. At middle temperatures, the LC is in any intermediate states i.e smectic A/C or nematic state which falls between the crystalline solid and isotropic liquid state. [1-3]

There can be several types of LCs in the world, n-alkyl-cyanobiphenyl (nCB) LCs have drawn more attention in research and applications due to its use in the electronic and physical world. The typical three states of nCB LCs are solid crystalline state, a nematic state, and an isotropic state. In the solid crystalline state, the LC's molecules are packed close together and fully organized. The nematic state begins to have less order and organization; the molecules display short-range order which means some molecules are organized neatly but not all are organized the same. The molecules progress to a completely disorganized isotropic state. Some LCs also show a Smectic A or smectic C phase before going to the nematic phase and then the isotropic phase. Like the nematic phase, it is less organized and has short range order, but now the molecules will be grouped together in layers. These layers become tilted on an axis when it reaches smectic C phase. Finally, the isotropic phase is the liquid phase. This is the least organized phase with no order, no layers, and the flexibility to slip past each other. [2-4] Due to having several atoms in the molecule and more than one functional group, the LC molecule looks like a rod or oval shaped molecule. The typical structure and molecular alignment in different states from solid to liquid state of a LC can be seen in Figure 1.

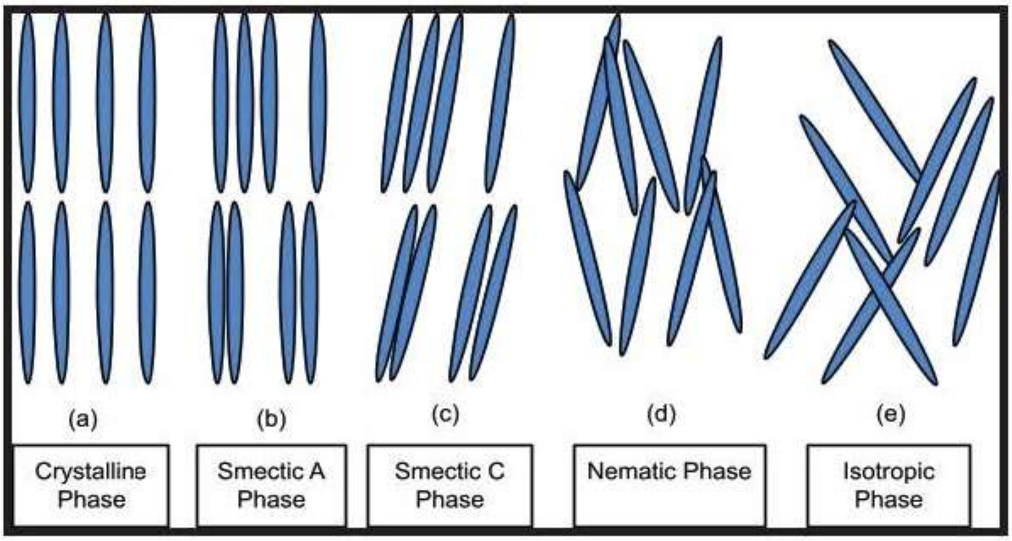

Figure 1: The molecular arrangements of a typical liquid crystal: the crystalline phase (a), smectic A phase (b), smectic C phase (c), nematic phase (d), and isotropic phase (e).

Octyl-cyanobiphenyl (8CB) has been studied a lot in the past and has been used in world applications for decades [4]. Whereas other members of LC, classified as alkyl-oxy-cyanobiphenyl (nOCB), showed less study in literature. [5-8] The youngest member of nCB is pentyl-cyanobiphenyl (5CB) and it is studied by some authors so far, [7-9] whereas the youngest member of nOCB, pentyl-oxy-cyanobiphenyl (5OCB) has not been studied much in literature as of yet. The 5CB liquid crystal has a tail consisting of 5 carbons connected to two phenyl rings; the head of this molecule is an amine. Whereas the 5OCB has almost the same structure but its 5-carbon tail is connected to an oxygen which then connects to the phenyl rings. [5-9] The molecular structure of 5CB and 5OCB is compared in Figure 2.

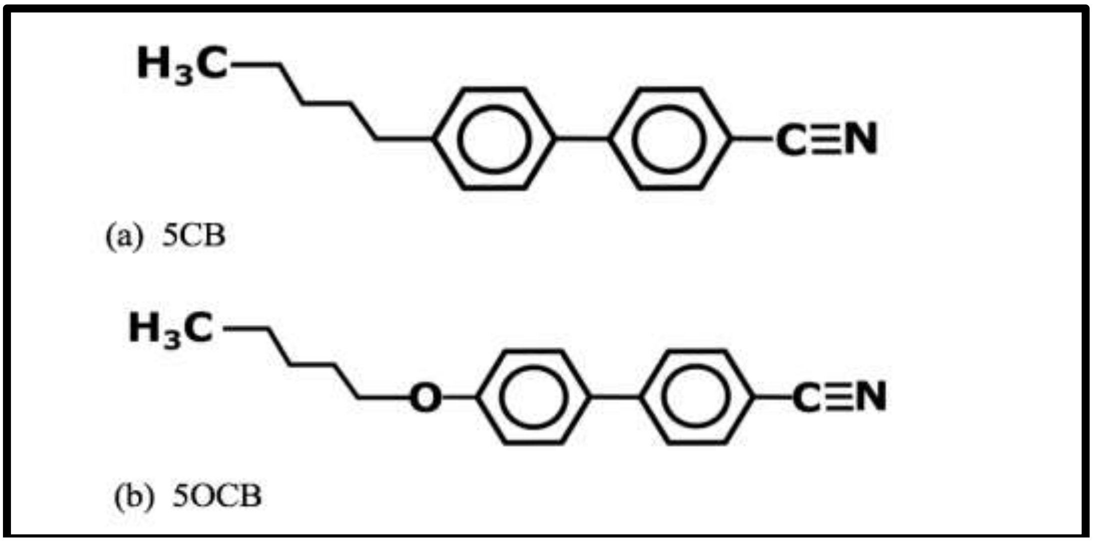

Figure 2: The molecular Structure of the (a) 5CB and (b) 5OCB liquid crystals.

The two liquid crystals have an identical number of carbons in its tail, being 5; the two structures are also similar with their biphenyl rings and cyano group heads. The main difference between the molecules can be seen easily as 5OCB has an oxygen in between the tail and rings.

Our interest is to study detailed behavior of 5OCB, as it has not been sufficiently studied in the past and find out its hidden facts. Since 5CB has been studied by some authors recently, a comparative study parallel to those studies of 5CB can be seen with 5OCB in this paper. [5-9]

To find detailed results of the 5OCB LC, the data taken from the Differential Scanning Calorimetry (DSC) is used for this paper. DSC is an instrument that is used to analyze types of material in research, to see their thermal behavior and types of transitions and phases they have. The instrument works by heating a sample by a certain rate (℃/min) to see how much heat flow passes through them in terms of peaks and dips. After heating, the sample is cooled using the same rate. The DSC graphs obtained as a result of heating and cooling are represented as heat flow versus temperature, showing details of the types of phases of the material. [10] We are using the DSC technique to gather data of 5OCB for this paper and find more details of how 5OCB can be used in the technical world.

In the real world, people use research results of LCs in the smart devices that are called Liquid Crystal Display (LCD) to get better resolution images in LCD TV, LCD smart watch or laptops. An LCD screen is a thinner alternative to CRT screens, which made technology bulky in the past, because it housed the cathode ray tube. LCD screens are thinner and more efficient; they take a thin layer of nematic LCs on two plates and press them together. Light is shown from behind the screens and images are made in the nematic range of LCs. LCDs have been integral in the development of 'smart technology' meaning the technology is more efficient and compact than previous versions. [11-13] Scientists and engineers use LCs in the nematic state and use nematic range for smart devices in their application. It is important to know the details of the nematic state and how long the nematic range is for the LC that is being used in LCDs. [11-13] So, to find whether 5OCB is useful for LCDs or not, this research is focused on detailed results of the nematic phase and nematic range of 5OCB. The data of the transitions found from DSC are analyzed using the Logger Pro data analysis software tool in this paper.

LoggerPro is a software that graphs data and performs analysis on the graphical data produced. It allows for a user to create their own data columns in a data table and then graph the data for visualization. LoggerPro has built in analysis tools like 'peak integration' which can quickly find the area under a curve. Most students are introduced to LoggerPro through their physics course in colleges because it also has the ability to track and graph data from a video by tracking, however it is a useful software that can be used in research. Our other goal of this research is to see if Logger Pro fit to analyze research data to find more interesting details of LCs and 5OCB. [10-13]

Experimental Section:

Pure sample of 5OCB liquid crystal is used to run a Differential Scanning Calorimetry (DSC) instrument from TA instruments, model number MDSC 2920, in the Chemistry and Biochemistry department of WPI in order to study its phase transitions. For DSC experiments, a small amount of 5OCB is loaded into pans and sealed with lids and placed inside a DSC instrument for heating and cooling. The sample of 5OCB is then heated from -40 °C to 80 °C and then cooled from the same temperature, 80 ℃ to -40 °C. with a constant heating and cooling rate. The DSC instrument is calibrated before the start of the experiment. The data is collected from DSC as flow of heat as a function of temperature.

The results of DSC data show that 5OCB shows some endothermic peaks on heating and then some exothermic peaks on cooling. The DSC runs are repeated to see accuracy of these peaks and are found the same as before for the same rates. The sample of 5OCB is then reheated three more times to see the effect of reheating and cooling just after each heating run. The idea of this procedure is to see how 5OCB behaves when it is heated and cooled multiple times. Some additional peaks are found on the 2nd, 3rd and 4th heating and cooling. More details of these peaks will be shown in our next paper.

Theory and Molecular Details:

This research involves Thermodynamics of liquid crystal and theory of DSC instruments.

<u>Using DSC Theory and Thermodynamics:</u>

$dQ/dt = m*Cp*dT/dt$ (1)

Equation 1 is the heat flow from DSC. Here Q, t, m, Cp, T are heat, time, mass, specific heat capacity, and absolute temperature respectively. dQ/dt and dT/dt are heat flow and heating rate respectively.

$(1/m)*(dQ/dt) = Cp*(dT/dt)$ (2)

Equation 2 shows the calculation for normalizing heat flow, with the mass of the material from equation 1 plugged in equation 2 which is used in DSC.

$[(1/m)*(dQ/dt)]/(dT/dt) = Cp$ (3)

Equation 3 shows the specific heat capacity calculation of the sample from DSC.

$\mathbf{Cp = [(1/m)*(dQ/dt)]/(dT/dt)}$ (4)

Equation 4 shows the rearranged equation 3 for the specific heat capacity equation for DSC runs.

Units used for each term in these equations are given as: dQ/dt in Watt = J/s, it can also be called heat flow in mW. After normalizing the heat flow by the mass of the sample, the heat flow = W/g. The unit of the specific heat capacity = J/g℃. Mass is in g, time is in s, and temperature can be in K or ℃.

We are focusing on details of the nematic phase transition of 5OCB LC in this paper and comparing it with the 5CB nematic phase as published by other authors. [7-8] The chemical formula of 5CB and 5OCB can be seen in Figure 3 showing how many carbons and how many functional groups there are in their molecules.

$$\text{(a)}\quad C_5H_{11} - (C_6H_4)_2 - CN$$

$$\text{(b)}\quad C_5H_{11} - O - (C_6H_4)_2 - CN$$

Figure 3:The molecular formula of (a) 5CB and (b) 5OCB liquid crystals where 5OCB has an Oxygen that is absent in 5CB.

The other interest of this research is to see how the presence of oxygen brings differences in the nematic phase when it is present in the molecule of 5OCB, compared to 5CB.

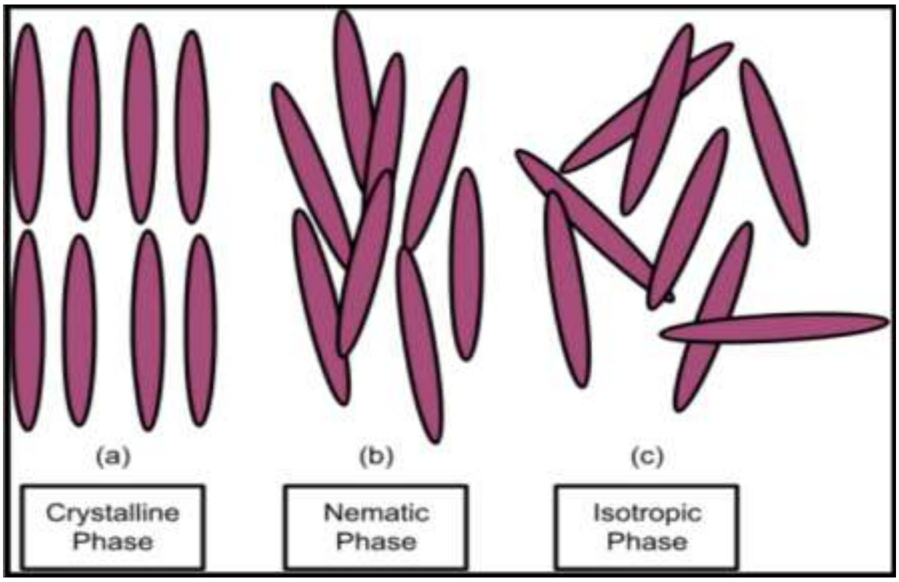

Figure 4: Molecular arrangement of 5OCB liquid crystal molecules in (a) Crystalline, (b) Nematic, and (c) Isotropic phases.

The phase states for 5OCB can be seen in the form of a drawing in Figure 4 that shows the molecular alignment of (a) Crystalline state, (b) Nematic state, (c) Isotropic state of 5OCB liquid crystal. 5OCB goes through just three phase changes when heated from crystalline to the isotropic state. 5CB also shows similar phase transitions as shown in Figure 4 except it doesn’t have any oxygen in its molecule.

II. Results and Discussion:

The small amount of 5OCB liquid crystal was run in DSC for heating and cooling from -40 ℃ to 80 ℃ and then back to -40 ℃. The DSC graph can be seen in Figure 5, which shows the heating and cooling of 5OCB. Figure 5 shows the first run in DSC for heat and cool at a rate of 20 ℃/min, with the sample being heated first and then cooled back down. The bottom of the graph shows the liquid crystal as it is heated, and the top of the graph shows the crystal as it is being cooled. The DSC data shows two endothermic peaks in heating and two exothermic peaks in cooling. These peaks can be named as a Melting peak (M), a Nematic peak (N) on heating, a Nematic cool peak (N), and a Crystalline peak (C) in cooling respectively. The peak temperature of these peaks can be considered as their peak values of the transition where these phase transitions occur to their 50% stage. The temperature ranges from one peak to another peak can be considered as the range of that phase. 5OCB stays in the solid crystalline state until the melting peak comes and then it changes to the nematic state; it stays in the nematic phase until the nematic peak comes and then it changes to the isotropic state which completely melts the state of 5OCB.

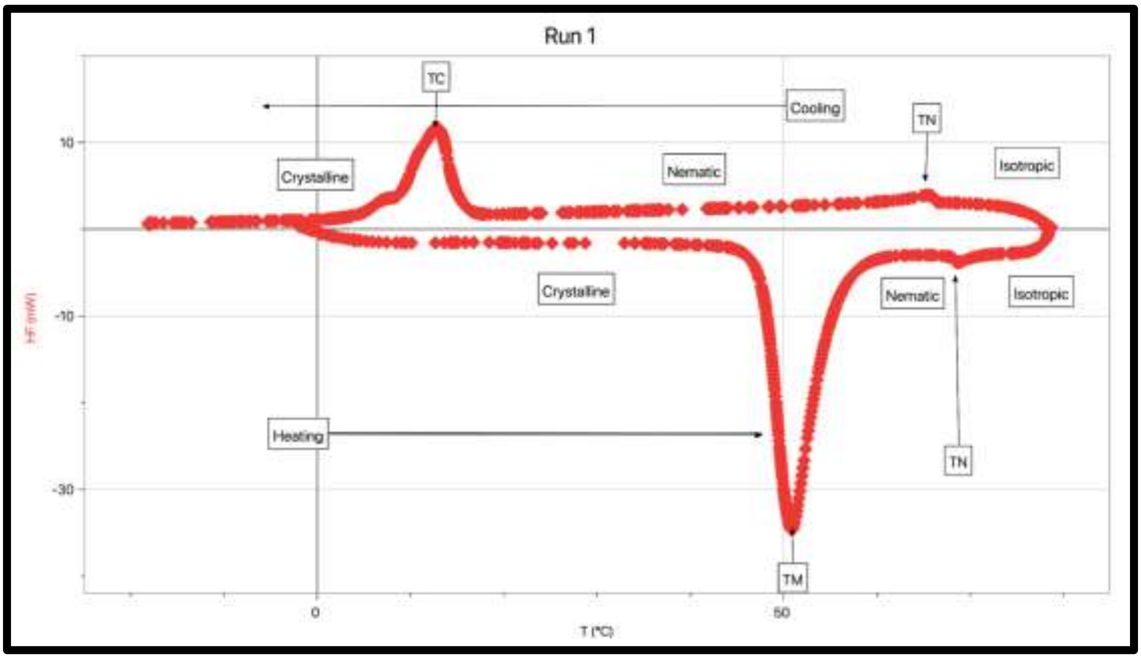

Figure 5: Heat and cool of 5OCB LC for the first run using the DSC plotted as heat flow Vs temperature plot.

The zoomed in graph of the first heating of 5OCB is shown in Figure 6, with the progression of state changes labeled. The normalized heat flow was calculated by dividing the heat flow recorded by the DSC by the sample's mass, which was 4.8 mg. The first run of heating and cooling shows the typical progression of a liquid crystal through its molecular arrangement: crystalline to nematic, nematic to isotropic, then isotropic back to nematic, and nematic back to crystalline. The peak temperatures for the melting, nematic peak is labeled as TM, TN, and TC respectively.

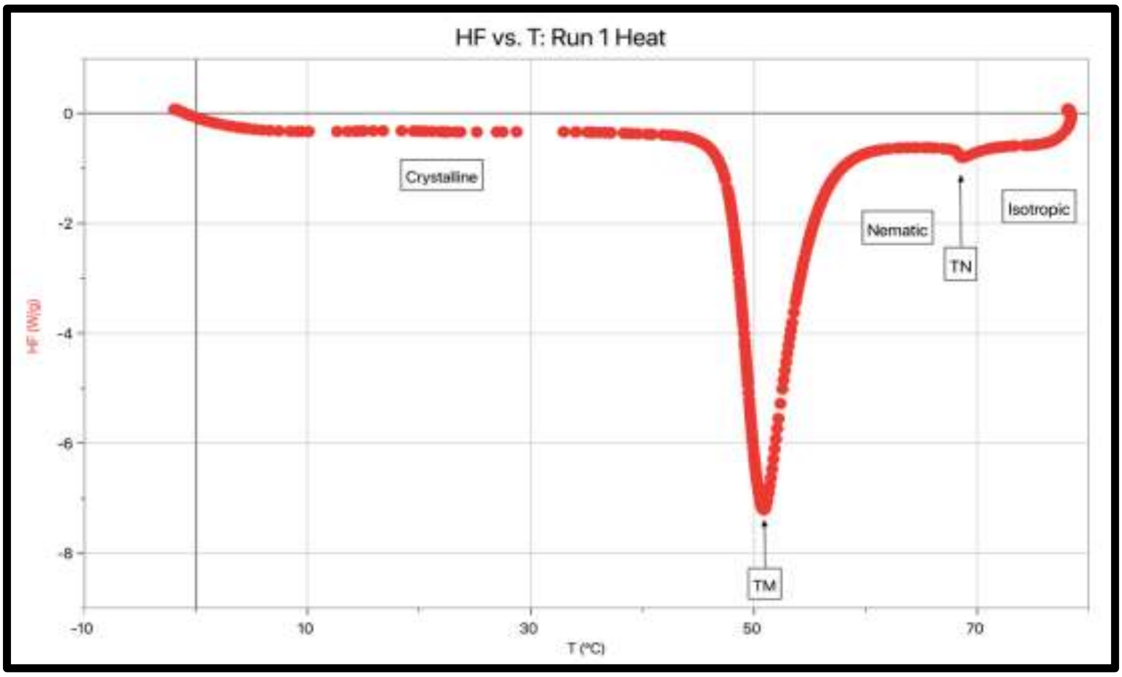

Figure 6: Normalized heat flow vs temperature plot for first Run for heating only.

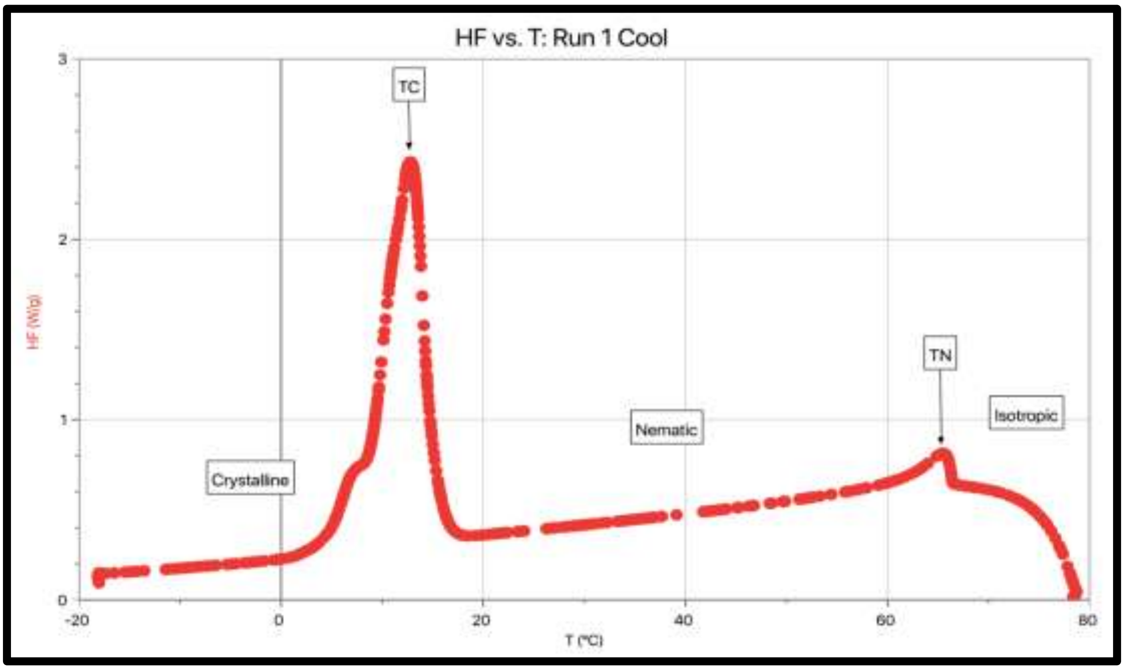

Figure 7: Normalized heat flow vs temperature plot for first run for cooling only.

The normalized heat flow calculated from run 1's cooling of 5OCB is shown in Figure 7 with essential peaks denoting a change in state being labeled. The three typical states of 5OCB are observed through the first run's graphs with the sample being cooled from isotropic to nematic and finally crystalline. The two peaks seen in the figure are the Crystalline peak (TC) and the Nematic peak (TN).

Using the normalized heat flow data discussed previously in the theory section, the specific heat capacity of each run could be calculated. Figure 8 shows the heat capacity vs. the temperature of the first heating of 5OCB using the DSC. The heat capacity was determined by multiplying the normalized heat flow by the reciprocal of the rate at which the sample was being heated and cooled. The specific heat capacity of run 1 is Figure 8.

Each run was broken into their respective heating and cooling portions. Figure 9 shows the cooling portion of run 1, with the specific heat capacity on the y-axis and the temperature on the x-axis. The normalized heat flow of run 1's cooling was multiplied by the reciprocal of the rate and then graphed in LoggerPro. All peaks and states of the LC are labeled in Figure 9.

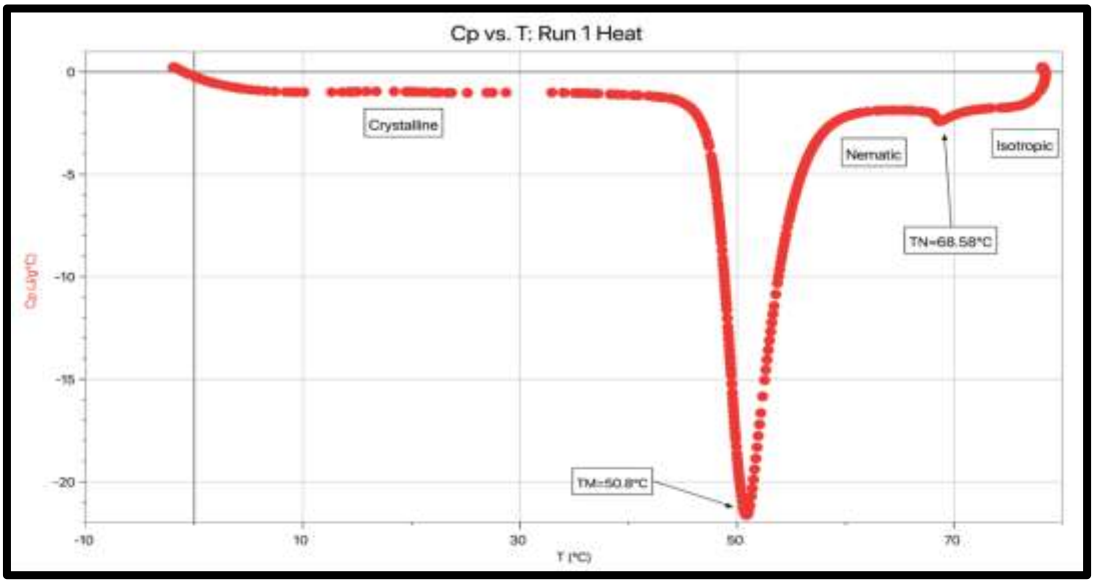

Figure 8: Specific heat capacity vs temperature plot for the first run for heating only with peak temperatures.

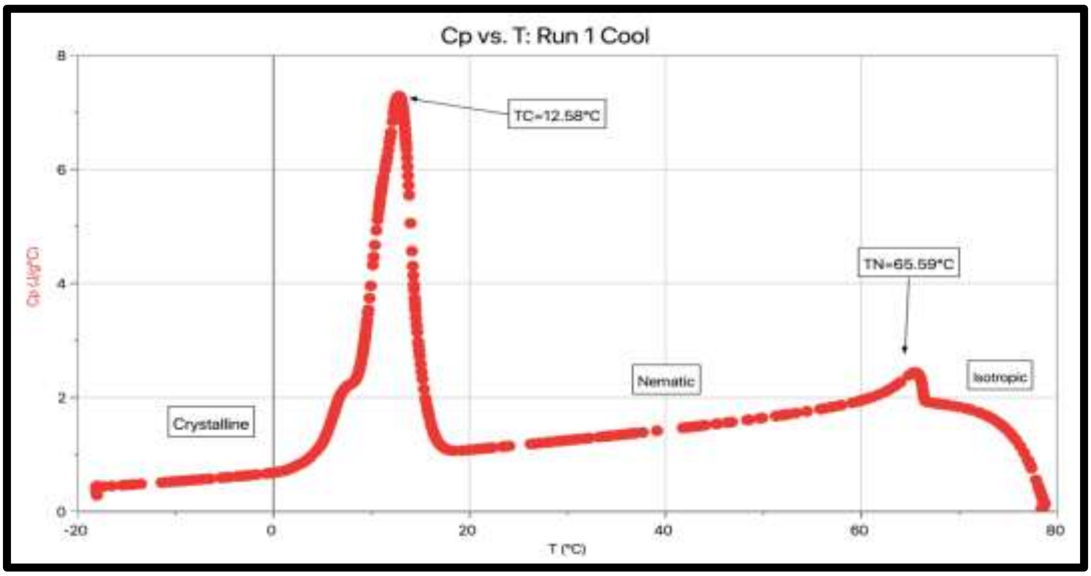

Figure 9: Specific heat capacity vs temperature plot for the first run's cooling only.

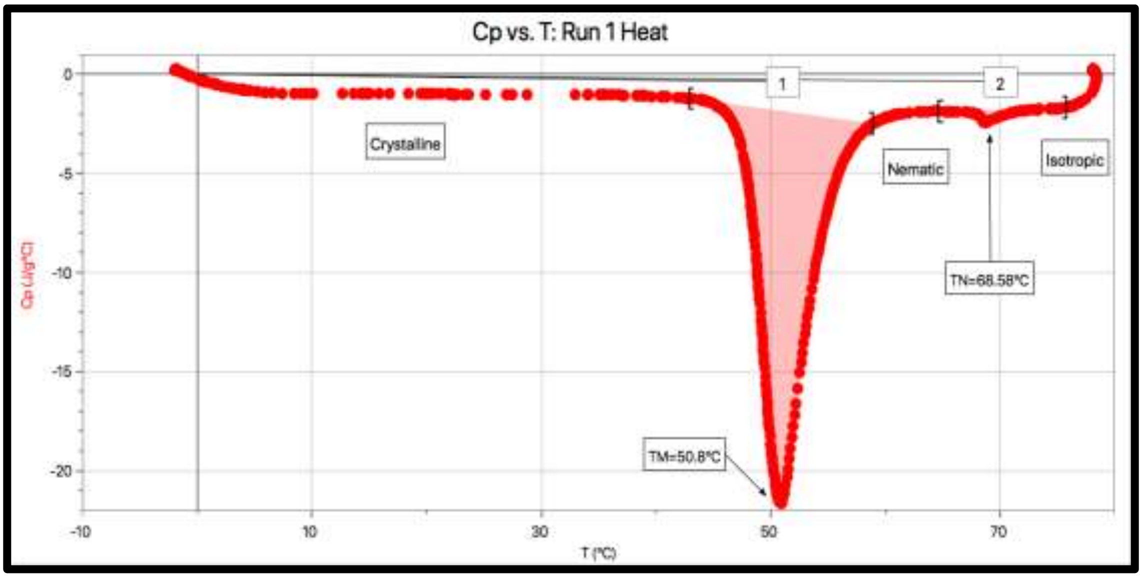

Figure 10: Enthalpy of the melting and the nematic transitions during heating for run 1 of 5OCB.

Run 1's specific heat capacity graph is shown again in Figure 10, but the peaks of the graph have been integrated using the 'peak integration' tool on LoggerPro. The melting peak is large and can be easily seen shaded by the tool; the nematic peak was analyzed as well, however its size makes the shading hard to see. The integrated peak shows how much energy is absorbed by LC molecules during heating as endothermic peaks for melting and nematic transitions.

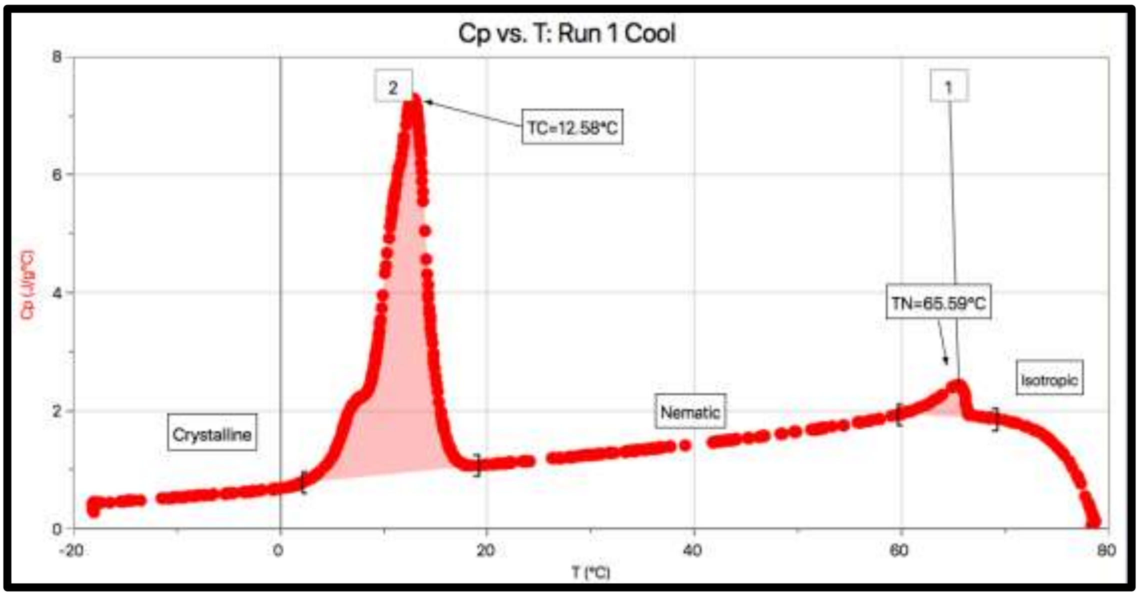

Figure 11: Enthalpy of nematic and crystalline peaks for run 1's cooling.

The peaks of run 1 during their cooling are displayed in Figure 11 and the crystalline and nematic peaks were chosen to be analyzed using peak integration. The nematic peak integration can be seen really well with light red shading, but the crystalline peak is much larger. All other runs had their peaks analyzed in this way. The integrated area shows the amount of energy released by LC molecules during cooling as exothermic peaks.

Since it was hard to see the integrated part of Nematic peak in heating and cooling, the zoomed in part of the integrated nematic peak is shown for heating in Figure 12. The states of the LC have been labeled as it heats up from the nematic state to the isotropic state. The peak is much smaller than the melting peak for the same run and can be hard to see as a result. The peak was plotted using LoggerPro by isolating the points that occurred during the nematic peak and creating their own separate figure. Using LoggerPro's analysis features, the peak was integrated, and the area was found as a result. The area of the peak is equal to its enthalpy. The wing jump of the peak has also been labeled with 'WJN' pointing to the starting point and ending point of the peak. The wing jump shows the difference between the level of energies found before and after the nematic phase is reached as the wings of the endothermic peak. It is clearly seen that the wings before and after peak have a vertical gap that is called a wing jump.

Figure 13 shows a zoomed in perspective of the nematic peak that occurred during run 1 while 5OCB was being cooled from an isotropic state to a nematic state. The graph shows specific heat capacity vs. temperature and the nematic peak is labeled with 'TN'. The behavior of the peak is more visible when graphed on its own plot instead of next to the large crystalline peak. The shaded part of the graph shows the area of the peak or the enthalpy of the transition. The starting point and ending point have been marked with 'WJN' for the peak's wing jump.

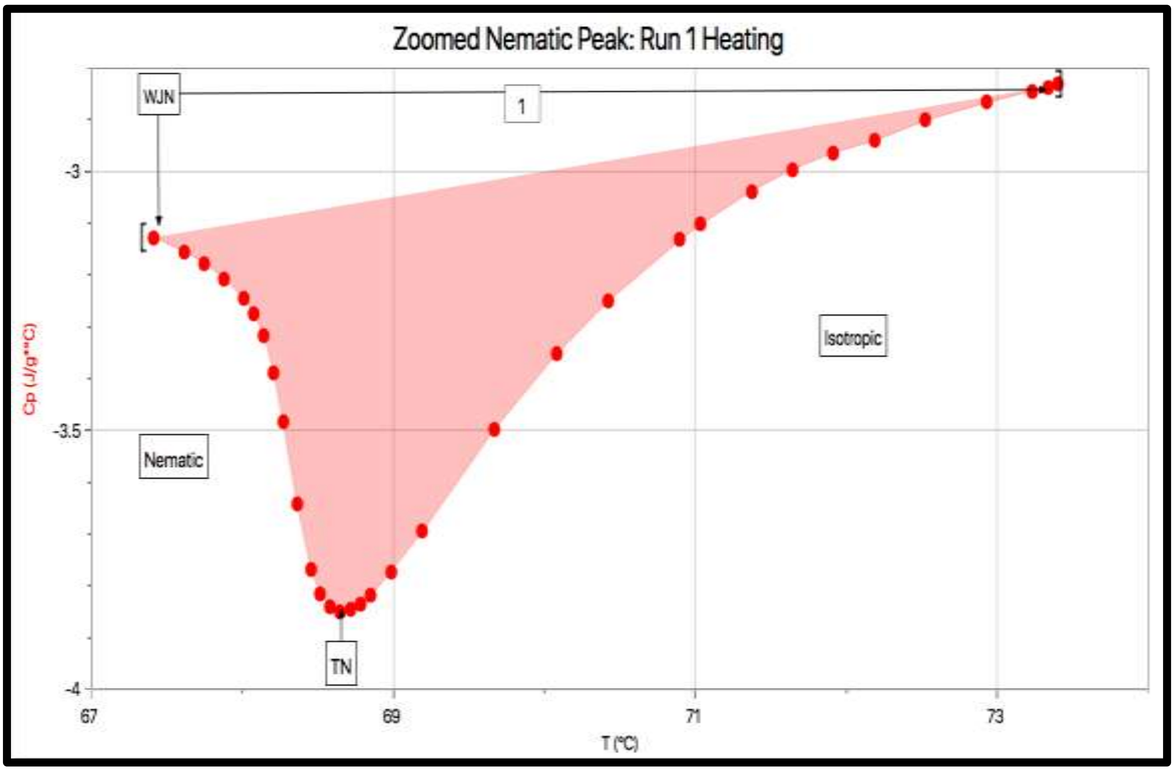

Figure 12: Enthalpy of run 1's nematic peak for heating of 5OCB.

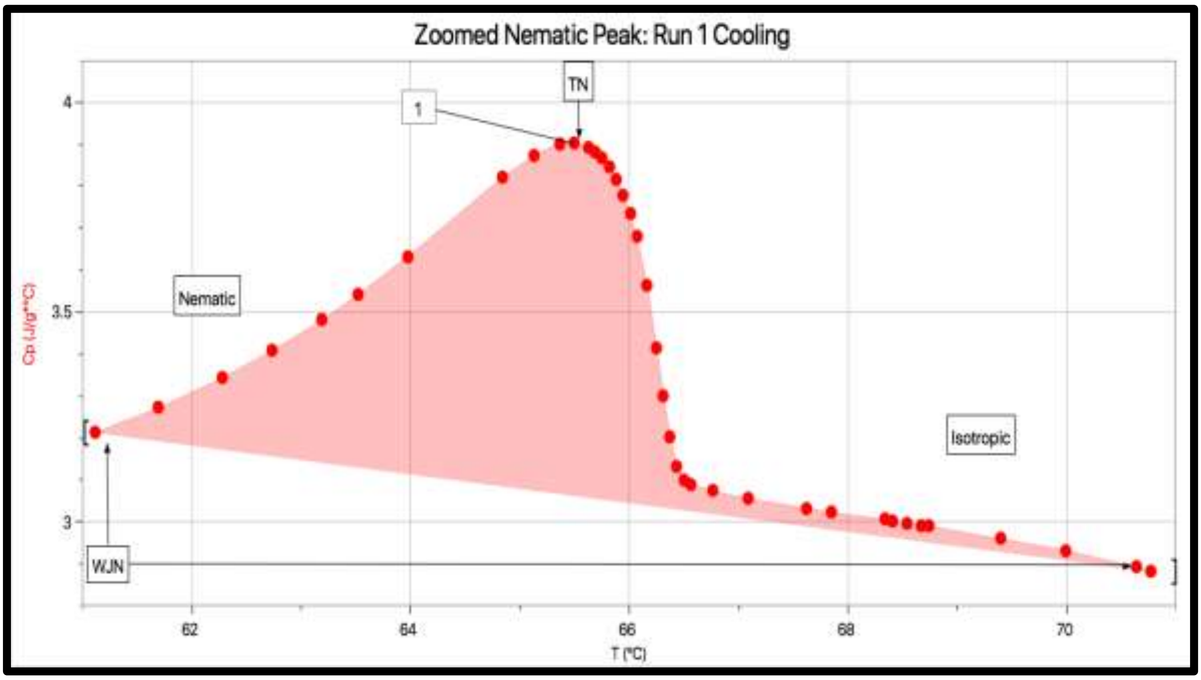

Figure 13: The enthalpy of the nematic peak for 5OCB's first run during cooling.

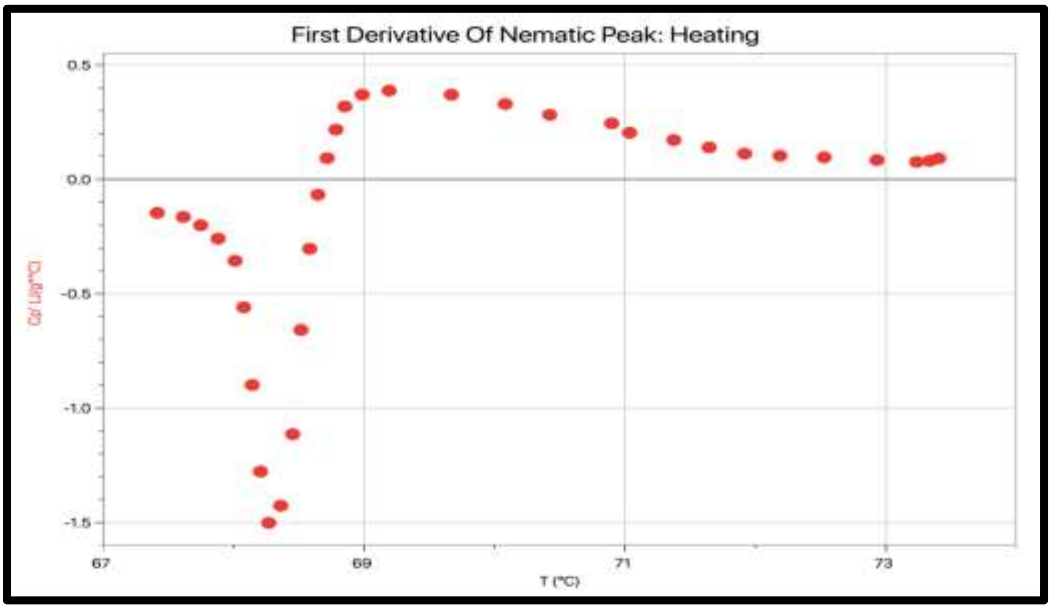

Figure 14: The first derivative of run 1's nematic peak during heating of 5OCB.

The data plotted in figure 12 was used along with LoggerPro to calculate a new column: the first derivative of the peak's specific heat capacity during run 1. The graph in Figure 14 shows this calculated first derivative data for the nematic phase in heating on the y-axis vs. the temperature on the x-axis. The plot is shown in red to match with the previous run 1 data. The 1st derivative shows the dynamics of the nematic peak in heating with the same slope (speed of heating) as the graph that was plotted in Figure 12.

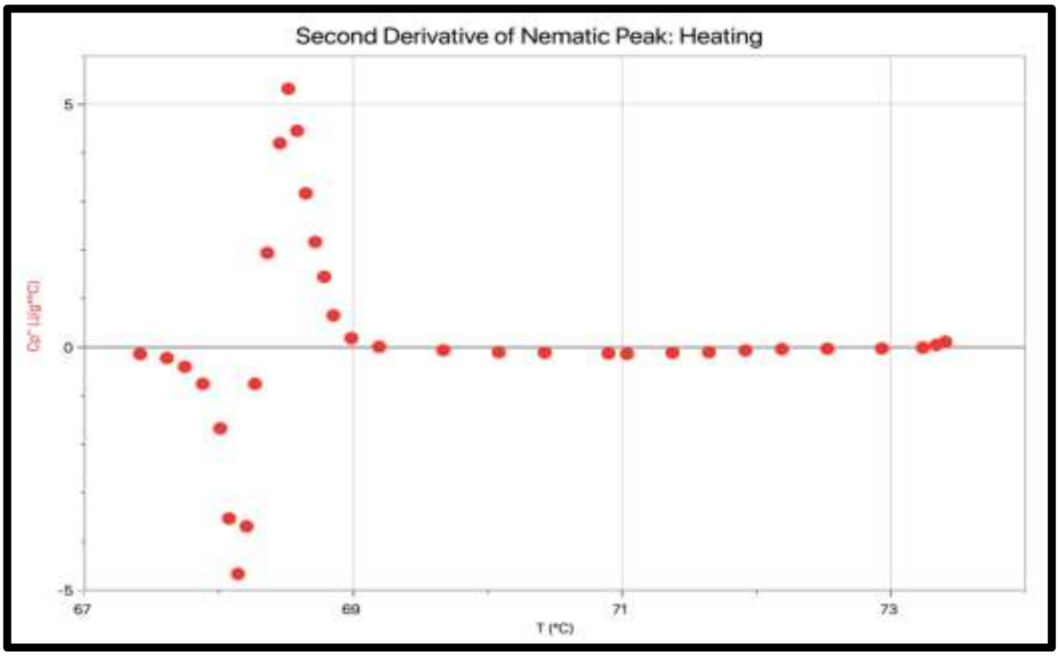

Figure 15: The second derivative of run 1's nematic peak during heating of 5OCB.

Figure 15 shows the second derivative of run 1's nematic peak, with the second derivative of the peak's specific heat capacity on the y-axis and the temperature of the peak on the x-axis. LoggerPro was used again to create a new calculated column and the second derivative function was performed on the specific heat capacity data. The 2nd derivative of Figure 12 or the derivative of Figure 14 shows a slope of acceleration of heat flow, showing how sharp a slope for the nematic transition has or how quickly the nematic phase changes with temperature and time.

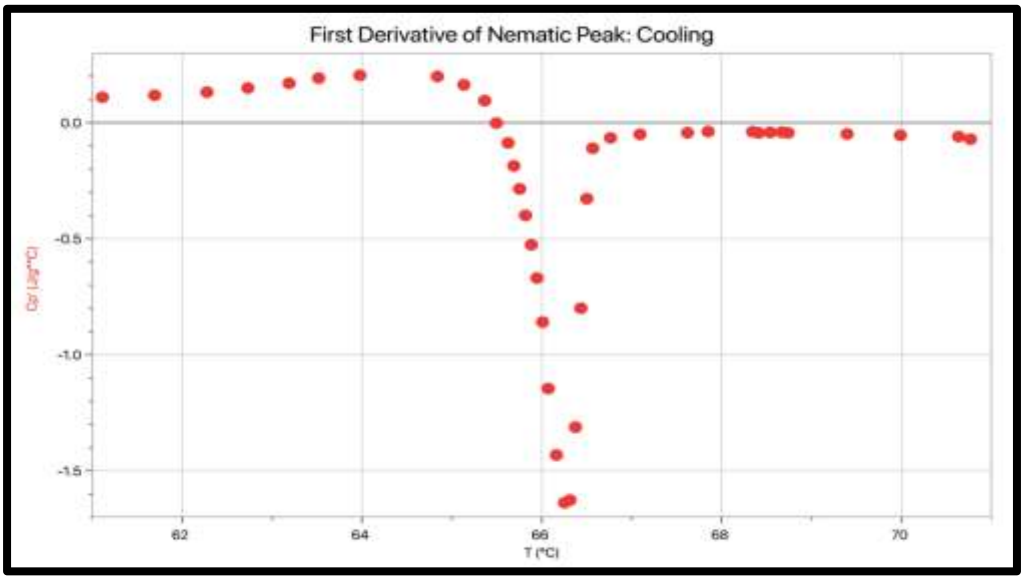

Figure 16: The first derivative of run 1's nematic peak during cooling of 5OCB.

Similar to Figure 14, Figure 16 displays the first derivative of run 1's nematic peak. Figure 16 shows the nematic peak from the cooling portion of run 1, with the first derivative of the specific heat capacity on the y-axis and the temperature of the run on the x-axis. The calculated column function was used on LoggerPro, and the first derivative was taken of the peak's specific heat capacity.

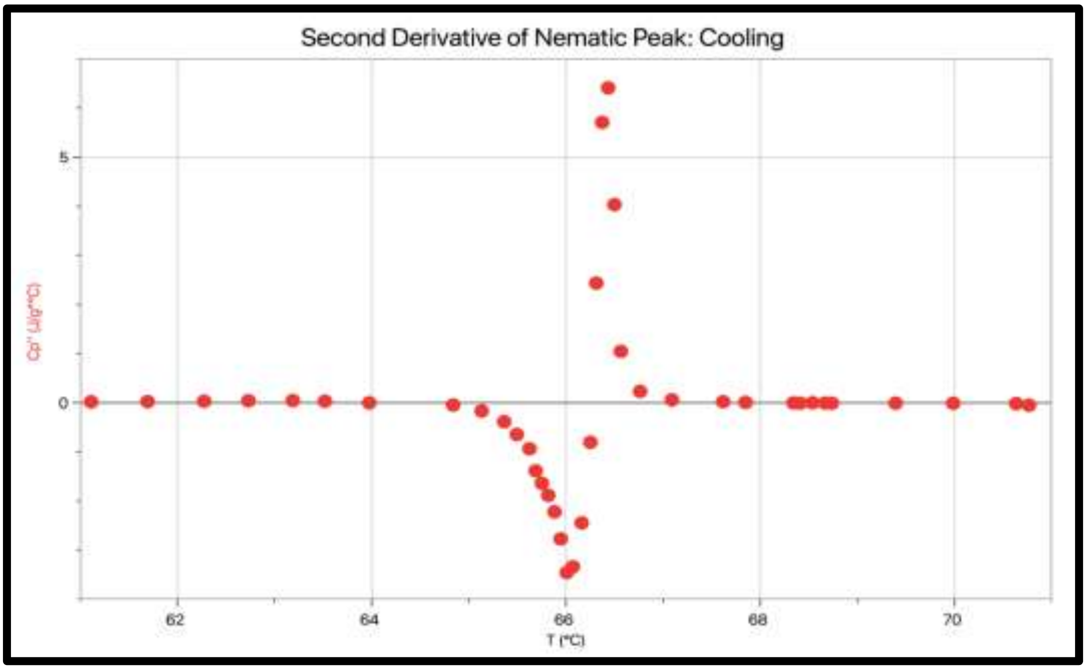

Figure 17: The second derivative of run 1's nematic peak during cooling of 5OCB.

Similar to Figure 15, the second derivative of run 1's nematic peak was taken. Figure 17 shows the second derivative of this peak's specific heat capacity during run 1's cooling of 5OCB. The calculated column was created in LoggerPro, and the second derivative function was used on the nematic peak's specific heat capacity. The second derivative of the specific heat capacity is on the y-axis and the temperature is on the x-axis.

The first derivative shows how sharp or broad the peaks were for the heat flow plots of the nematic transitions for heat and cool. The second derivative shows how sharp the nematic peak is in the first derivative plot of the nematic peak for heat and cool. Physically, the meaning of the 1st and 2nd derivatives are how the slopes of the nematic peak, or curve, are changing in heating and cooling. The slopes can later be given a term as speed and acceleration of the peaks and how they are changing with time and temperature. Higher slopes mean sharper change, longer lines mean deeper change.

To show a comparison between 5CB and 5OCB nematic phase transition, Figure 18 is plotted as specific heat capacity vs. the temperature for 5CB to show what the nematic peak looks like for 5CB. The nematic peak is labeled as 'TN' and the states of the LC have been labeled as it progresses from nematic to isotropic and back again. Figure 18 shows the shape, size, appearance, and location of the nematic peak in heating and cooling for 5CB, which has no oxygen in its molecule.

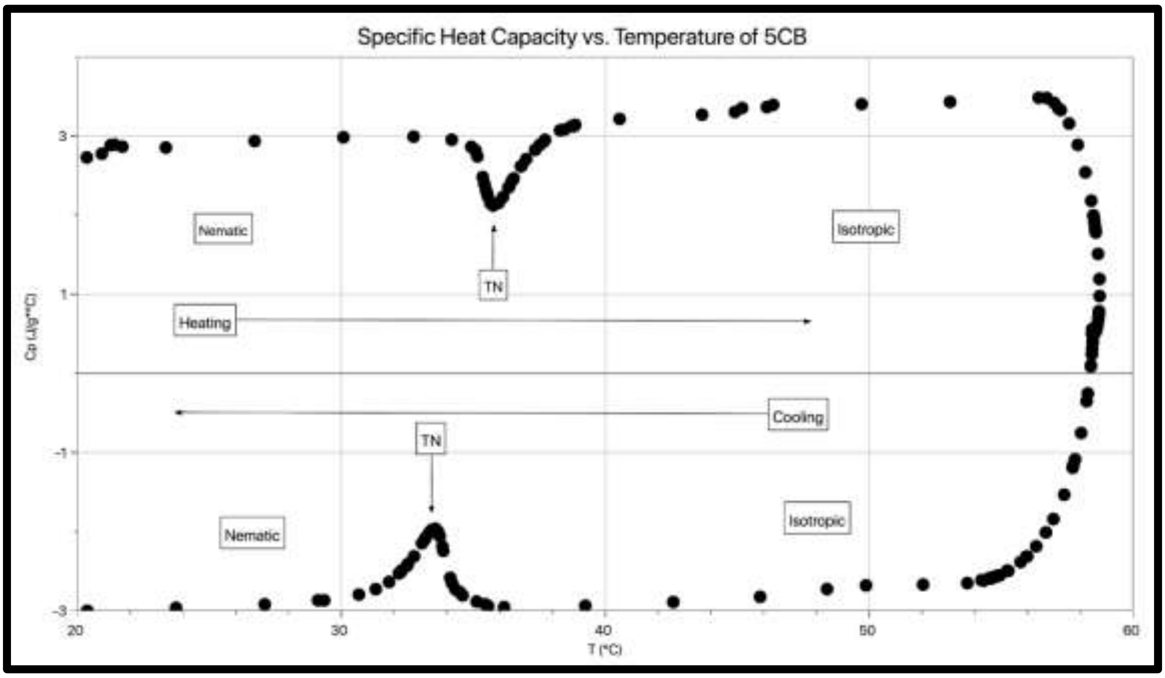

Figure 18: The specific heat capacity vs. temperature of 5CB being heated and cooled.

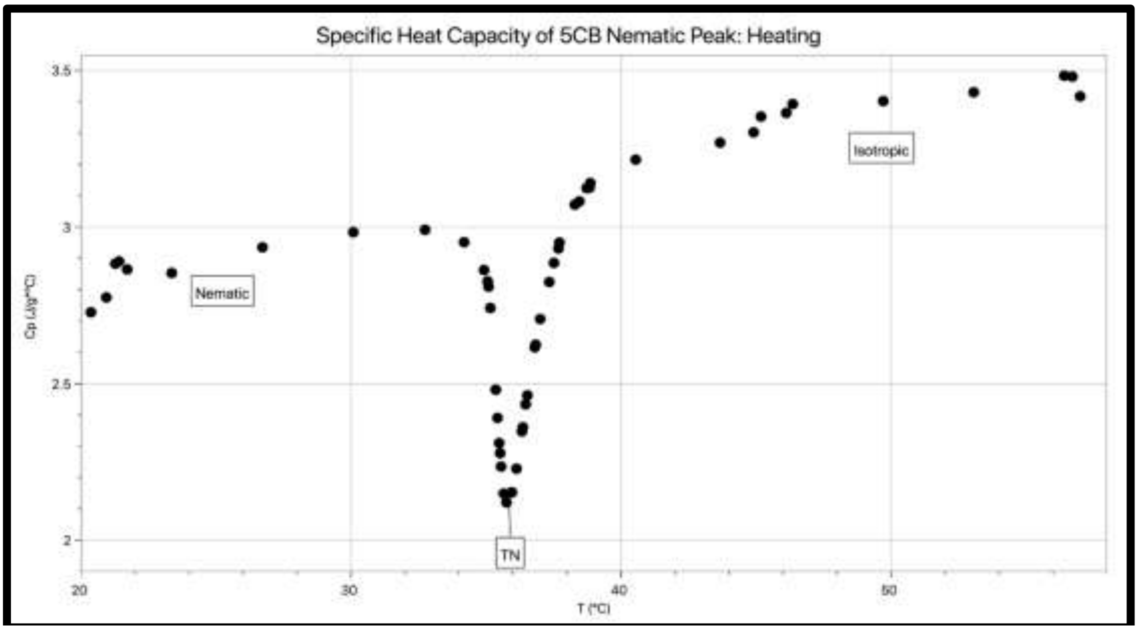

Figure 19: The specific heat capacity of the nematic peak from heating 5CB.

Figure 19 shows the zoomed in part of the nematic peak of 5CB from Figure 18, when it was being heated using the DSC instrument. The specific heat capacity of the transition is on the y-axis, while the temperature of the transition is on the x-axis. The states that the LC shifts to during this transition were labeled as nematic and isotropic.

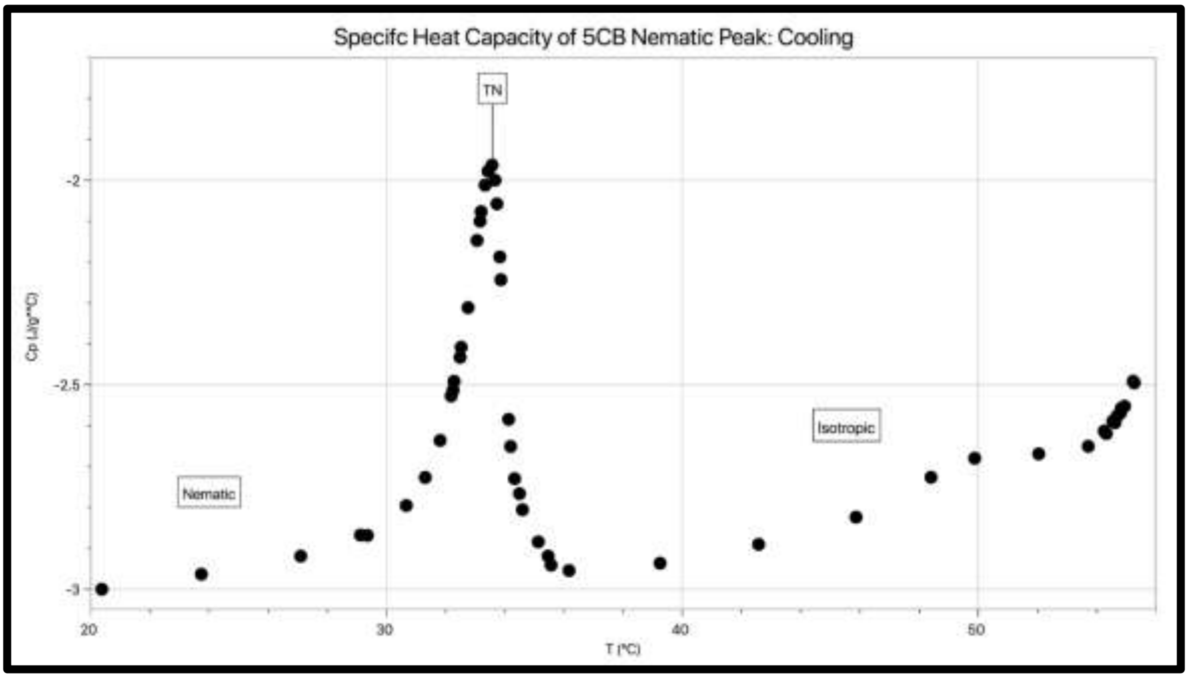

Figure 20: The specific heat capacity of the nematic peak for the cooling of 5CB.

The zoomed in nematic peak that occurred during the cooling of 5CB is shown in Figure 20. The peak has been labeled as 'TN' for the nematic peak and the plot shows the LC as it cools from an isotropic state to a nematic state. The shape of the nematic peak for cooling 5CB can be seen.

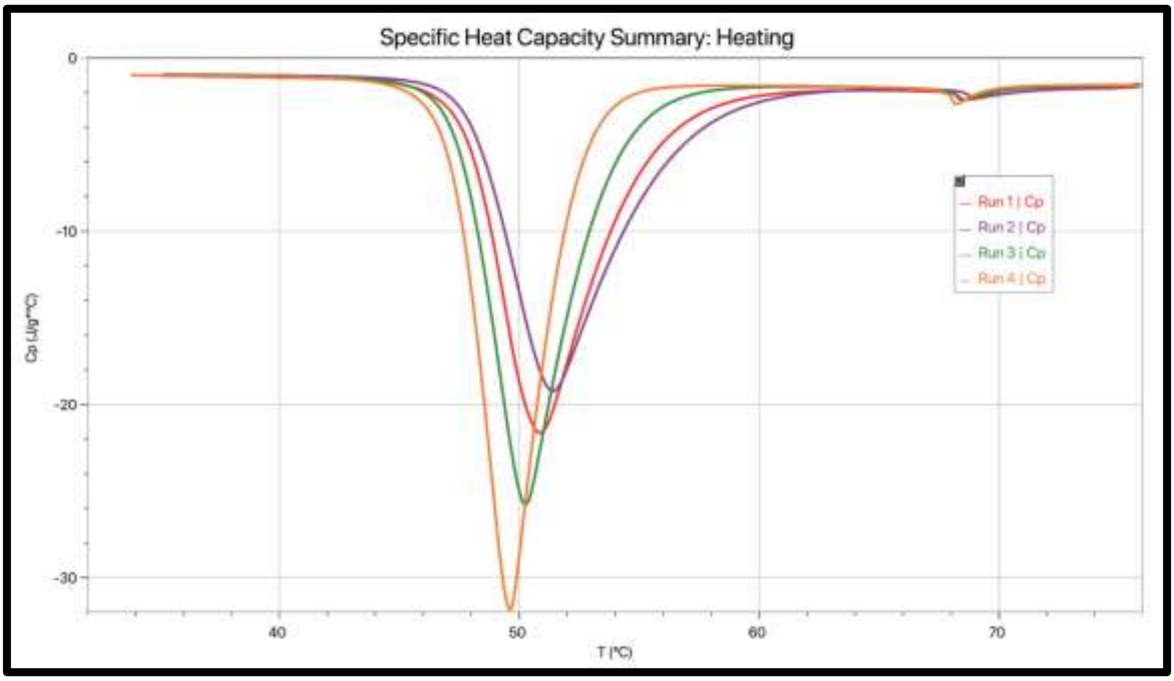

Figure 21: Specific heat capacity of 5OCB for all 4 runs for heating.

To see a clear comparison between the four heating runs' melting and nematic peaks, Figure 21 is plotted using LoggerPro. The specific heat capacity for each run's heating of 5OCB vs. its temperature is shown in Figure 21; with run 1 in red, run 2 in purple, run 3 in green, and run 4 in orange. Graphing all runs together allows for easy comparison of each run and how the sample behaved in these two-phase transitions. The mixed solid-state peak is only present for runs 2-4 and run 4 has the biggest melting peak. All runs had a relatively similar nematic peak, but it is hard to see in this figure as the nematic peak is smallest in the graph. Although it can be seen that the shapes and sizes of the melting and nematic peaks are changing as the number of runs are changing from first run to fourth run.

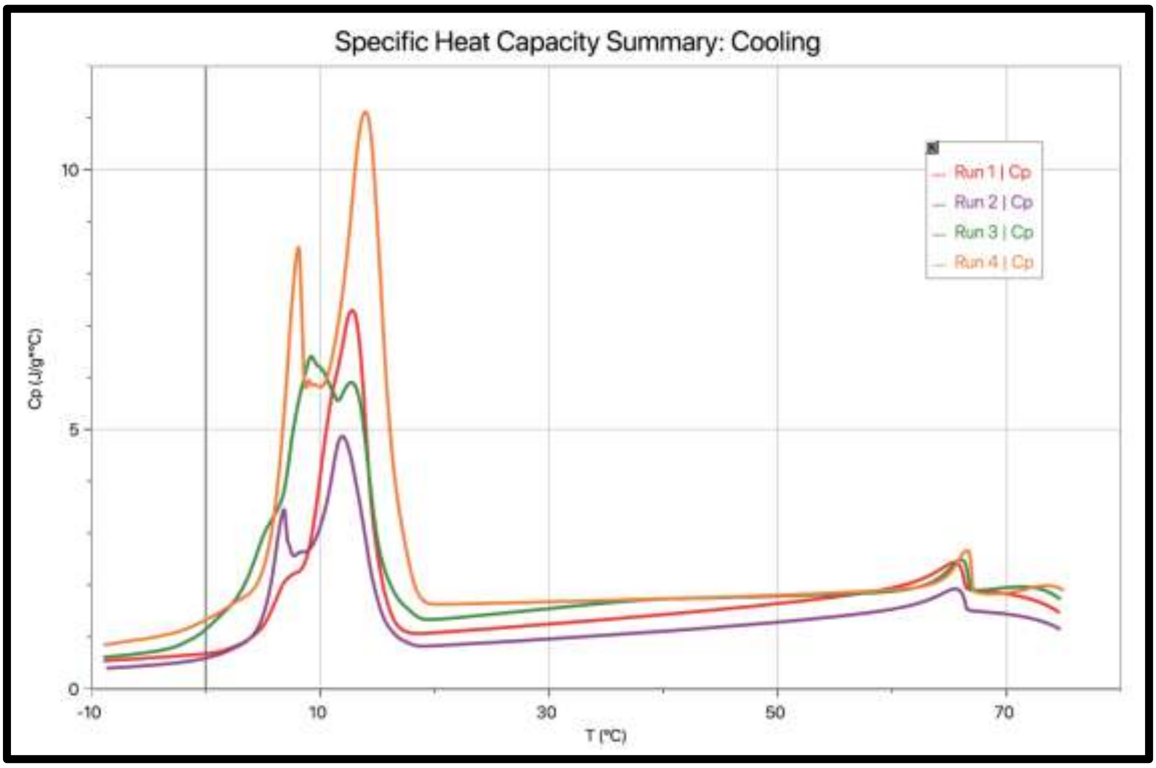

Figure 22:Specific heat capacity of 5OCB for all 4 runs for cooling.

Similar to the graph in Figure 21, Figure 22 is plotted to see a proper comparison of the cooling transitions of all runs for 5OCB. The specific heat capacity vs. the temperature for the cooling of 5OCB for all four runs is shown in Figure 22, with a legend detailing run 1 in red, run 2 in purple, run 3 in green, and run 4 in orange. The nematic peaks show deviation in behavior throughout the different runs and are hard to see as it is the smallest peak in this graph. In addition, the crystalline peaks are very distinct to their complementary run. Run 1 is the only singlet crystalline peak, while the others show a double peak.

Since it is hard to see nematic peaks in Figure 21 and Figure 22, being the smallest peaks in the graphs, the zoomed in graphs of Figure 21 and Figure 22 are plotted separately to see the effect of multiple heating and cooling on the nematic phase transition and its shape and size. The zoomed-in figures for the nematic peaks that occurred during the heating of 5OCB for each run are shown in Figure 23 with run 1 in red, run 2 in purple, run 3 in green, and run 4 in orange. Graphing all nematic peaks in one place provides for easy comparisons to be made between each peak. The first two runs are broader than runs 3 and 4, while the last two runs have a greater specific heat capacity magnitude than runs 1 and 2.

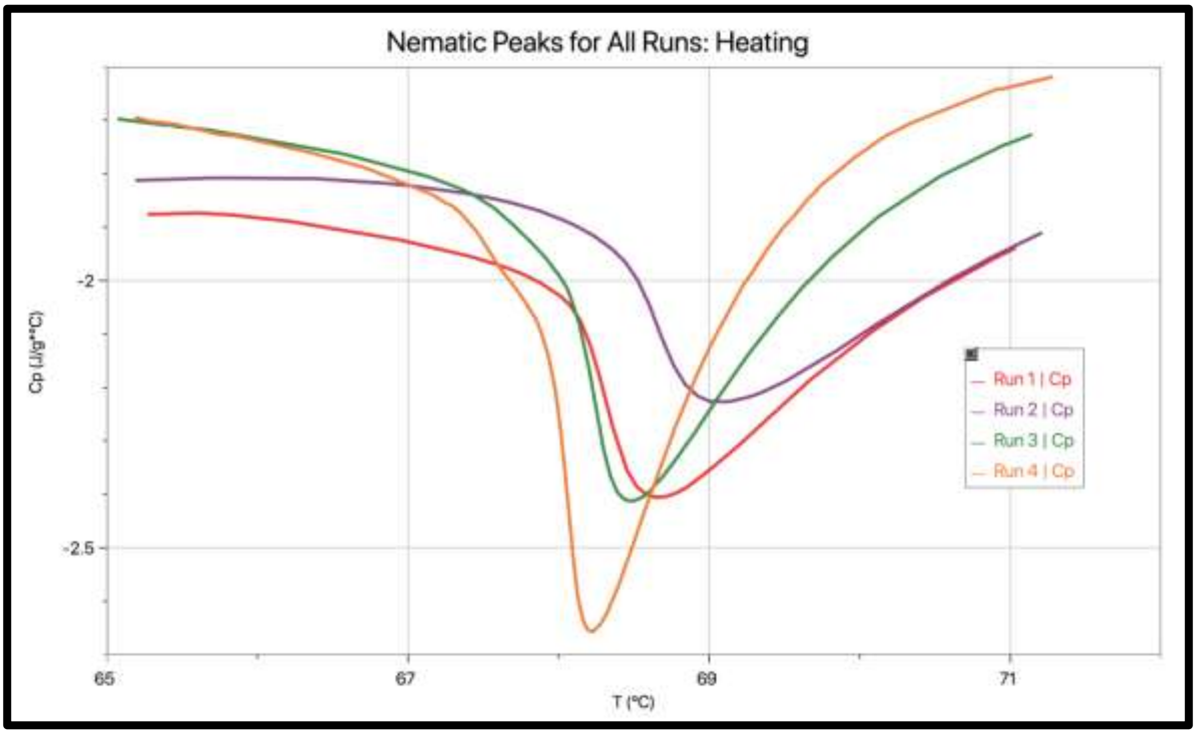

Figure 23: The zoomed in peaks for the nematic peak for all heating runs of 5OCB.

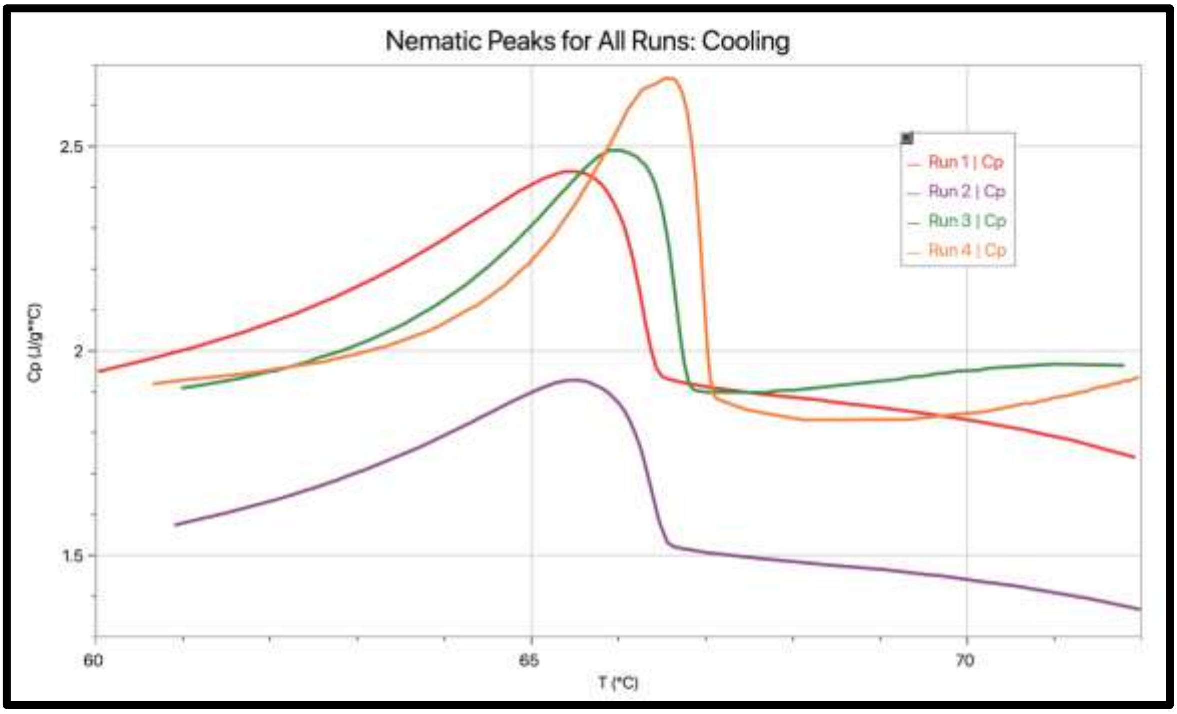

Figure 24: The zoomed in peak for the nematic peak for all runs of 5OCB being cooled.

Figure 24 shows the zoomed in nematic peaks of 5OCB when it was being cooled during all runs of the experiment; run 1 is in red, run 2 is in purple, run 3 is in green, and run 4 is in orange. The graph of Figure 24 shows that run 1, 3, and 4 had nematic peaks that were close in specific heat capacity value, while run 2 was by itself.

After comparing the position, shape, size, depth, width, wing jump, and energy absorbed or released for the nematic transition for all four runs for 5OCB, some summary graphs are plotted to see significant results and any trend behavior.

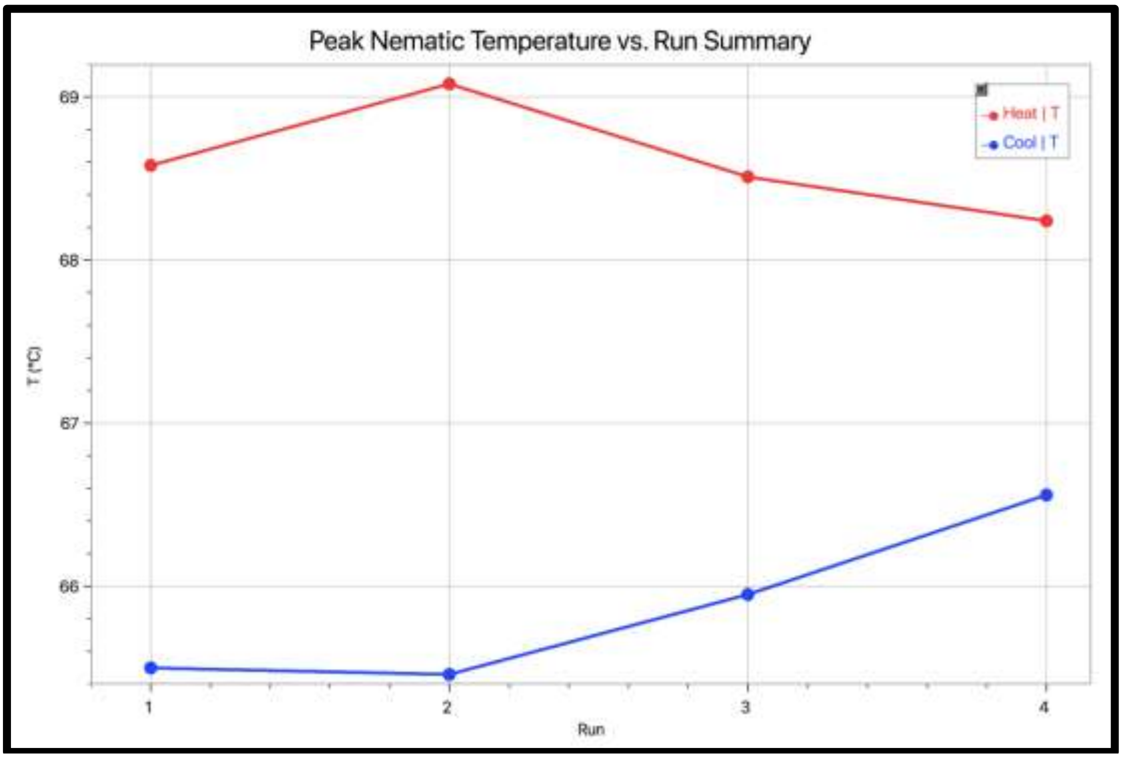

Figure 25: The peak temperature for a run's nematic peak vs. its run.

Figure 25 shows the peak temperature for the nematic transition of every run of 5OCB through the DSC instrument. The temperature values obtained from the nematic peaks from the heating of 5OCB is shown in red, while the ones obtained from cooling are shown in blue. The nematic peaks that occurred during heating, had a greater peak temperature than those that occurred during the cooling of 5OCB.

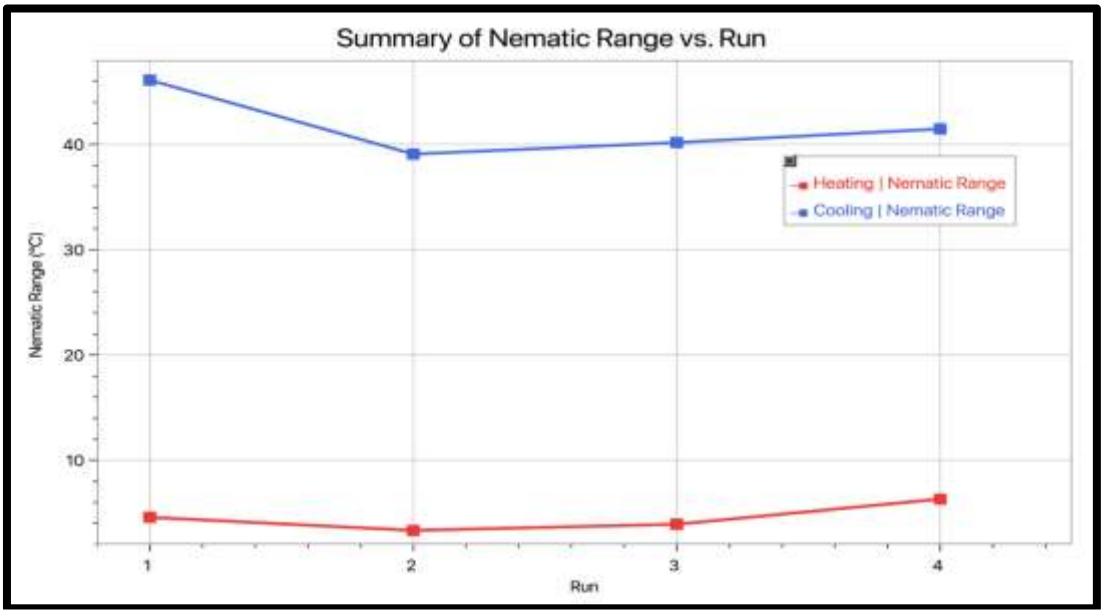

Figure 26: Summary graph of 5OCB's nematic range for heating and cooling for all four runs.

The nematic range for each run of the 5OCB sample is shown in Figure 26 with the nematic range for the heating portion in red and the nematic range for the cooling portion shown in blue. The nematic range occurs between the melting peak and the nematic peak during heating, and between the nematic peak and crystalline peak during cooling. The summary graph illustrates the large difference between the nematic range when the sample was being heated vs. when it was being cooled. The sample stayed in the nematic range much longer when it was being cooled.

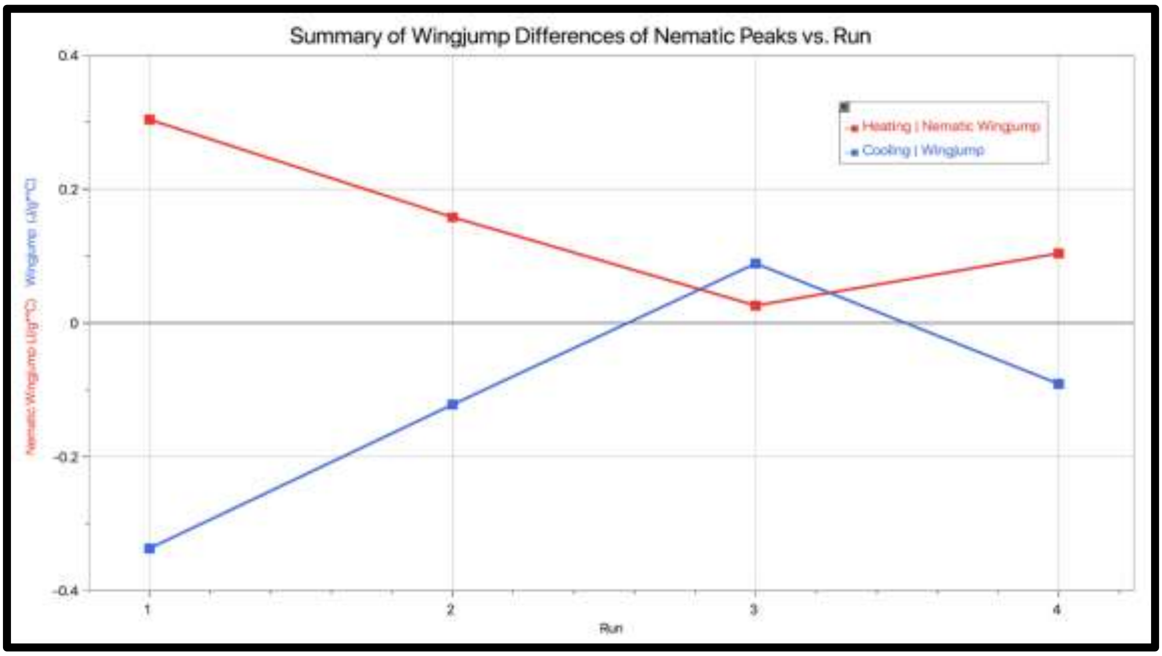

Figure 27: 5OCB's wingjump differences for the nematic peaks of heating and cooling for all runs.

The wing jump difference of each nematic peak of 5OCB's heating and cooling is displayed in Figure 27, blue is the values for the nematic peaks in cooling and red is the nematic peaks in heating. The wing jump is found by subtracting the starting value from the ending value of the points belonging to the peak. The cooling portion shows a general increase in wing jump differences, while the heating portion shows a general decrease in values.

Data details can be seen in **Table 1**, showing the peak melting temperature (TM) and peak nematic temperature (TN) for heating and cooling of all four runs. The table has each run-in chronological order with their heat value displayed first and the cool value displayed second. RN refers to the nematic range, WJN refers to the nematic wing jump, and HN refers to the enthalpy of the nematic peak.

Table 1: Data on melting and nematic states of heating and cooling for all runs.

Run	TM (°C)	TN (°C)	RN(°C)	WJN (J/g*°C)	HN (J/g)
1 Heat	50.8	68.58	4.58	0.304	-42.68
1Cool	-	65.5	46.11	-0.337	-44.11
2 Heat	51.42	69.08	3.33	0.158	-33.83
2 Cool	-	65.46	39.08	-0.122	-29.91
3 Heat	50.31	68.51	3.92	0.026	-24.6
3 Cool	-	65.95	40.18	0.089	-34.75
4 Heat	49.69	68.24	6.31	0.104	-26.88
4 Cool	-	66.56	41.47	-0.091	-48.71

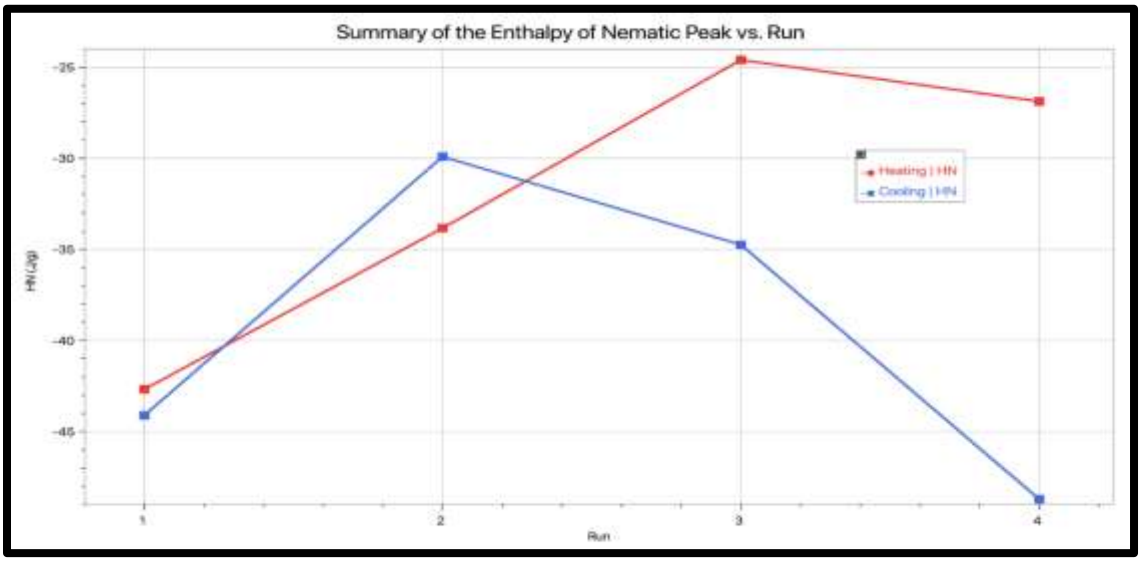

Figure 28: Enthalpy of the nematic peaks of 5OCB for the heating and cooling of all runs.

A summary of the enthalpy, or area under the nematic peak, is displayed in Figure 28. The run is shown on the x-axis and the value for the enthalpy of each nematic peak is on the y-axis. The values that belong to the cooling portion of the runs are shown in blue and the heating portions are shown in red. The nematic peaks that resulted from heating 5OCB were typically larger than the enthalpy of the nematic peaks in cooling.

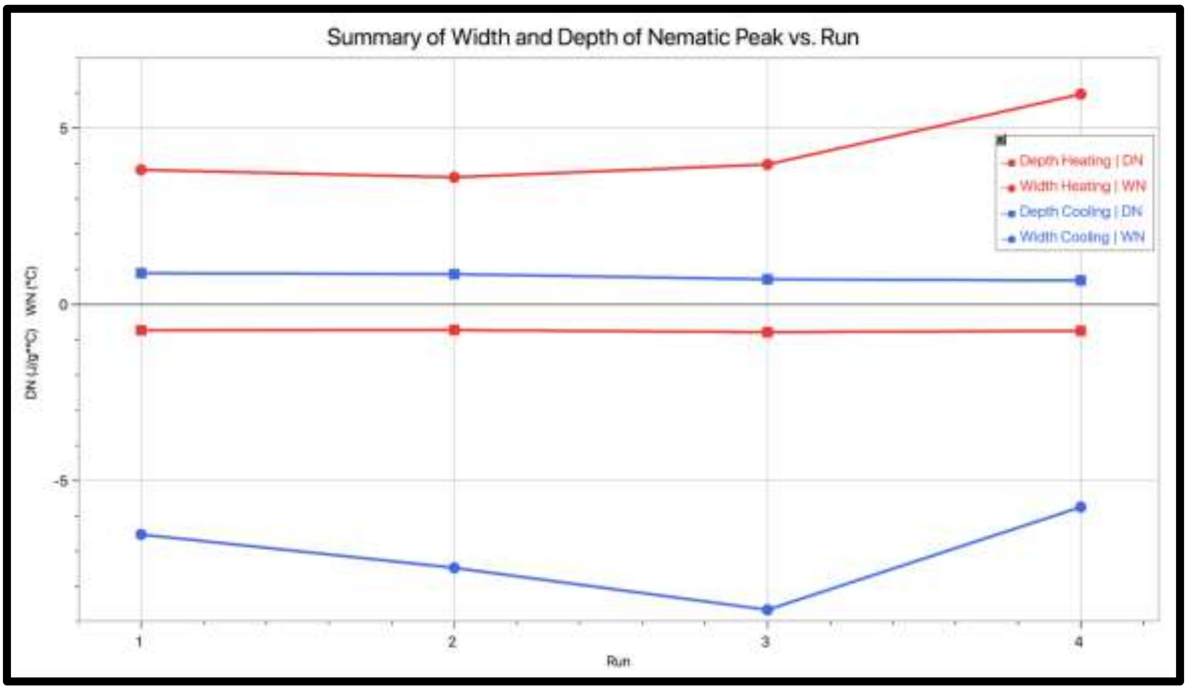

Figure 29: Width and depth of 5OCB's nematic peaks for the heating and cooling of all runs.

The values obtained from analyzing the width and depth of 5OCB's nematic peaks is displayed in Figure 29; the width of the nematic peaks is shown with a filled circle point symbol and the depth of the nematic peaks is shown with the filled square point symbol. The red color represents the nematic peak being a part of the heating, while the blue color denotes the nematic peak as having occurred during cooling. The width and depth had a similar behavior whether it occurred during cooling or heating, but the width of the peaks in cooling was less than the width of the nematic peaks in heating. Conversely, the depth of the nematic peaks in cooling was greater than those in heating.

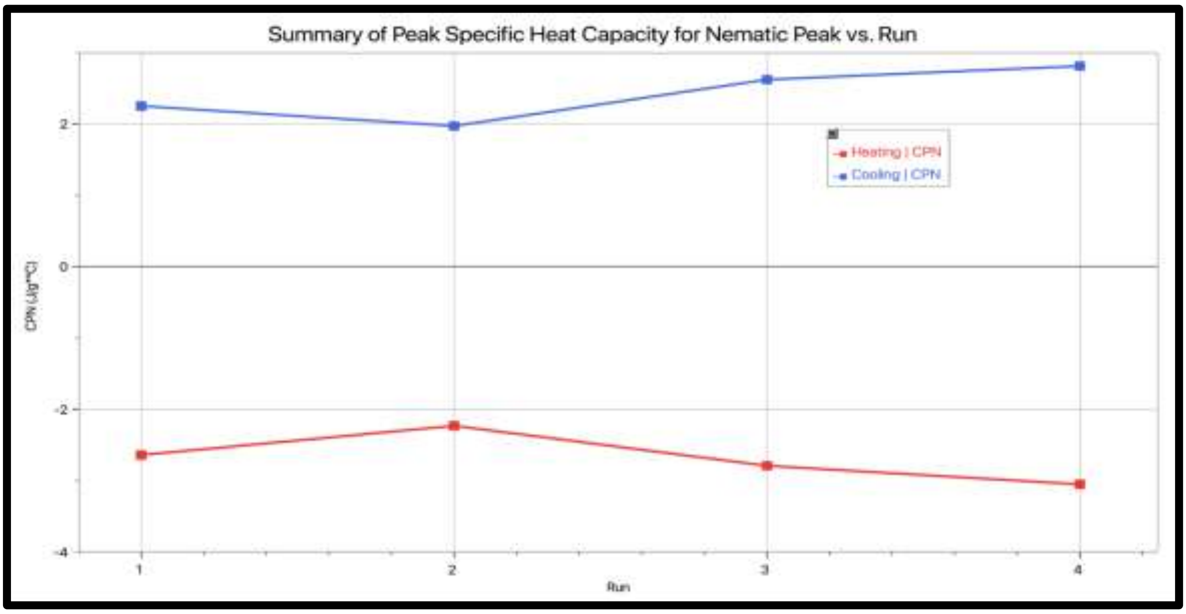

Figure 30: Peak specific heat capacity of 5OCB for each run's nematic peak for both cooling and heating.

The peak specific heat capacity value for each of 5OCB's nematic peaks for heating and cooling is shown in Figure 30, with the corresponding run or trial on the x-axis. The red data set is for the values that belong to the heating of 5OCB and the blue points are for the cooling of 5OCB. The peak specific heat capacity for the nematic peaks is found by locating the maximum or minimum of the peak and recording its y-value. The cooling peak specific heat capacity values are greater than those of the heating and generally increase, while the heating's values are decreasing.

Table 2: Width, depth of the nematic peaks of 5OCB and their peak specific heat capacity.

Run	ΔT(°C)	Δ*CP* (J/g*°C)	*CPN* (J/g*°C)
1 Heat	3.817	-0.732	-2.64
1 Cool	-6.524	0.887	2.25
2 Heat	3.606	-0.726	-2.23
2 Cool	-7.47	0.86	1.97
3 Heat	3.971	-0.786	-2.79
3 Cool	-8.66	0.713	2.62
4 Heat	5.965	-0.748	-3.05
4 Cool	-5.746	0.68	2.81

The data details in **Table 2** can be seen for the nematic peaks of 5OCB during heating and cooling using the DSC instrument. ΔT is the width of the peak, while ΔCP is the depth of the nematic peaks. *CPN* stands for the peak specific heat capacity value of the nematic peaks for each run. The runs have been organized in the order that they were performed.

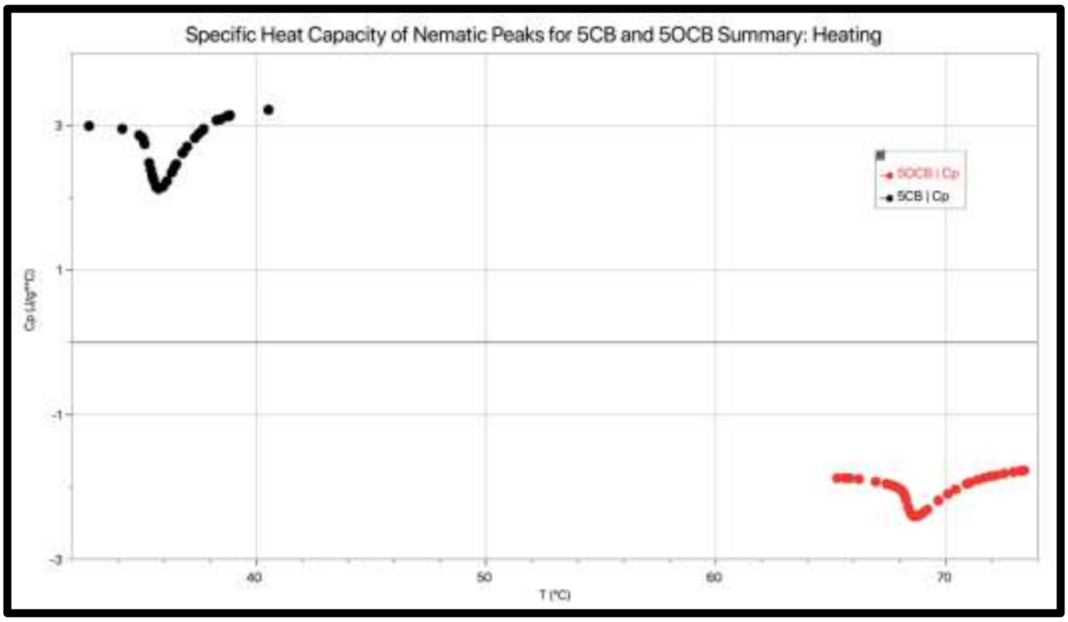

Figure 31: The nematic peaks of 5OCB and 5CB being heated summary graph.

The nematic peak of both liquid crystals is shown in Figure 31, with the nematic peak for 5OCB in red and the nematic peak for 5CB in black. The specific heat capacity of the phase transition is on the y-axis, while the temperature for each peak is on the x-axis. The summary graph allows for easy comparison between 5OCB and 5CB.

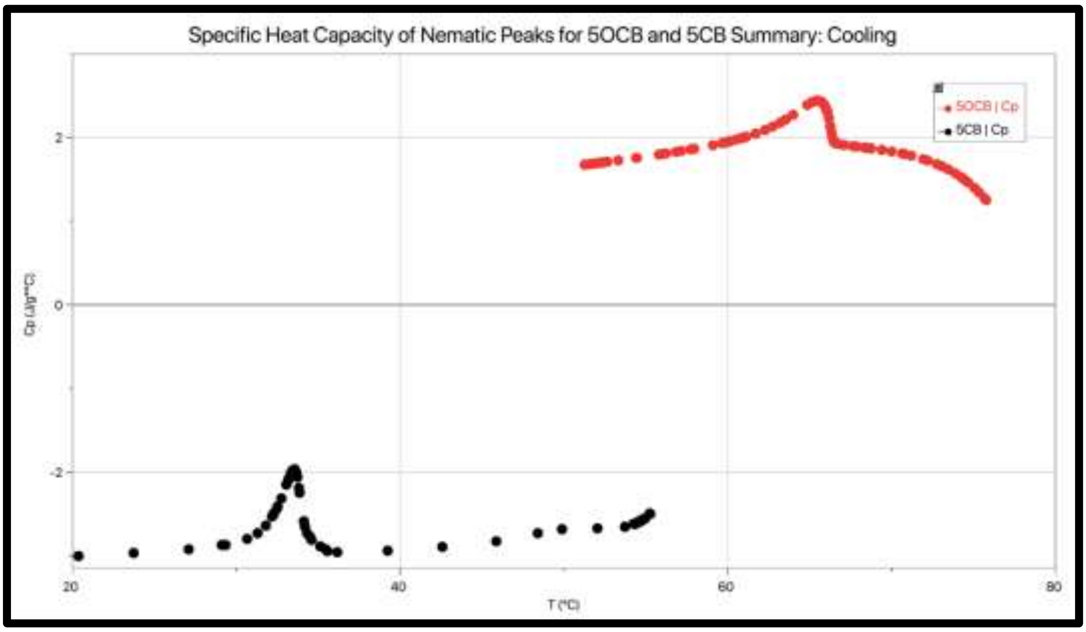

Figure 32: The nematic peaks of 5OCB and 5CB being cooled summary graph.

Figure 32 shows the nematic peaks for 5OCB and 5CB when they are being cooled using the DSC. The data for 5OCB is in red and 5CB is in black, with the specific heat capacity of the peak on the y-axis and the temperature on the x-axis. The difference between the nematic peaks is large but could be attributed to the difference in ramp rates (5OCB had one of 20 ℃/min and 5CB had a rate of 10 ℃/min).

he data details in **Table 3** shows the comparison between the nematic peaks of 5OCB and 5CB. Since 5CB was heated and cooled at a rate of 10°C/min, the fourth run of 5OCB was used since it had the same ramp rate. The peak temperature, peak specific heat capacity, nematic range, nematic wing jump, depth of the peak, width of the peak, and enthalpy of the nematic peak are shown in the columns of Table 2. The molecular weight is also shown in Table 3.

Table 3: Comparing the nematic peaks of 5CB and 5OCB.

Samples	Molecular weight (g/mol)	T_N (°C)	|CPN| (J/g*°C)	R_N (°C)	W_{JN} (J/g*°C)	|ΔT|(°C)	ΔC_P (J/g*°C)	|H_N| (J/g)
5CB Heat	249.35	35.66	2.097	29.75	0.579	18.14	-0.824	0.37
5CB Cool	249.35	33.55	1.955	15.38	0.024	15.48	0.989	1.98
5OCB Heat	265.35	68.24	3.05	6.31	0.104	5.965	-0.748	26.88
5OCB Cool	265.35	66.56	2.81	41.47	-0.091	5.746	0.68	48.71

III. Conclusion:

In this paper, the detailed results of the nematic phase transition and nematic range during heating and cooling in 5OCB liquid crystal are reported. The results are then compared with the results of 5CB's nematic phase transition to see how the presence of oxygen brings changes in the behavior of the 5OCB liquid crystal. The effect of multiple heating and cooling on 5OCB is also reported along with the effect of heating and cooling on the nematic range. It is found that when 5OCB is heated and cooled from -40 °C to 80 °C and then from 80 °C to -40 °C, it shows the nematic peak shifts towards lower temperatures in cooling and shows almost 11 times larger nematic range in cooling. The peak temperatures for the nematic transition of the 1st run is found at 68.5 °C and 65.5 °C for heat and cool respectively. The nematic range is found to be 4.58 °C in heating and 46.11 °C in cooling for run1. When 5OCB is heated and cooled four times continuously without a break, it shows that all values reported in data tables 1 and 2 go down as the number of runs increases. This can be explained by the molecules not getting enough time to relax when they are heated and cooled continuously. This effect is why values decrease but not significantly. When 5OCB is compared with 5CB's nematic phase and nematic range, it is found that the presence of oxygen in 5OCB makes it heavier, more stable and more consistent with a lower wing jump, lower width and depth, and lower heat capacity. However, 5OCB shows greater enthalpy and, more interestingly, larger nematic range when being cooled. **Based on the results discussed above in this paper, 5OCB can be a good fit for the LCD world. When it is used in its cooling state, it shows a larger nematic range; the nematic range is most important for the LCD world when trying to show high resolution images.**

Acknowledgement:

We like to acknowledge Professor John C. MacDonald from the department of Chemistry and Biochemistry, WPI for providing his lab and DSC instrument model MDSC 2920 TA Instruments to run 5OCB liquid crystal to obtain data. The student is thankful to Dr. Dipti Sharma for supervising this summer research internship to get some valuable research experience on analyzing data using Logger pro.

References:

[1]. Andrienko, D. (2018). Introduction to liquid crystals. Journal of Molecular Liquids, 267, 520–541. https://doi.org/10.1016/j.molliq.2018.01.175

[2]. New Vision Display. (2018, May 30). What is "liquid crystal"? https://www.newvisiondisplay.com/liquid-crystal/

[3]. Miller, N., Admin. (2021, May 17). Nematic vs Smectic Phase in LCDs. Nelson Miller. https://nelson-miller.com/nematic-vs-smectic-phase-in-lcds/

[4]. Sharma, D., MacDonald, J. C., &Iannacchione, G. S. (2006). Thermodynamics of Activated Phase Transitions of 8CB: DSC and MC Calorimetry. The Journal of Physical Chemistry. B, 110(33), 16679-16684. https://doi.org/10.1021/jp062862d

[5]. Doran, M. C., Seide, M., & Sharma, D. (2022). Reporting Strange and Unique Behavior of 4CB Liquid Crystal using Logger Pro. International Journal of Research in Engineering and Science (IJRES), 10(5), 27–41.

[6]. Oweimreen, G., &Morsy, M. (2000). DSC studies on p-(n-alkyl)-p′-cyanobiphenyl (RCB's) and p-(n-alkoxy)-p′-cyanobiphenyl (ROCB's) liquid crystals. Thermochimica Acta, 346(1–2), 37–47. https://doi.org/10.1016/s0040-6031(99)00411-6

[7]. Sharma, D. (2010). Non-isothermal kinetics of melting and nematic to isotropic phase transitions of 5CB liquid crystal. Journal of Thermal Analysis and Calorimetry, 102(2), 627–632. https://doi.org/10.1007/s10973-010-0837-2

[8]. Seide, M., Doran, M. C., & Sharma, D. (2022). Analyzing Nematic to Isotropic (N-I) Phase Transition of nCB Liquid Crystals Using Logger Pro. European Journal of Applied Sciences, 10(3), 98-124. https://doi.org/10.14738/aivp.103.12373

[9]. Zhao, Y., & Farrell, J. A. (2007). Self-Organizing Approximation-Based Control for Higher Order Systems. IEEE Transactions on Neural Networks, 18(4), 1220–1231. https://doi.org/10.1109/tnn.2007.899217

[10]. Differential Scanning Calorimeters. (2022). TA Instruments. Retrieved July 5, 2022, from https://www.tainstruments.com/products/thermal-analysis/differential-scanning-calorimeters/?gclid=Cj0KCQjwhLKUBhDiARIsAMaTLnGYmidYCIiDpYBdEqbT7ZmL4ynF-A_4PikOVRRRceDNC6PP6QCFWeIaAo4lEALw_wcB

[11]. Lorch, M. (2013, March 22). Shades of Gray, The Curious History of LCDs – Chemistry Blog. Chemistry Blog. http://www.chemistry-blog.com/2013/03/22/shades-of-gray-the-curious-history-of-lcds/

[12]. Tyson, J., & Carmack, C. (2021, September 16). How Computer Monitors Work. HowStuffWorks. https://computer.howstuffworks.com/monitor5.htm

[13]. liquid crystal display | electronics. (2022, February 2). Encyclopedia Britannica. Retrieved July 5, 2022, from https://www.britannica.com/technology/liquid-crystal-display.