International Journal of Research in Engineering and Science (IJRES)
ISSN (Online): 2320-9364, ISSN (Print): 2320-9356
www.ijres.org Volume 10 Issue 12 ǁ December 2022 ǁ PP. 449-461

"Plotting DSC Results using Logger Pro for a Binary Liquid Crystal System (BLCS)"

Mathew C. Doran 1 and Dipti Sharma (PhD) 2*
[1] *Undergraduate student, Emmanuel College, Boston, MA, USA*
[2] *Supervisor, Emmanuel College, Boston, MA, USA, * Corresponding Author: dsharmaphd@gmail.com*

ABSTRACT
This paper shows detailed results from Differential Scanning Calorimetry (DSC) of a Binary Liquid Crystal System (BLCS) that are plotted using Logger Pro data analysis software. This paper also focuses on how to plot graphs using Logger Pro that are also obtained from DSC. It then shows a comparison between the graphs obtained from DSC data to the graphs plotted with Logger Pro to check if graphs obtained from DSC instruments can be replotted in a similar way using Logger Pro. In conclusion, results show that Logger Pro is a good data analysis tool and laboratory software that can also be used to plot graphs and analyze research data for different materials.

KEYWORDS
Differential Scanning Calorimetry (DSC), Liquid Crystals (LCs), Binary Liquid Crystal System (BLCS), LoggerPro, Heat Flow, Endothermic, Exothermic, Melting, Nematic state, 1st Derivative, 2nd Derivative, 3rd Derivative

---

Date of Submission: 11-12-2022 Date of acceptance: 26-12-2022

I. INTRODUCTION

Differential Scanning Calorimetry (DSC) is a technique used to detect and analyze endothermic and exothermic transitions of an intended sample given a certain temperature change, to see if the sample shows any phase change. DSC helps obtain more accurate and detailed information of the state and thermal properties of material like transition temperatures and enthalpies. DSC uses a reference facing the same conditions as the sample of interest. Typically, DSC is used in polymer and academic research, like glass transition determination or analyzing melting and crystallization behavior. [1-6]

One of the two main DSC measurement methods is Heat-Flux DSC which involves a temperature-controlled furnace for the sample and reference to sit in, whereas power-compensated DSC controls the temperature of each crucible by providing a specific amount of electrical current to maintain the temperature. [1] Running a sample through a DSC will help determine phase change and other thermal behavior of that sample, which has been done numerous times in studies showing DSC analyzed phase transitions for certain types of materials. Several authors and researchers showed their work using DSC and some can be seen in these publications. [3-6] DSC is a good technique to see transitions or changes of state in any material, where one example of material can be given as Liquid Crystals.

Liquid crystal (LC) is a material that shows multiple states of matter based on the type of LC when it goes from solid to liquid state. [3-10] Liquid crystals have technological as well as biological applications.For instance, many proteins and cell membranes are LCs. Things like soap and related detergents, some clays and even technology as advanced as Liquid Crystal Displays (LCDs) are composed of LCs. [10] Years of research led to the discovery of 4-octyl-4-cyanobiphenyl (8CB) and 4-pentyl-4-cyanobiphenyl (5CB) liquid crystals that are used in a variety of LCD applications. We would like to search for a different LC by mixing two pure LCs together in a certain ratio to see if this sample is better for the LCD industry or not. We thought to combine two LCD-viable liquid crystal molecules 5CB and 4-heptyl-4-cyanobiphenyl (7CB) in a 1:1 ratio by weight to form a Binary Liquid Crystal System (BLCS). After making this BLCS, this sample was run into a DSC instrument and heat flow data was collected. Our next intention is to investigate the analysis capabilities of LoggerPro using the DSC results of this BLCS to see if results obtained from DSC can be plotted similarly using Logger Pro. [11-13] LoggerPro lab software is a computer program widely used in academia, mainly in physics and chemistry labs to collect and analyze data. The details of the paper can be seen below.

II. METHODS

Differential Scanning Calorimetry (DSC) is a smart instrument that conducts thermal experiments by providing heat flow to a sample and measuring a change in heat flow between the sample and a reference and then displaying that sample's heat flow results as a function of temperature or time. If data obtained from DSC shows a flat line with no change in the graph that means, there is no change in the state of the sample, or no phase transitions are taking place. Any change in the flat portion of the plot as mentioned above represents a change in the heat flow which signifies the change in the state of the sample and a presence of phase transitions.

In this paper, research is conducted with a mixture of two Liquid Crystals (LCs) to see how data and thermal results come using DSC. The same amount of 4-pentyl-4-cyanobiphenyl (5CB) and 4-heptyl-4-cyanobiphenyl (7CB) liquid crystals are added by weight to make a composition of 1:1 and then placed into a DSC 214 instrument from the NETZSCH company that is at WPI's Chemistry and Biochemistry department. The molecular weights of the 5CB and 7CB components individually are 249.36 and 277.41 g/mol respectively. The sample of 5CB+7CB was run at three different ramp rates as 5 °C/min, 10 °C/min and 20 °C/min from -30 °C to 100 °C and then back from 100 °C to -30 °C. The DSC instrument gave some plots and results that can be seen in this paper in pdf form. Our goal is to see if the plots obtained from the DSC instrument can be plotted further in detail using Logger Pro. The detailed results that are obtained from DSC and then plotted from Logger Pro can be seen in the result section.

III. RESULTS

Results obtained from DSC are plotted with Logger Pro in detail to see each component of results separately. All detailed results and graphs plotted with Logger Pro can be seen below.

In Figure 1, the three different heating and cooling results with three different ramp rates are plotted together in a row as a function of heat flow and time. The peaks appearing upwards are endothermic and the peaks appearing downwards are exothermic. Endothermic means the sample is absorbing heat whereas exothermic means the sample is releasing heat while they are heated or cooled. Endothermic peaks appeared in heating and exothermic peaks appeared in cooling. The first endothermic peak is a melting peak, and the second endothermic peak is a nematic peak in heating whereas the one exothermic peak is the nematic in cooling. Similar patterns of endothermic and exothermic appeared two more times for two different ramp rates with DSC in the same plot shown as larger peaks in the same Figure 1.

Figure 2 is a zoomed-in version of Figure 1 to show the melting and nematic phase transitions of the LC mixture at R=5°C/min only. The tall peak represents the melting phase that requires more energy input than both heating and cooling nematic phase transitions. The vertical section of the plot that switches from positive to negative heat flow shows when the DSC went from heating to cooling.

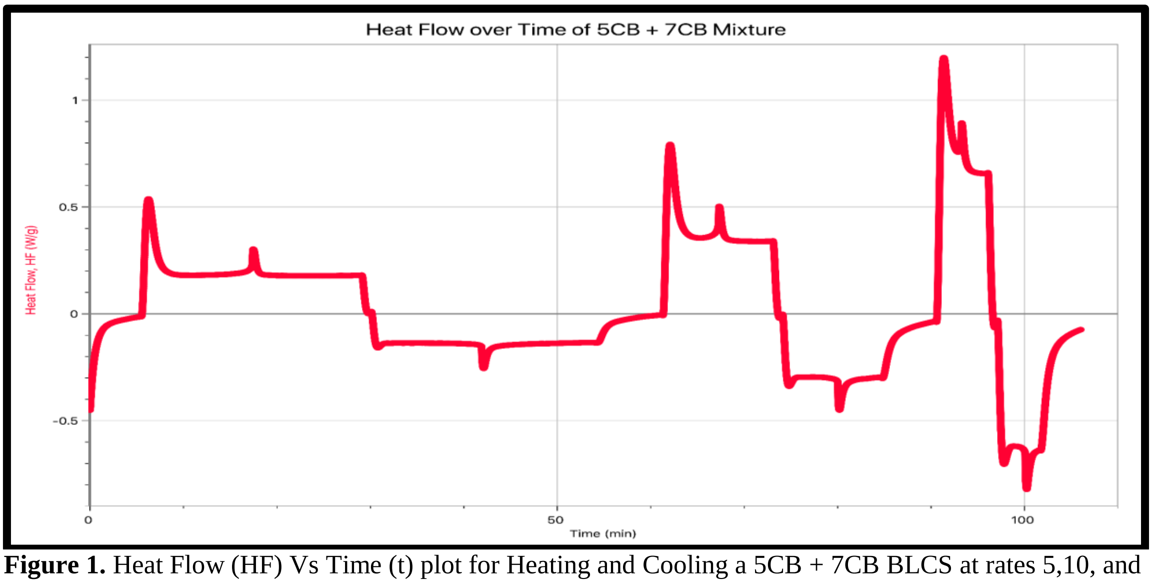

Figure 1. Heat Flow (HF) Vs Time (t) plot for Heating and Cooling a 5CB + 7CB BLCS at rates 5,10, and 20°C/min.

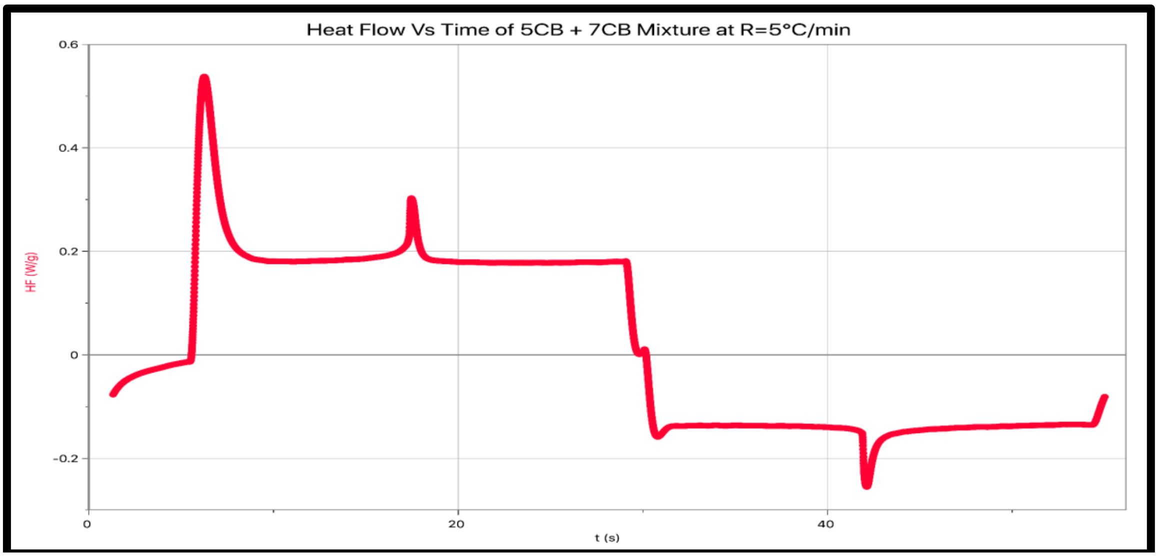

Figure 2. HF Vs t plot for Heating and Cooling a 5CB + 7CB BLCS at R=5°C/min.

Figure 3 shows the first derivative of Figure 2 withsharp, steep peaks where there are phase transition peaks in Figure 2. The first derivative of the heat flow is on the y-axis and the time is on the x-axis, plotted using the calculated column in LoggerPro. Moving from left to right the tall peaks represent the melting, heating nematic and cooling nematic phase transitions.

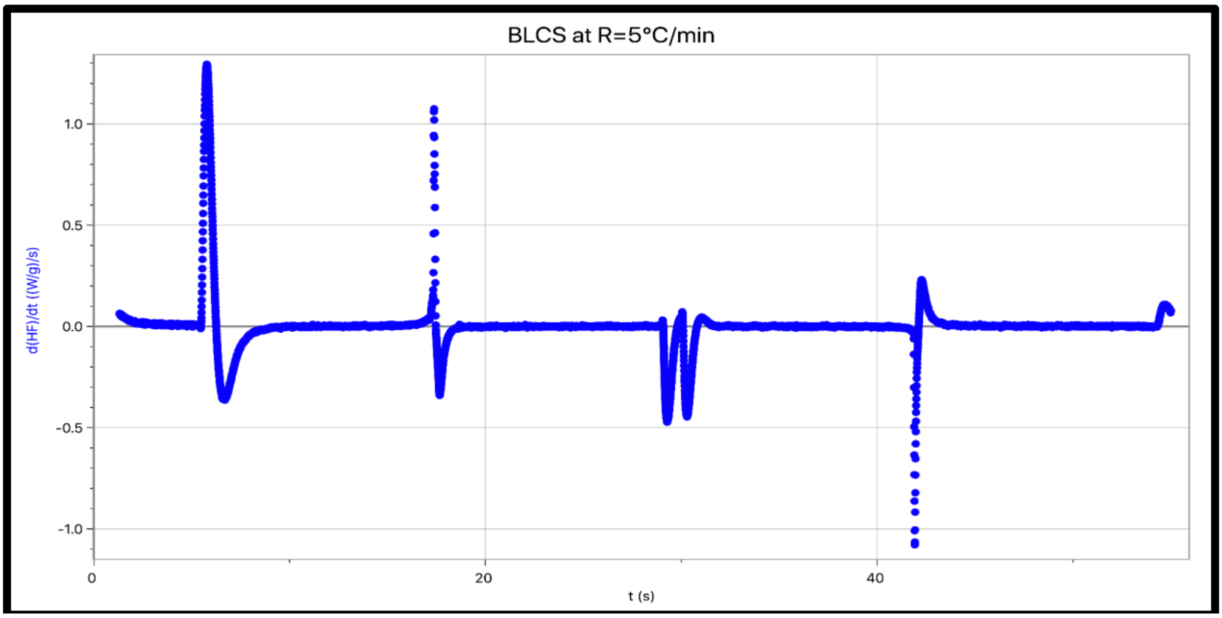

Figure 3. First derivative of heat flow **[**d(HF)/dt Vs t] for heating and cooling a 5CB + 7CB BLCS at R=5°C/min.

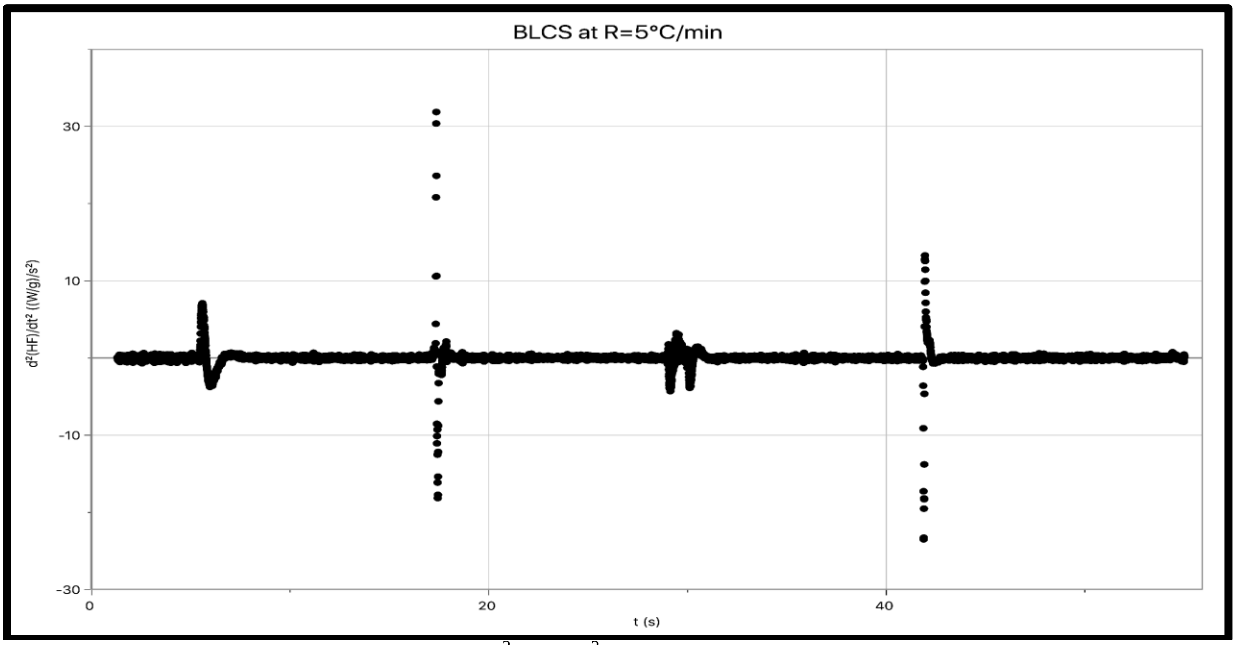

Figure 4. Second derivative of heat flow **[**$d^2(HF)/dt^2$ Vs t] for heating and cooling a 5CB + 7CB BLCS at R=5°C/min.

Figure 4 shows the second derivative of Figure 2 and shows steep peaks where the nematic transition peaks are in Figure 2. Unlike the first derivative, the plot is less tall where the melting transition peak lies in Figure 2. The second derivative of the heat flow is on the y-axis and the time is on the x-axis. The plot was made using the calculated column function in LoggerPro.

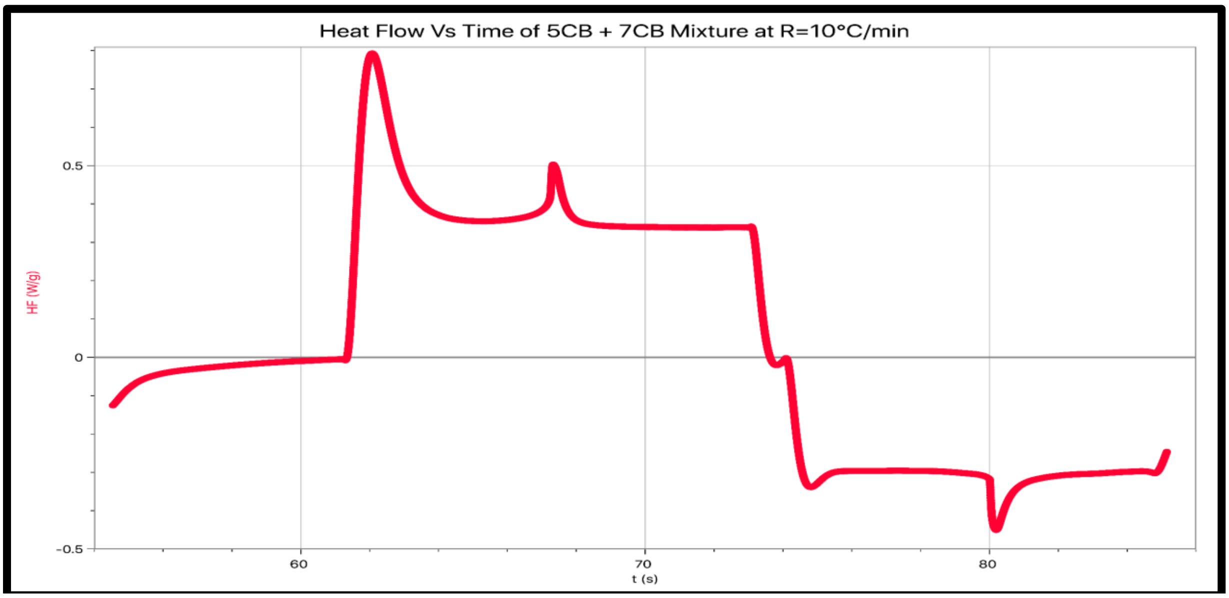

Figure 5. HF Vs t plot for Heating and Cooling a 5CB + 7CB BLCS at R=10°C/min.

Figure 5 is an enlarged version of Figure 1 to show the melting and nematic phase transitions for the LC mixture at R=10°C/min. The melting and nematic transition peaks are wider and closer together compared to the peaks seen in Figure 2 for R=5°C/min.

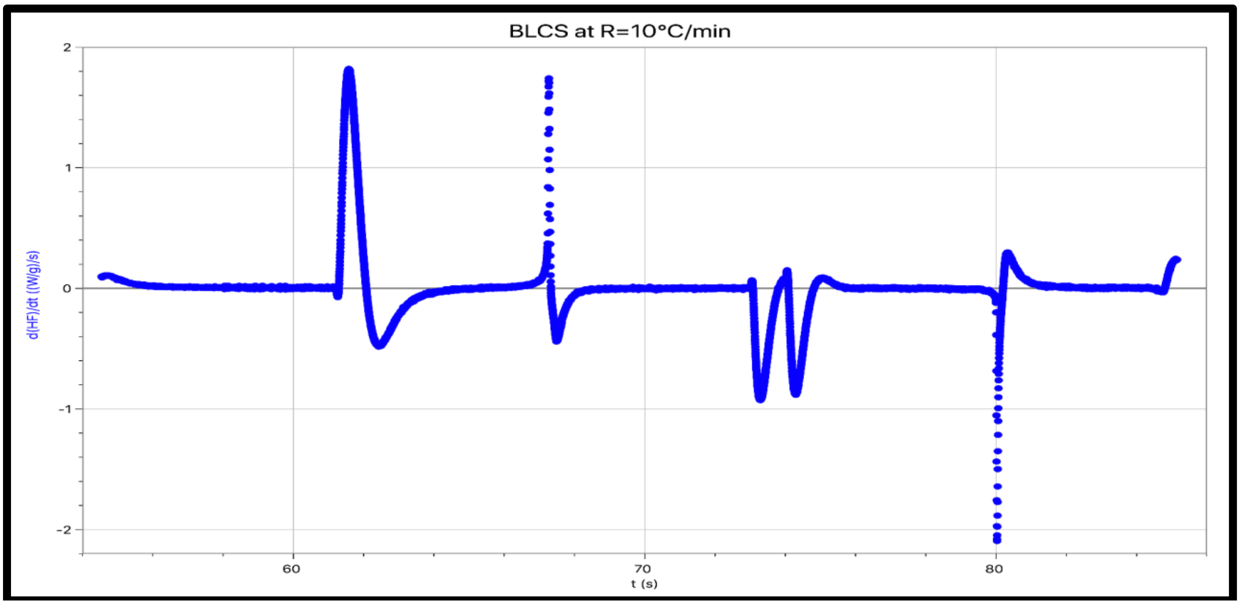

Figure 6. First derivative of heat flow [d(HF)/dt Vs t] for heating and cooling a 5CB + 7CB BLCS at R=10°C/min.

Figure 6 shows the first derivative of Figure 5 and shows sharp, slightly fewer steep peaks where there are phase transition peaks in Figure 2. The first derivative of the heat flow is plotted on the y-axis and the time on the x-axis using the calculated column.

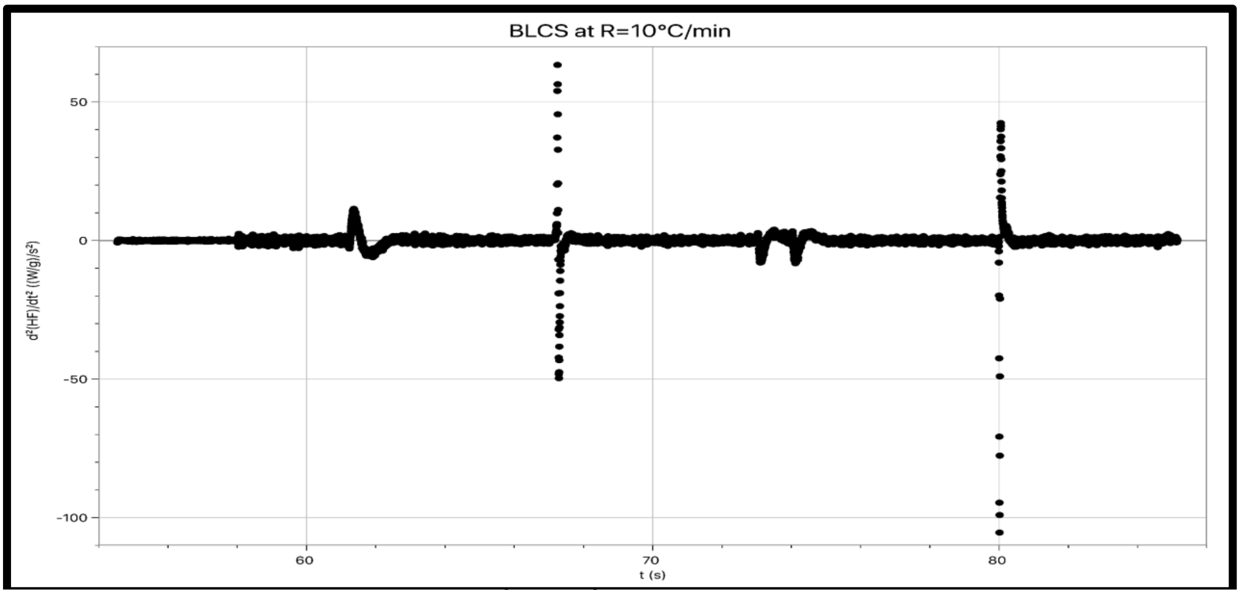

Figure 7. Second derivative of heat flow [d^2(HF)/dt^2 Vs t] for heating and cooling a 5CB + 7CB BLCS at R=10°C/min.

Figure 7 shows the second derivative of Figure 5 and shows sharp peaks where the nematic transition peaks are in Figure 5. Unlike the first derivative, the plot is shorter where the melting transition peak lies in Figure 5. Using a calculated column, the second derivative of the heat flow was plotted on the y-axis with the time on the x-axis.

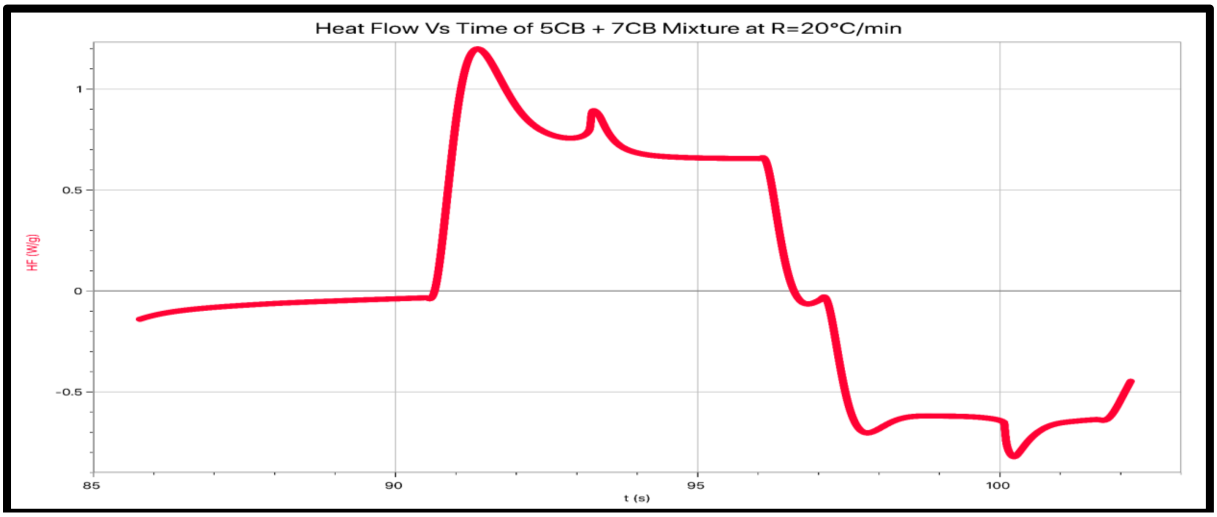

Figure 8. HF Vs t plot for Heating and Cooling a 5CB + 7CB BLCS at R=20°C/min.

Figure 8 is an enlarged version of Figure 1 to show the melting and nematic transition peaks for the LC mixture at R=20°C/min. These melting and nematic phase transition peaks are even wider and closer in proximity than the phase transitions of the other ramp rates. The vertical portion of the plot shows where the calorimeter went from heating to cooling the binary LC system.

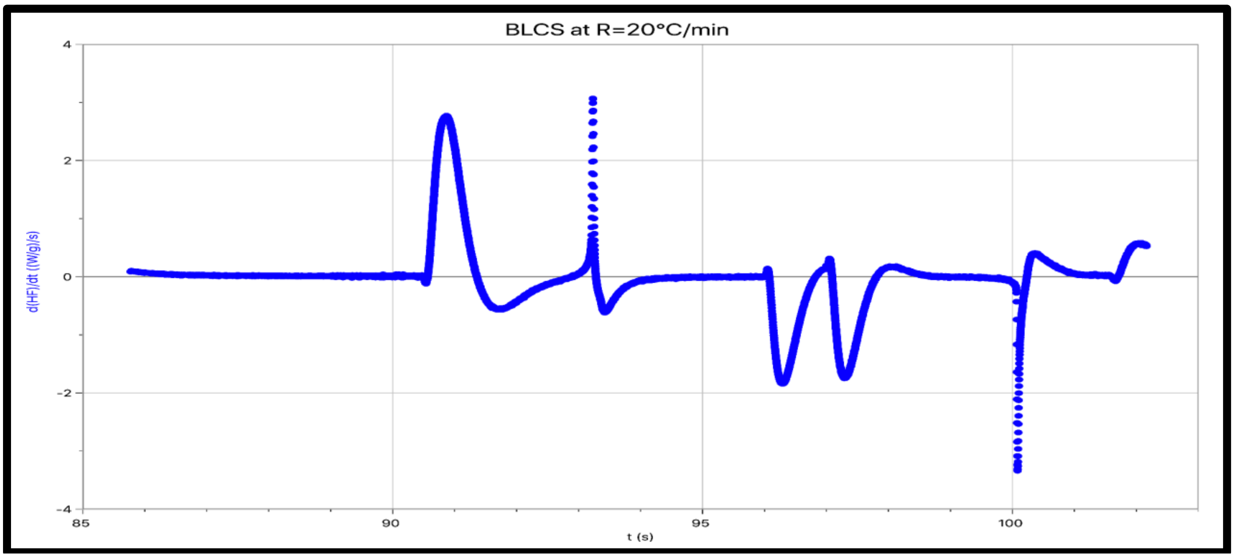

Figure 9. First derivative of heat flow [d(HF)/dt Vs t] for heating and cooling a 5CB + 7CB BLCS at R=20°C/min.

Figure 9 shows the first derivative of Figure 8 and shows steep peaks for nematic transition but less sharp peaks for melting than in Figure 3 and 6. The first derivative of the heat flow is on the y-axis and the time is on the x-axis. The plot was made using the calculated column function in LoggerPro.

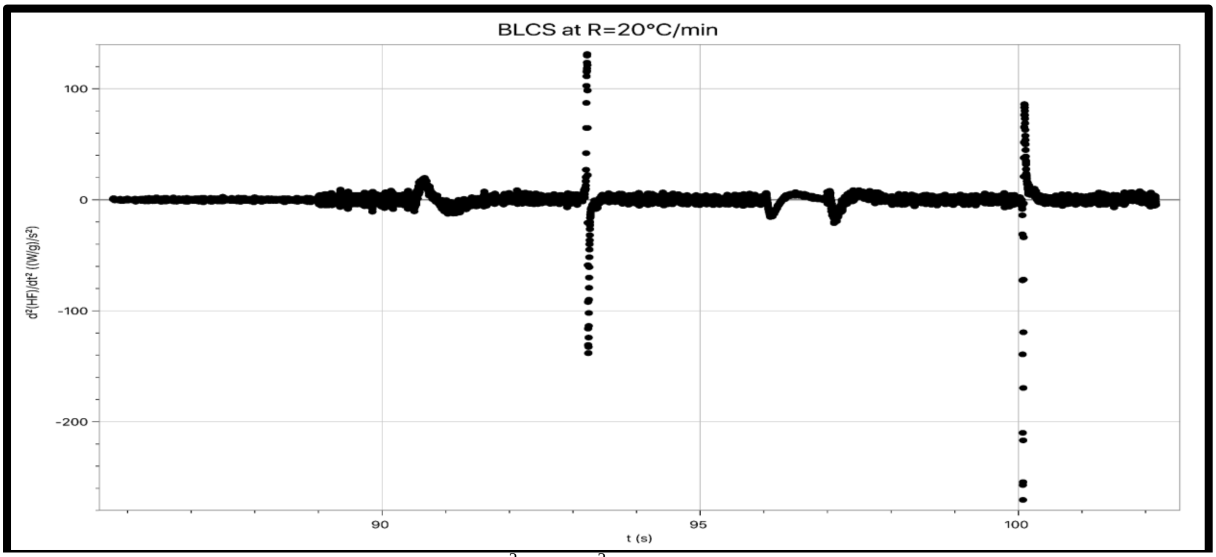

Figure 10. Second derivative of heat flow [$d^2(HF)/dt^2$ Vs t] for heating and cooling a 5CB + 7CB BLCS at R=20°C/min.

Figure 10 shows the second derivative of Figure 8 and shows sharp, steep peaks where the nematic transition peaks are in Figure 8. Not like the first derivative, the plot is shorter where the melting transition peak lies in Figure 8. The second derivative of the heat flow was a calculated column (y) in Logger Pro with time on the x-axis.

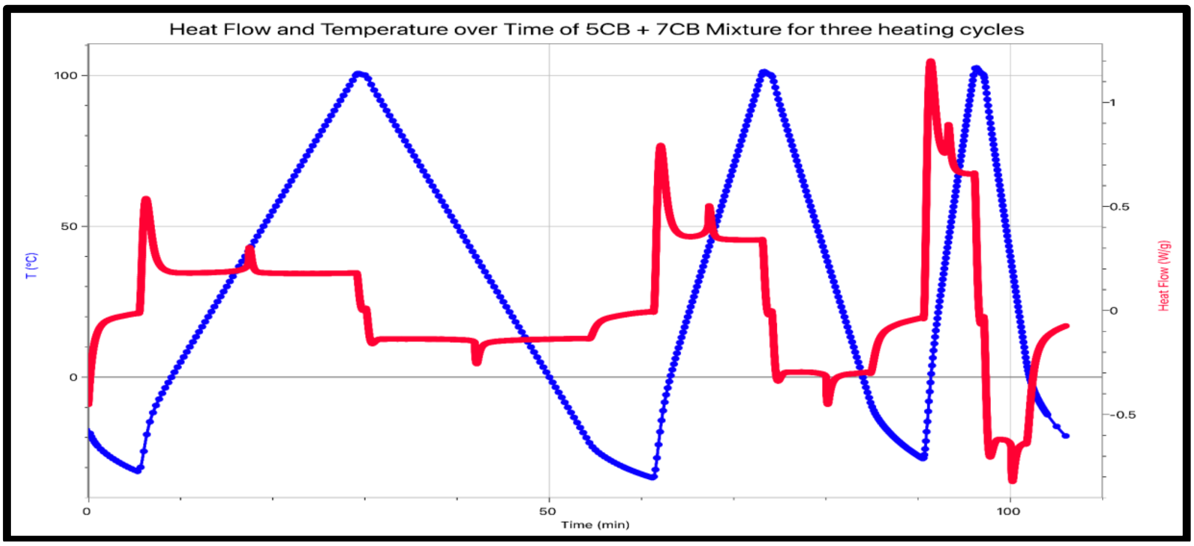

Figure 11. HF and T Vs Time of three varied rate heating runs for a 5CB + 7CB mixture.

Figure 11 shows the temperature and heat flow over time for each heating run. Where the blue temperature plot is wider it shows that heating and cooling took longer, representing heating at R=5°C/min. So, moving to the right the heat flow and temperature graphs get squished horizontally showing an increase to R=10°C/min and then R=20°C/min. An increase in heating rate suggests a decrease in time.

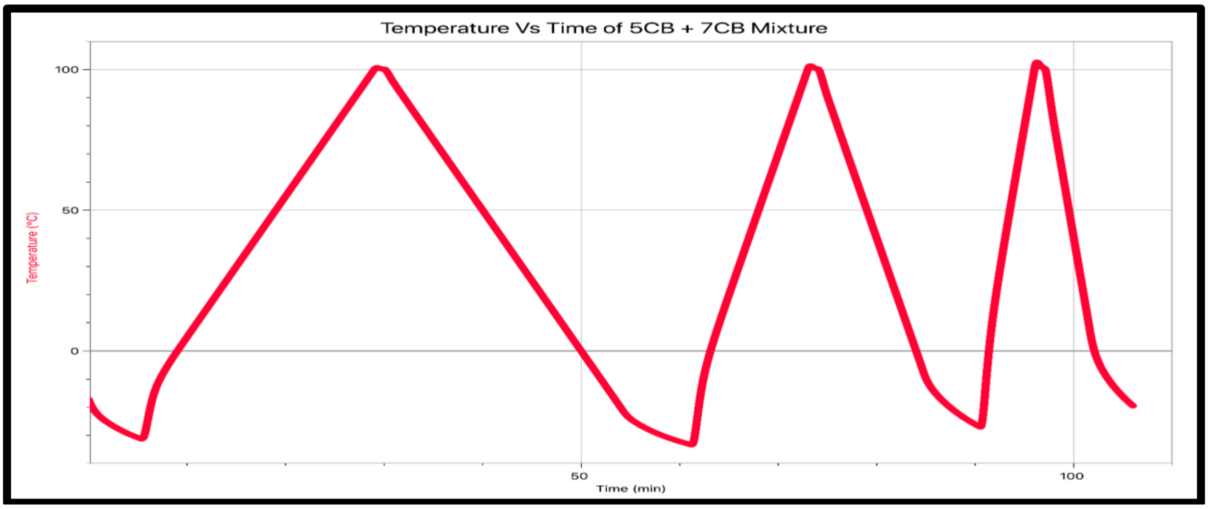

Figure 12. Temperature Vs Time for Three Heating cycles of 5CB + 7CB BLCS at three different rates.

Figure 12 shows the three separate heating and cooling cycles with increasing ramp rates from left to right. An increase in ramp rate increases the rate of heating of the LC sample which is why the waves are getting thinner as the ramp rate increases.

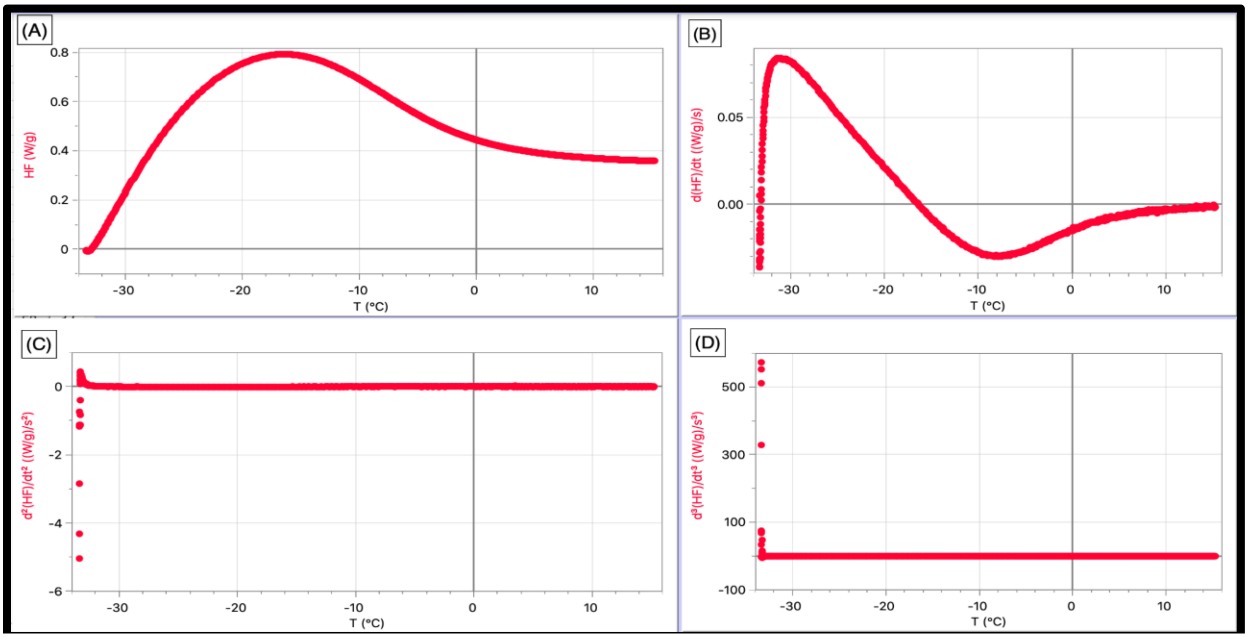

Figure 13. Comparing (a) HF Vs T for Melting transition of 5CB + 7CB BLCS at R=10°C/min to its (b) first, (c) second and (d) third derivatives.

Figure 13 shows detailed results of BLCS for ramp rate 10°C/min as four sub-parts from A-D. These parts show how Logger Pro is used to analyze heat flow data for the 1st, 2nd, 3rd derivatives of heat flow. The top left plot has the HF Vs T of the melting transition peak. The top right graph shows the 1st derivative of that melting transition, the bottom left shows the 2nd derivative, and the bottom right shows the 3rd derivative. The derivative plots were created through LoggerPro's calculated column function. These heat flow derivative plots prove a phase change appeared in BLCS for melting.

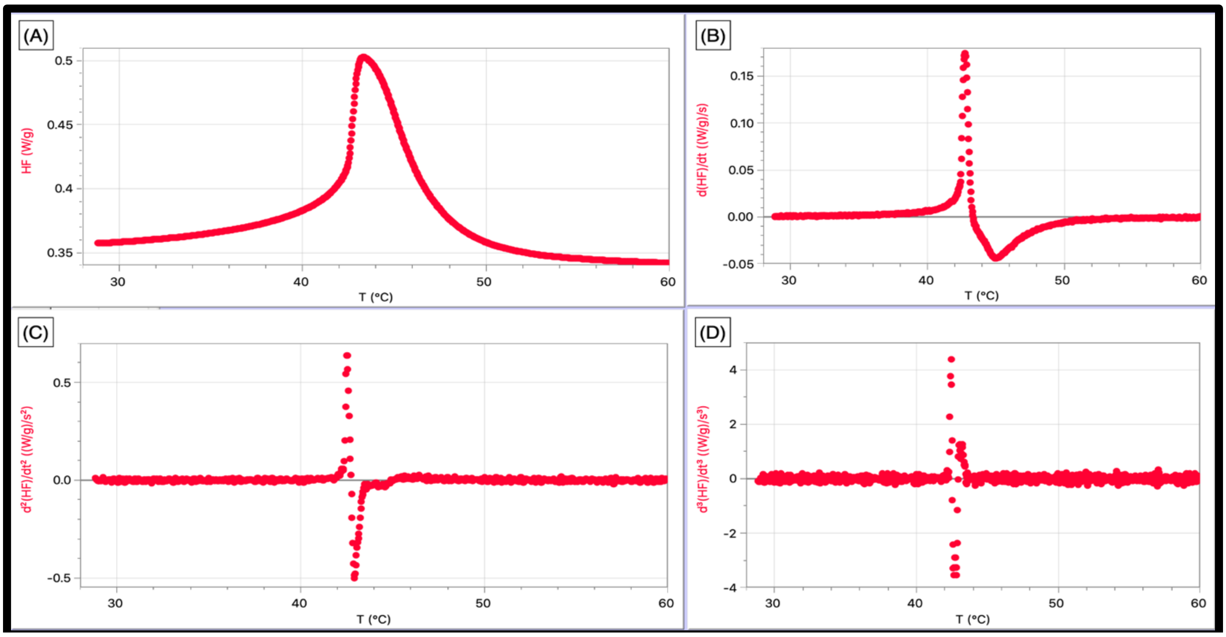

Figure 14. Comparing (a) HF Vs T for Heating Nematic transition of 5CB + 7CB BLCS at R=10°C/min to its (b) first, (c) second and (d) third derivatives.

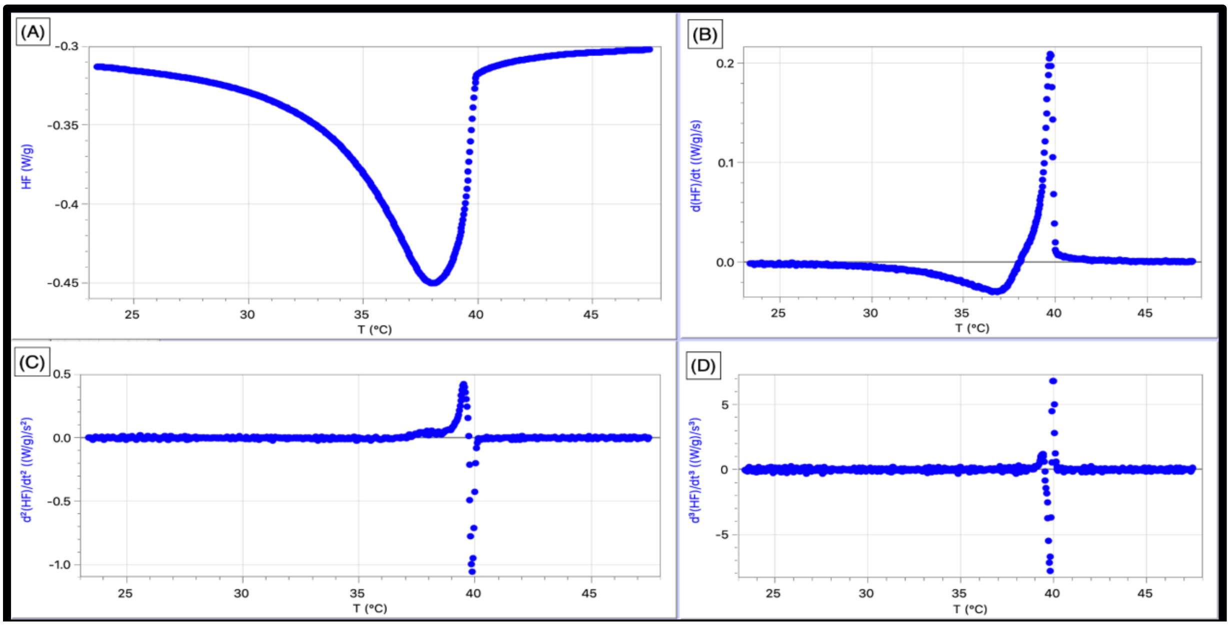

Figure 15. Comparing (a) HF Vs T for Cooling Nematic transition of 5CB + 7CB BLCS at R=10°C/min to its (b) first, (c) second and (d) third derivatives.

Figure 15 shows the Logger Pro analysis of the cooling nematic phase transition peak of the 5CB + 7CB mixture at R=10°C/min. The top left plot has the HF Vs T of the cooling nematic transition peak. The top right shows the 1st derivative of that nematic transition, the bottom left shows the 2nd derivative, and the bottom right shows the 3rd derivative plots calculated in columns in LoggerPro.

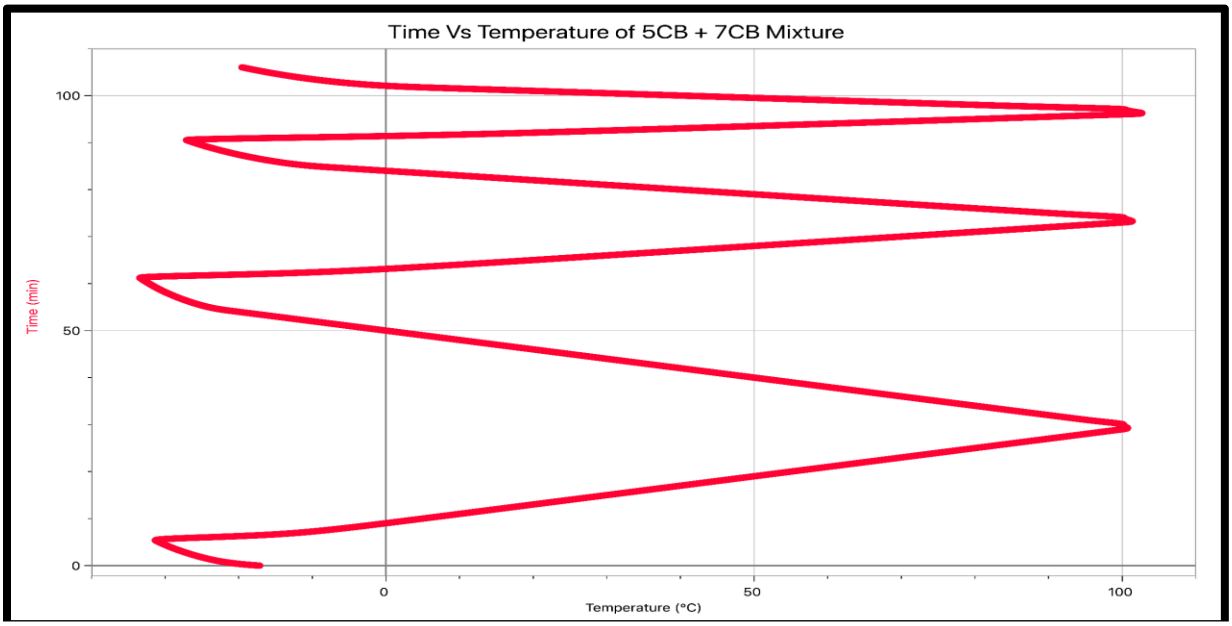

Figure 16. Time Vs Temperature of three separate rate heating cycles of 5CB + 7CB BLCS.

Figure 16 displays the opposite x and y-axis orientation of Figure 12 for heating the 5CB + 7CB BLCS three times at different ramp rates. Starting from the bottom of the plot the R=5°C/min run continues for one full oscillation from -30°C to 101°C then back to -30°C. The R= 10 and 20°C/min DSC cycles are the other two, shorter waves in order moving up the plot. This Figure 16 also shows how ramp rate looks when it is plotted as time vs temperature plot for three ramp rates for BLCS.

All figures shown above from Figure 1 to Figure 16 are the detailed results plotted with Logger Pro; those were obtained as heat flow vs time/temperature data from DSC. The following graphs and results are plotted by DSC and taken from the DSC instrument in pdf form to see how similar data can be plotted with Logger Pro. The graphs obtained from the DSC instrument are shown below as Figure 17 and Figure 18.

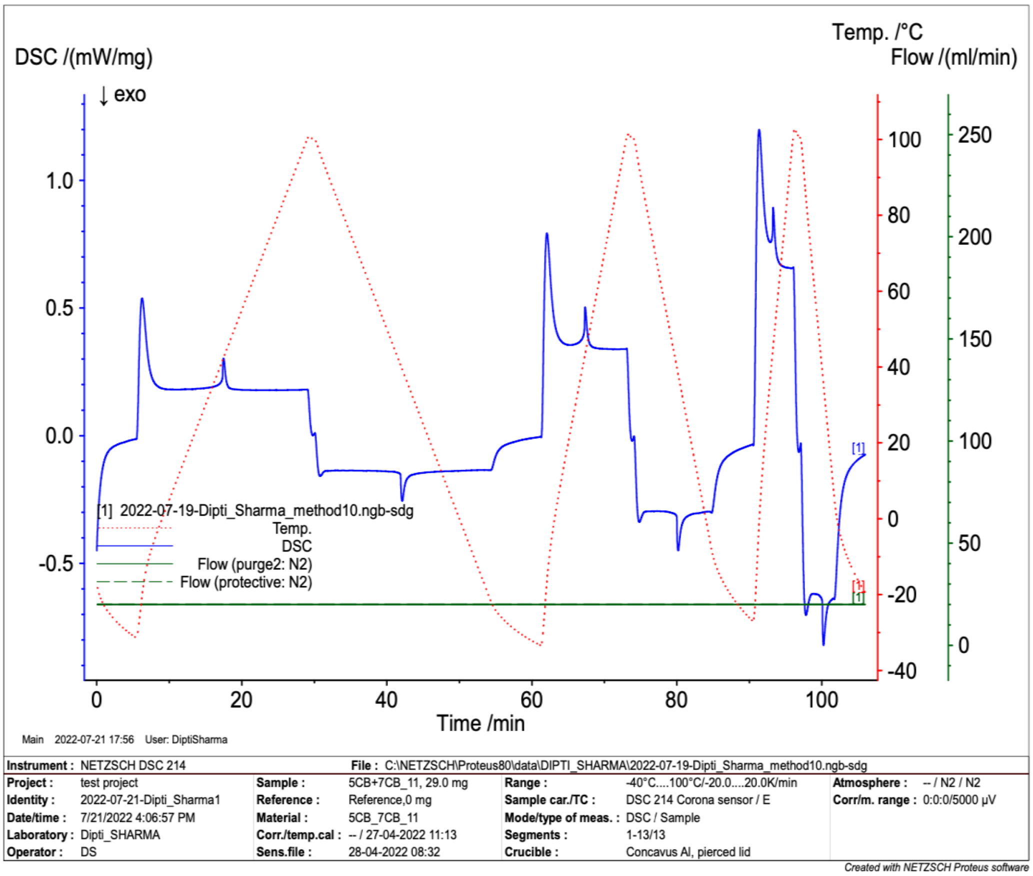

Figure 17. Combined all results of BLCS obtained from DSC shown in the form of a pdf file taken from DSC for all three ramp rates 5,10 and 20°C/min as heat flow versus time and temperature plot.

In this Figure 17, it can be seen that the left side Y axis shows heat flow and X axis shows time whereas the right-side Y axis shows temperature and Nitrogen flow. Our intention is to see how the heat flow of BLCS changes with time and temperature for three ramp rates for heating and cooling. If all detailed results plotted as Figure 1 to Figure 16 are compared with Figure 17, all Figures from Figure 1-6 follow the similar trend and nature of the sample in analyzed data.

Figure 18 is obtained from DSC including two derivatives of heat flow for BLCS. Figure 18 shows DSC results that are combined Figures 3,6,9 and 11. Using Logger Pro, we can split these graphs and show more details of BLCS. Graphs plotted with Logger pro are found like the graphs obtained by DSC.

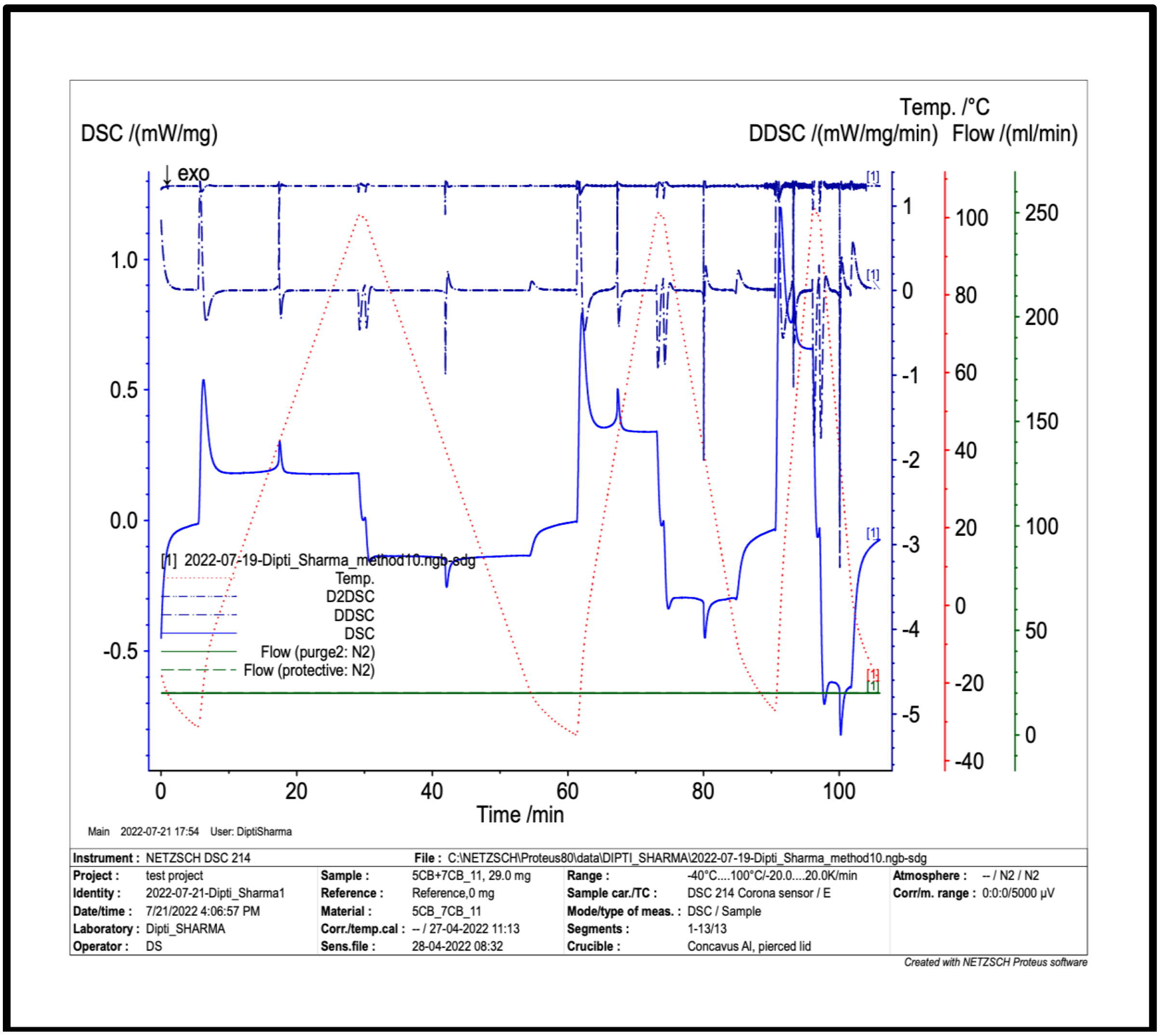

Figure 18. Adding twoderivatives of heat flow for the BLCS, all results of BLCS shown in this pdf file are taken from DSC at ramp rates 5,10 and 20°C/min as heat flow versus time.

IV. CONCLUSION

The data and graph obtained from the DSC instrument was plotted with Logger Pro for BLCS at three different ramp rates in detail. It is found that all graphs found in DSC appear in a similar way when plotted with Logger Pro. Logger Pro can be used for further analysis of BLCS to show more details of each result obtained from DSC. The data obtained from DSC can be plotted as a single or as individual graphs using Logger Pro. Similarities in DSC and Logger Pro graphs can be seen between Figure 18 and Figures 3, 6, 9 and 11. Logger Pro is useful to analyze each component of DSC data in detail, proven in the details of each phase transition (Figures 13-15), rather than using an entire heating and cooling cycle to discover more about the thermal behavior of a BLCS. Overall, Logger Pro is found to be a good tool for research analysis and can be used to analyze DSC data further in detail for any sample.

ACKNOWLEDGEMENT

Authors like to acknowledge Professor John C. MacDonald from the Chemistry and Biochemistry department and Andrew Butler from Life Sciences and Bioengineering Center, WPI, Worcester, MA for helping with the Differential Scanning Calorimetry instrument. Authors also like to acknowledge NETZSCH company for DSC 214 instruments, and pans and lids. The student author likes to acknowledge Dr. Dipti Sharma for supervising this research internship with Liquid Crystal, and Emmanuel College for running internship programs.

REFERENCES

[1]. Differential scanning calorimetry - how does it work? LinseisMessgeräte GmbH. (2020, November 26). Retrieved March 4, 2022, fromhttps://www.linseis.com/en/methods/differential-scanning-calorimetry-dsc/

[2]. Haines PJ, Reading, M, Wilburn FW. Differential thermal analysis and differential scanning calorimetry. In Brown ME (ed): Handbook of Thermal Analysis and Calorimetry, vol 1. The Netherlands: Elsevier Science BV, 1998;279–361.

[3]. 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

[4]. 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

[5]. 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

[6]. 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

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

[8]. What Are Liquid Crystals? (n.d.). Kent State University. Retrieved October 31, 2022, from https://www.kent.edu/amlci/what-are-liquid-crystals

[9]. Libretexts. (2020, August 15). Liquid Crystals. Chemistry LibreTexts. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Physical_Properties_of_Matter/States_of_Matter/Liquid_Crystals

[10]. Wikipedia contributors. (2022, October 30). Liquid crystal. Wikipedia. https://en.wikipedia.org/wiki/Liquid_crystal

[11]. Sharma, D., & Doran, M. (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.

[12]. Sharma, D., & Mello, J. (2022). Details of Nematic Phase Transition and Nematic Range of 5OCB Liquid Crystal using Logger Pro. International Journal of Research in Engineering and Science (IJRES), 10(9), 197–217.

[13]. Sharma, D., & Mello, J. (2022a). Effect of Reheating and Ramp Rates on Phase Transitions of 5OCB Liquid Crystal using Logger Pro. International Journal of Research in Engineering and Science (IJRES), 10(9), 218–236.