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PhasIR: An Instrumentation and Analysis Software for High-throughput Phase Transition Temperature Measurements

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ABSTRACT

We have designed an open-source and high-throughput thermal analysis system for fast and accurate estimation of phase transition temperatures for up to 96 samples analyzed simultaneously. The results are comparable to current state of the art systems such as differential scanning calorimetry (DSC), which is costly and time-consuming. The PhasIR hardware system utilizes an infrared camera to optically record thermal processes that result from the melting/freezing and/or evaporation of samples, while the accompanying open-source software package allows for subsequent batch analysis and processing to extract phase transition temperatures. The PhasIR system showed good agreement with DSC results for both pure substances and mixtures, such as deep eutectic solvents (DES). The all-in-one hardware and software system can be easily replicated and built using relatively inexpensive components at a total estimated cost of $1,080 USD. Implementation of the PhasIR system will allow for increased throughput in material thermal characterization and broader investigation of material design spaces.

METADATA OVERVIEW

Main design files: *https://github.com/pozzo-research-group/phasIR*

Target group: Scientists requiring high-throughput thermal analysis of organic samples (e.g. pharmaceuticals, polymers, food ingredients, greases, solvents).

Skills required: CNC machining, 3D printing, basic electronics and programming.

Replication: No builds known to the authors so far.

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KEYWORDS:
High-Throughput Experimentation; Thermal Analysis; Thermal Imaging; Melting Point Determination; Deep-Eutectic Solvents

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(1) OVERVIEW

INTRODUCTION

Performing thermal analysis of organic samples is an integral part of materials characterization. This is routinely used to determine melting/boiling points, phase transitions, to assess sample purity, and thermal stability, which are all important features to a number of research and technology areas including the development of pharmaceuticals, advanced materials, and foods. The industry standards for this type of analysis are usually based on differential scanning calorimetry (DSC) and differential thermal analysis (DTA), both of which measure temperature differences of a reference and a sample material under identical thermal cycles [1]. While DSC and DTA allow for accurate and precise results, measurements can take upwards of an hour per sample to complete. This becomes extremely time consuming and expensive to run for very large sample sets. While additional instrumentation could be added to increase throughput of these measurements, such as autosamplers, the technology as a whole is currently not conducive to high-throughput experimentation, which has become increasingly powerful for materials discovery when it is coupled with data science and machine learning algorithms [2–6].

Recently, the concept of optically determining melting points and other thermal properties with an infrared (IR) camera has been proposed. The first to introduce this method was K. Kawakami in 2010 [7]. Kawakami used an IR camera to observe the melting process of common active pharmaceutical ingredients on a programmable hot plate. As the samples melted, an increase in their thermal conductivity resulted in a temporary spike in the temperature, from which the melting point could be estimated. The estimated melting points showed good agreement with melting points obtained through DSC. Because the technique used thermal imaging as a basis, it was proposed by the authors that it could be used to sample multiple materials at once. Similarly, Hou et al. also used this method to estimate melting points and other thermal properties for common materials using a dedicated aluminum pan with 16 wells for holding samples [8]. While these proof-of-concept systems have emphasized the high-throughput potentials for this unique method, the demonstration of a fully integrated and open-source system that can be easily replicated by other users is still lacking. Moreover, the analysis also needs to be optimized for reliable automatic data interpretation so that the bottlenecks for sample analysis are not simply transferred from the measurement to the user that is interpreting the results.

In this paper we describe the design, construction, software development, and implementation of a high throughput and open-source thermal analysis system, called PhasIR. The system consists of a Raspberry Pi microcomputer, a FLIR Lepton 3.5 IR camera, an Echotherm IC25 Peltier plate, and aluminum multi-well plates as the basic elements, ***Figure 1***. Our design allows for simultaneous measurement and data acquisition which can be subsequently analyzed by an accompanying open-source Python-based software package. This all-in-one system can be easily replicated and modified as most of the hardware components are either relatively inexpensive or commonly found in many laboratories. In addition, the open-source nature of the software package allows for modularity and flexibility for the user when selecting hardware components.

OVERALL IMPLEMENTATION AND DESIGN

PhasIR System

The PhasIR system consists of a FLIR Lepton 3.5 IR camera that is placed at a fixed position above a Peltier plate to image a sample array. The Echotherm IC25 can be used with aluminum 96, 48 or 24 well plate systems that are fabricated from black anodized aluminum for high-throughput measurement of phase transition temperature(s), ***Figure 2***. Samples are collected on a metal plate with conical-shaped wells and then placed on the heat source. The conical structure of the wells was determined to be critical to maintaining sample positioning, in particular after melting transitions, to facilitate automatic analysis with reduced error. Once the temperature ramp is initiated, the IR camera feed is also launched to allow for simultaneous data collection for all samples. As the plate heats up, the temperature of the objects present in the camera field of view is measured and saved as a collection of frames in an *.HDF5* file format that is saved once the run is completed. The overall design of the PhasIR hardware system takes inspiration from DTA techniques that operated on a single sample at a time [9].

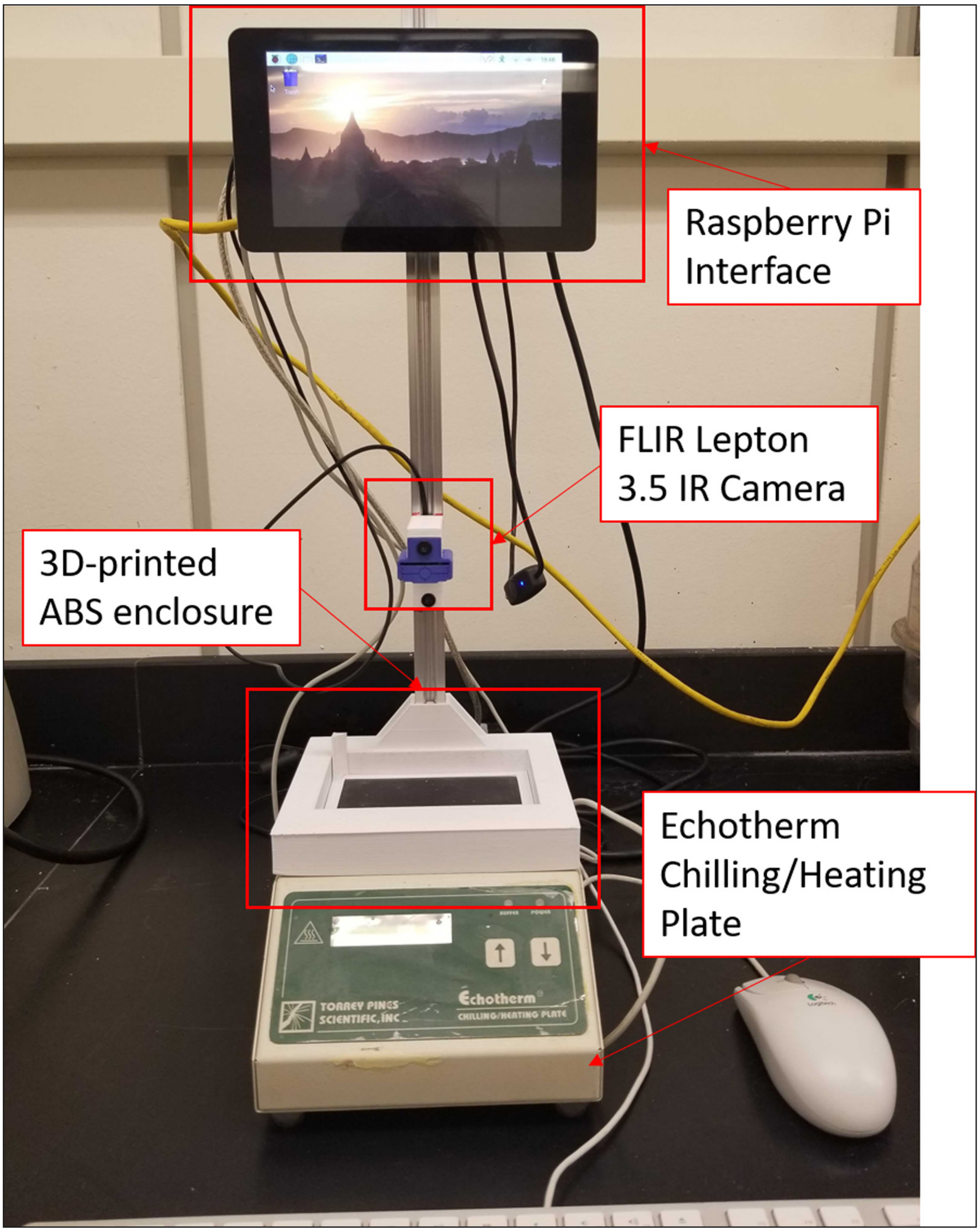

Figure 1 PhasIR Hardware System. This is composed of a Raspberry Pi Interface, an IR Camera, a 3D printed plate enclosure and a Peltier plate.

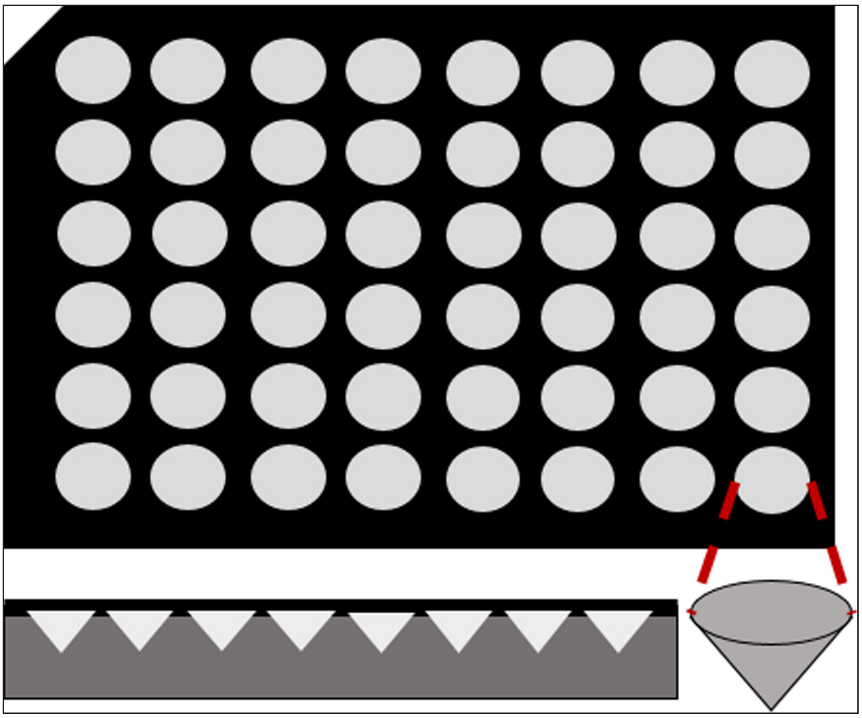

Figure 2 Schematics of the aluminum well plate design. The top of the plate is coated in black paint to obtain an emissivity of one. The wells have a conical shape to ensure consistent sample location throughout the phase transition process.

However, instead of using a furnace and a thermocouple system, the black anodized aluminum plate is used as the reference point for the plate temperature while the sample temperature is obtained at the center-point of the conical wells. All of this is collected simultaneously using the IR camera that captures the full view of the plate. The data file that is produced by the camera is then analyzed with the accompanying homonymous open-source software package. The PhasIR system also provides a 3D-printed Acrylonitrile Butadiene Styrene (ABS) enclosure that allows for consistent placement of the well plates below the IR camera and centered on top of the heating element. A consistent position of the plate allows for easier and more streamlined data collection.

Hardware Development

We utilized a FLIR Lepton 3.5 Radiometric IR camera procured from GroupGets to capture thermal processes occurring as a result of the simultaneous heating/cooling of samples in parallel, ***Figure 3a***. The Dynamic range of this camera varies from –10°C to +140°C in high-gain mode and –10°C to +400°C in low-gain mode, with radiometric accuracy of 5% and 10%, respectively. This is adequate for capturing a wide range of phase transitions occurring in organic materials. The image size obtained from the Lepton 3.5 is 160 × 120 pixels. The Lepton 3.5 camera core was integrated with the PureThermal 2 Smart I/O module procured from GroupGets in order to interface as a USB webcam, ***Figure 3c***. The Lepton 3.5 and PureThermal 2 board were both enclosed in a case that was also provided by GroupGets. To obtain a collection of thermal images and save them using the IR camera, the open-source software *purethermal1-uvc-capture* available on Github was used [10]. This software allows to start the camera, obtain a real-time frame of the system, as well as record and save the data collected into an .HDF5 file all from the same window, ***Figure 4***.

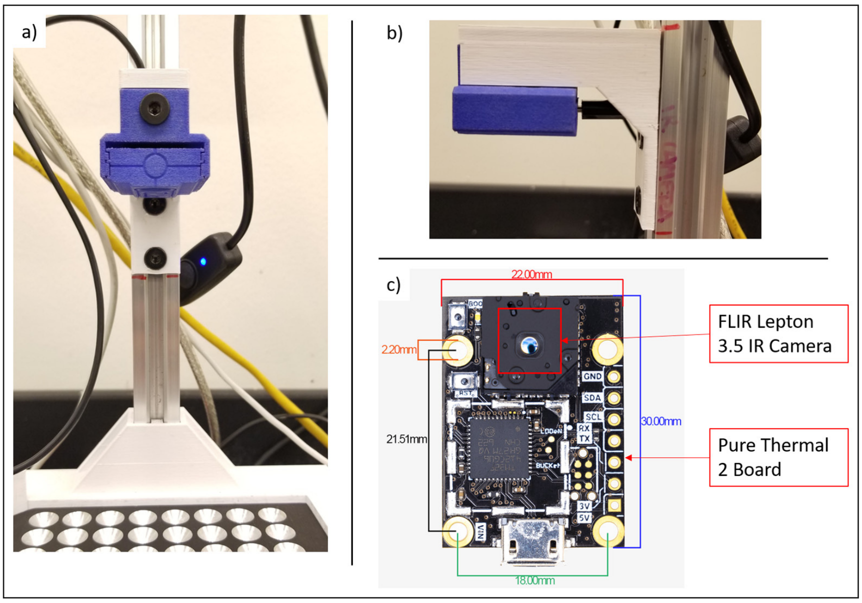

Figure 3 Lepton 3.5 and PureThermal 2. **a)** Front view of mounted camera and board. **b)** Side view of mounted camera and board. **c)** Schematic of Lepton 3.5 attached to PureThermal 2 board.

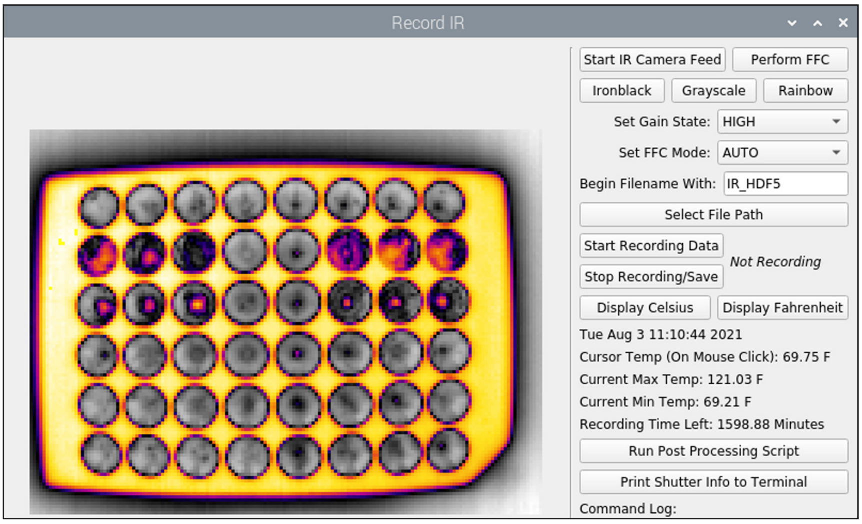

Figure 4 Example window of the image capture software purethermal1-uvc-capture. A real-time image of the system is displayed on the left, while the right panel allows the user to interact with the camera, start the data collection and save the results into an .HDF5 file.

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The well plates were designed from 6061 black anodized aluminum bars procured from McMaster Carr (#7083T47) with length, width, and height dimensions of 12 × 6 × 0.5 inches (30.48 × 15.24 × 1.27 cm). These aluminum bars were anodized with black dye to maximize the emissivity and minimize reflectivity of the system, which is critical for the IR camera to obtain a proper radiometric measurement. A Tormach 1100M CNC mill was used to machine the aluminum bars into the approximate length and width of the ANSI/SLAS standard microplates that are routinely used in biotech analyses, 5” by 3.4” (12.7 by 8.64 cm) [11]. Three well plates can be obtained from each stock piece of aluminum. Plate designs with 96, 48, and 24 conical wells were machined. These help to balance the need for high-throughput versus the improved accuracy that may be obtained from the use of larger samples and more averaged pixels in the subsequent analysis. The conical-well designs ensure that the samples constantly remain in the center of the well throughput the melting process. The wells were machined specifically with a 90-degree countersink end mill.

As for the heating element, a Torrey Pines Scientific Inc. Echotherm IC25 Chilling/Heating Peltier plate was used but other heating/cooling plates would also be suitable to use with minor modifications to the camera and plate stabilization hardware design, ***Figure 5***. The operable temperature range for this Echotherm plate is between –10°C to +100°C. The rectangular active heating element on the Echotherm measures approximately 4.3” by 2.8” (10.92 by 7.11 cm) which is very similar to the size of the designed well plates, making it ideal for integration into the PhasIR system.

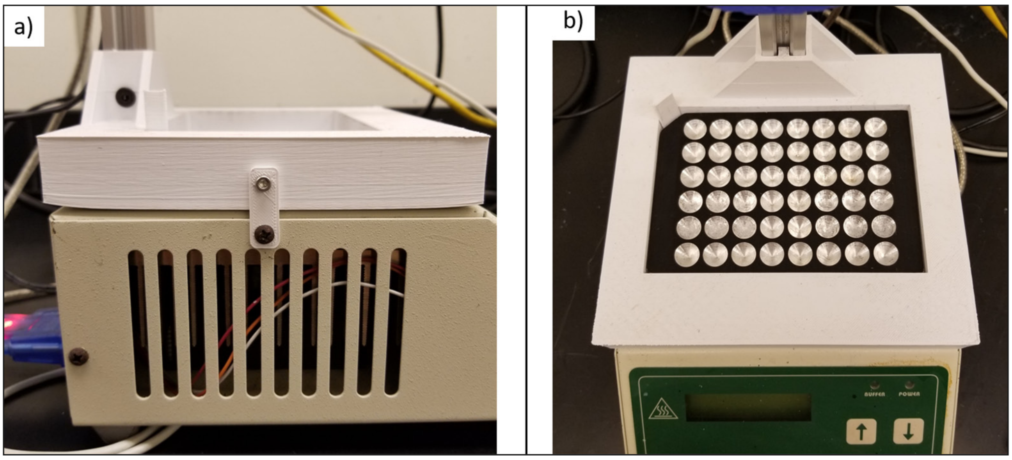

Figure 5 Enclosure and Conical Well Plate. **a)** Side view of enclosure mounted on to the Echotherm IC25 via a set of screws. **b)** Top view of the Echotherm IC25 and enclosure with conical-well 48 well plate inside.

Finally, these components were integrated together in order to design a compact all-in-one system. A 3-D printed enclosure was designed that is secured to the Echotherm via screws on the main body, ***Figure 5a***. This helps to hold the aluminum well plate in a consistent position during the entire measurement, prevents movements of the IR camera after it is locked in place, and also provides some thermal insulation on the sides of the aluminum plates to minimize lateral temperature gradients, ***Figure 5b***. The enclosure was printed from ABS filament, which is heat resistant to ~100°C with no noticeable deformation. Poly-lactic-acid (PLA) would not be suitable due to its low temperature stability. A 19-inch (48.26 cm) V-slot aluminum extrusion was used and secured vertically to the enclosure via a dedicated 3D-printed slot, which allows the Lepton 3.5 to be mounted facing directly above the aluminum well plate, ***Figure 3b***. The mount can be easily adjusted to give the Lepton 3.5 a larger or smaller field of view. At the top of the V-slot rail, a Raspberry Pi 3 B+ and the standard 7” (17.8 cm) touch-screen display are mounted in an additional 3D printed enclosure, ***Figure 6*** [12]. This integration allows the entire data collection process to be interfaced and initiated without the need for an additional computer.

Software Development

The PhasIR hardware is accompanied by the homonymous open-source Python-based package that allows for high-throughput analysis of the output video from the IR camera found on the set up. The package itself is designed to streamline the data exploration by allowing the user to extract and analyze the results directly from a Jupyter Notebook. The open-source package can be divided in two main sections: image analysis and thermal analysis.

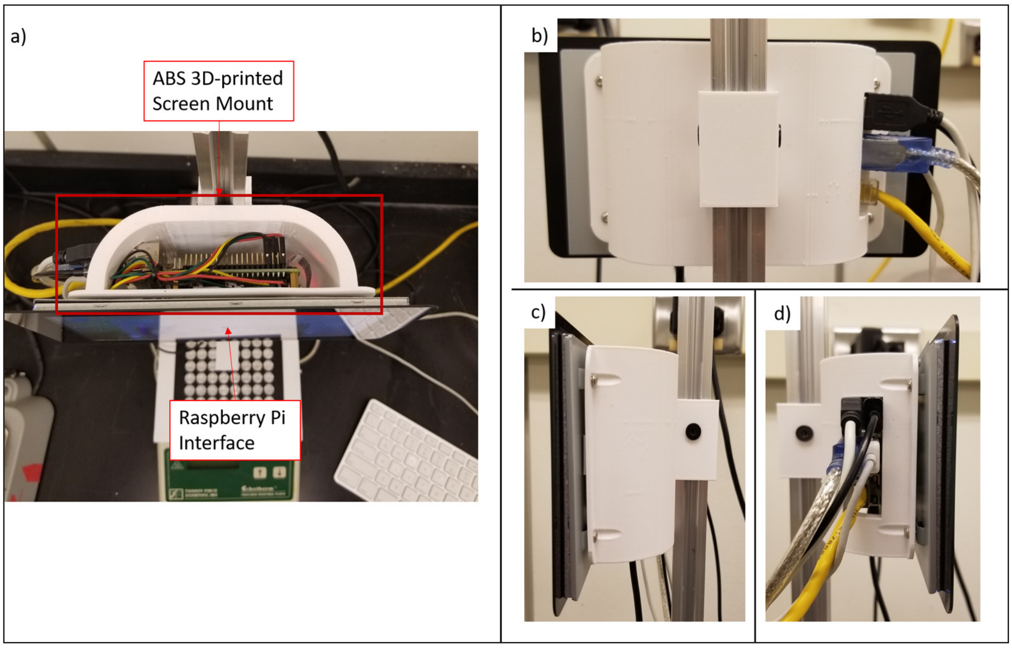

Figure 6 Raspberry Pi control system. **a)** Inside view of screen and Raspberry Pi 3B+ mount. **b), c), d)** Rear and side views of mount.

The former module allows for the initial analysis of the frames that are collected by the IR camera. The image can be cropped and resized to remove any objects in the field of view that are neither samples nor part of the well plate (e.g. insulating plastic enclosures). An example frame and intermediate steps of the image analysis module can be seen in *Figure 7a, b*. Next the position of the wells containing the samples can be obtained automatically or selected manually on a sample frame, *Figure 6c*. The average sample temperature is obtained from the average pixel values across a circular region of variable diameter that is positioned around each well's centroid across all frames of the video. For each well identified on the image, the plate temperature is identified as four equidistant points (red markers) placed diagonally with respect to the well centroid (black marker), see *Figure 8a*.

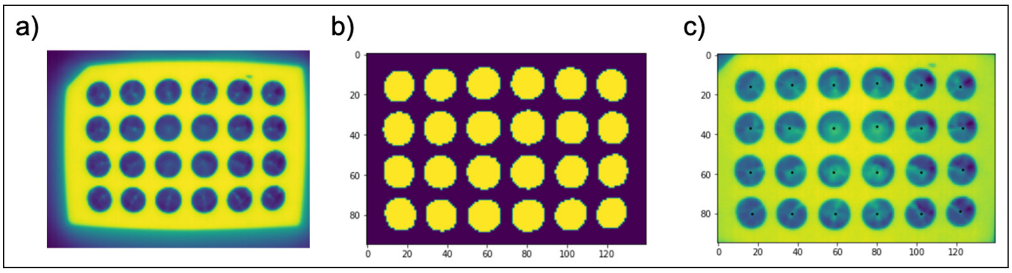

Figure 7 Example output of PhasIR image analysis module. **a)** Raw frame from .HDF5 video from Lepton 3.5 IR camera. **b)** Output of automatic object (well) recognition. **c)** Result of automatic centroid (black markers) fitting of each well in the plate.

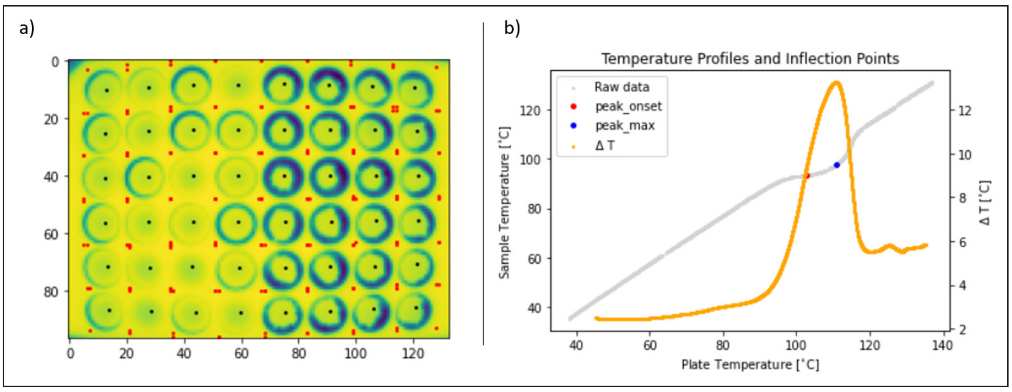

Figure 8 **a)** Example 48-well plate with centroid and plate temperature identification obtained through the PhasIR Image Analysis module. The black marker identifies the centroid of the well, whereas the red marked are used as the reference plate temperature for each well. **b)** Example result temperature curve for a single sample (Dodecanoic Acid). The phase transition temperature is the determined automatically as the onset of the peak in the curve (yellow).

The latter module allows us to measure the temperature profile for each well and to analyze the curve, plotted relative to the plate temperature, to identify the phase transition temperature of each sample. The temperature is encoded in the pixel value composing the frames collected by the Lepton IR camera. The final plate temperature is obtained as the average temperature of the four reference points for each well. Finally, the phase transition point is then obtained by

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identifying the onset of the peak that is formed by the curve that is obtained when subtracting the plate temperature from each sample temperature, ***Figure 8b***.

Finally, the data that is extracted from each experimental run can be saved and stored in a new. HDF5 file for subsequent sample characterization. Examples and further documentation of the open-source package can be found on the GitHub repository: *https://github.com/pozzo-research-group/phasIR*.

(2) QUALITY CONTROL

CALIBRATION

Quantitative Comparison to DSC

The industry standards of thermal analysis for melting point determination are the DSC and DTA. While these allow for accurate phase transition determination, full sample measurements can take upwards of an hour from start to finish for each individual sample. As the number of samples to be characterized increases, this type of measurement becomes extremely time consuming and costly to run. Moreover, most DSC instruments are not equipped with automatic sample changers (autosamplers) so that a user or technician would need to be present to manually change individual samples as they are being measured. Comparing results obtained from PhasIR to those from a TA Discovery 2500 DSC, it is noticed that the melting temperatures can be identified very accurately and rapidly, ***Figure 9***. The total experimental time for the samples ran in the PhasIR system was under 15 minutes. For pure substances, the results match within the limits of experimental error, with the highest discrepancy being less than 10%, which is below the temperature accuracy limit that is reported by the IR camera (***Table 1***). All measurements were performed in triplicates on 24-well plates. The precision of the PhasIR system was further demonstrated by performing 24 measurements each of xylitol and candelia wax on a fully loaded 48-well plate. The results are shown in ***Figure 10*** and ***Table 2***. The accuracy and precision of the 48-well plate are comparable to the previous measurements performed on the 24-well plates. In addition, these results show that spatial temperature variations across the plate are minimal and do not significantly affect the measurements with respect to where samples are placed on the plate.

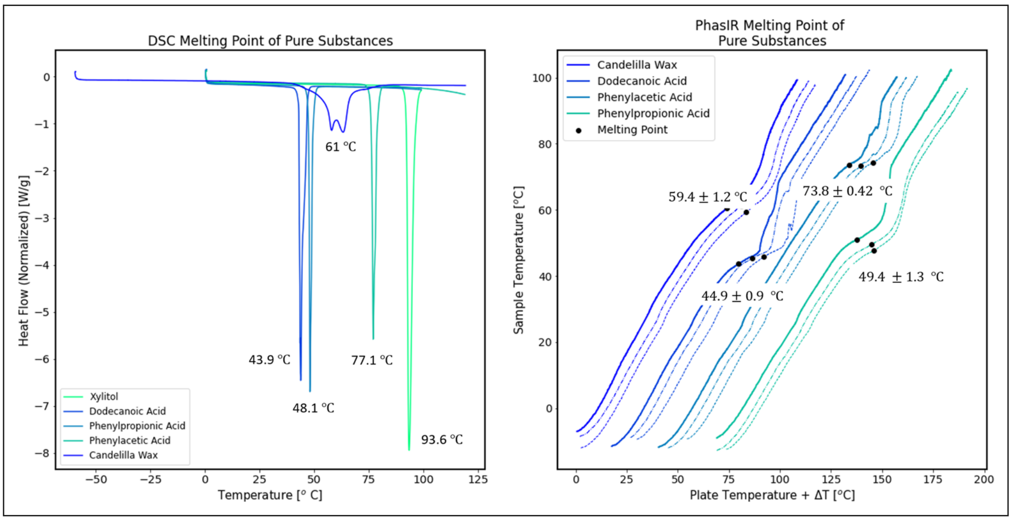

Figure 9 Results of melting point determination for pure substance using DSC (left) and PhasIR (right).

Table 1 Melting point comparison of pure substances obtained using DSC and PhasIR systems.

SAMPLE	DSC	PHASIR	LITERATURE	REFERENCE
[–]	[°C]	[°C]	[°C]	[–]
Candelia Wax	61	59.4 +/– 1.2	68–72	[13]
Dodecanoic Acid	43.9	44.9 +/– 0.9	44–46	[14]
Phenylpropionic Acid	48.1	49.4 +/– 1.3	45–48	[15]
Phenylacetic Acid	77.1	73.8 +/– 0.42	76–78	[16]

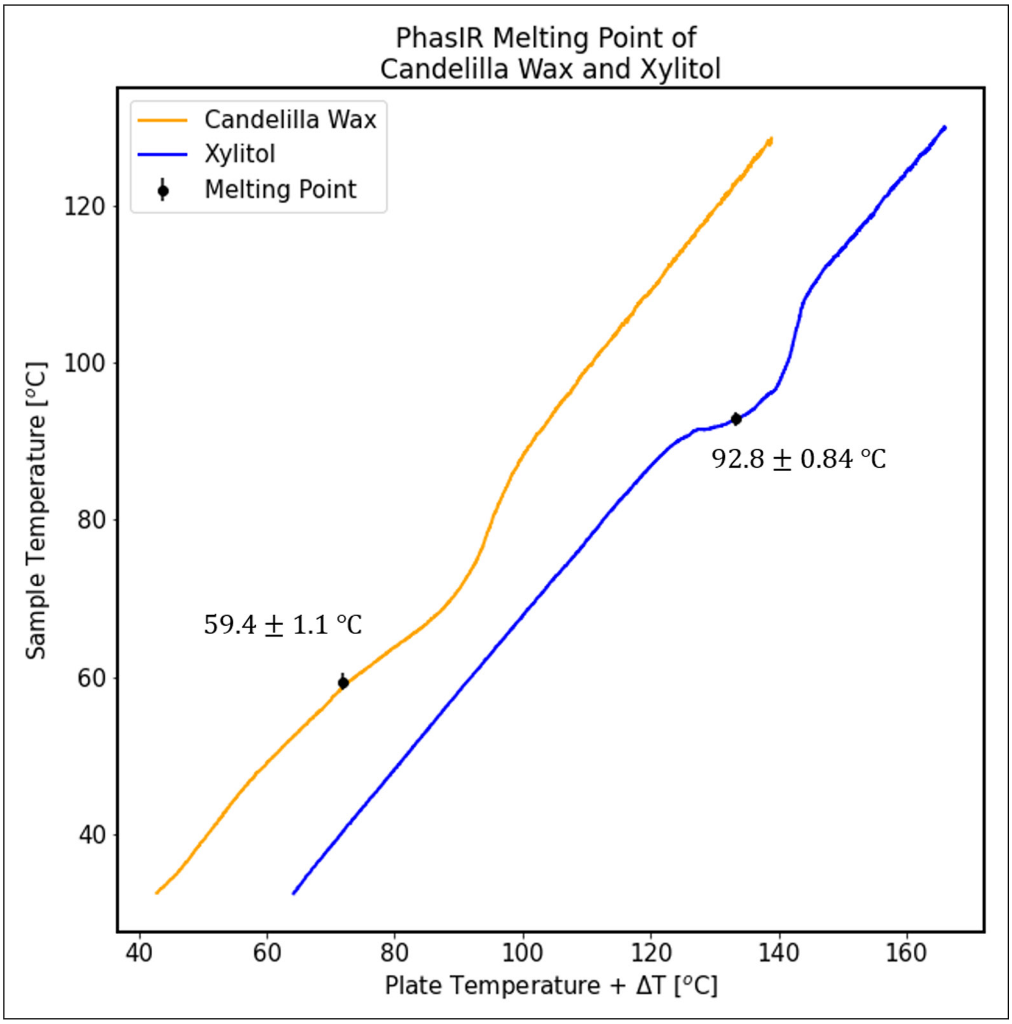

Figure 10 Results of melting point determination for candelia wax and xylitol on a 48-well plate.

SAMPLE	DSC	PHASIR	LITERATURE	REFERENCE
[–]	[°C]	[°C]	[°C]	[–]
Candelia Wax	61	59.4 +/– 1.1	68–72	[13]
Xylitol	93.6	92.8 +/– 0.84	94–97	[17]

Table 2 Melting point comparison of candelia wax and xylitol on a 48-well plate.

Error Management

The initial metal plate design implemented traditional cylindrical-shaped wells. However, issues arose when the samples were subjected to a temperature ramp. While still being able to undergo its phase transition, the position of the sample with respect to the center of the well was not consistent and could fluctuate throughout the duration of an experiment. Even though this did not pose complications with the hardware design, the data analysis was not able to be carried out in a streamlined manner as artifacts and errors would be introduced when determining the sample temperature profile. A workaround to this issue was the implementation of conical-shaped wells for the metal plates. These wells ensure a consistent position of the samples is maintained throughout the temperature ramp, see ***Figure 2***.

(3) APPLICATION

USE CASE(S)

Deep-Eutectic Solvents

While others previously have also demonstrated the use of optical methods to extract thermal properties of pure substances, the same analysis can also be extended towards the investigation of mixtures. For example, we have utilized the PhasIR system described herein to also obtain melting points for deep eutectic solvents. Deep eutectic solvents (DES) are composed of two or more substances, typically a molecular hydrogen bond donor and a quaternary ammonium salt. When mixed at a specific molar ratio, there is a large depression in the freezing point of the mixture, compared to that of the individual pure substances [18]. The design space for DES is incredibly large, and the utilization of high-throughput systems, such as PhasIR, will aid in the screening and discovery of low-melting point DESs that could find numerous uses as drug-delivery agents, clean energy electrolytes, green solvents, and many others [18–20].

In ***Figure 11*** we have estimated the melting point of three common DES in triplicates and compared PhasIR results with values obtained from DSC. Even though the DES are known to be highly hygroscopic samples, and therefore are susceptible to fluctuations in atmospheric conditions (i.e., humidity), the PhasIR results that are obtained in open air are still comparable to those obtained with the enclosed DSC system. In this case, the error between results from the two systems also remained below 10%, ***Table 3***. Thus, the PhasIR system can be a valuable screening tool for investigations involving thermal analysis of systems with a large material design space. It can provide valuable insight and estimation of phase transition temperatures for both pure substances and mixtures.

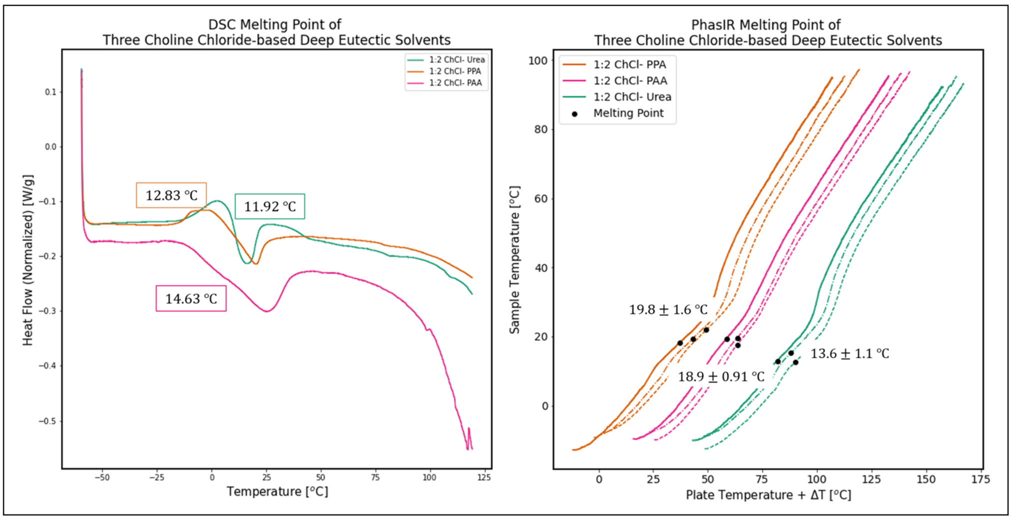

Figure 11 Results of melting point determination for three Choline Chloride-based Deep Eutectic Solvents using DSC (left) and PhasIR (right).

SAMPLE	DSC	PHASIR	LITERATURE	REFERENCE
[–]	[°C]	[°C]	[°C]	[–]
1:2 Choline Chloride- Urea	11.9	13.6 +/– 1.1	12	[21]
1:2 Choline Chloride- Phenylpropionic Acid	12.8	19.8 +/– 1.6	20	[22]
1:2 Choline Chloride- Phenylacetic Acid	14.6	18.9 +/– 0.91	25	[22]

Table 3 Melting point comparison of three Choline Chloride-based Deep Eutectic Solvents obtained using DSC and PhasIR systems.

REUSE POTENTIAL AND ADAPTABILITY

Many of the components in the PhasIR system consist of standard equipment that may already be found in many labs, allowing for a relative low-cost and simple transition into performing high-throughput thermal analysis. The PhasIR system is not limited to the specific heating plate demonstrated here, as virtually any heating source/plate can be adapted. This is especially convenient if larger plates are needed to characterize a greater number of samples, or if a heat source with specific heating ramp rates is required. While well plates based on standard dimensions were utilized here, any custom configuration can be introduced that fits within the frame of view of the IR camera. The IR camera itself is also not limited to the Lepton 3.5, as many other options exist on the market depending on the user's budget and resolution requirements. While we are specifically interested in the use-case of designing new deep eutectic solvents from a large chemical parameter space, there are numerous other potential use-cases for researchers to consider for PhasIR. With the ability to characterize a very large series of samples in under 15 minutes, the ability to perform routine quality control or purity testing for samples becomes much more approachable. The idea of running a series of carefully mixed samples can also be extended to other fields including sustainable 'green' engineering, pharmaceutical design, materials science, forensics, and polymer engineering among others. PhasIR can improve research efficiency and allow researchers to quickly locate and further focus research on critical sections of the sample space, which could be followed up with more costly industry standard tests such as DSC.

(4) BUILD DETAILS

AVAILABILITY OF MATERIALS AND METHODS

Construction of the custom hardware requires use of a 3D printer with temperature-resistant filament for the enclosures and a CNC mill to machine the aluminum well plates. Filament and starting materials are readily available and can be procured from Amazon and McMaster Carr. An IR camera is required to capture the melting process of samples, and while here we used the FLIR Lepton 3.5 for its low cost and compactness, there are a wide array of IR cameras on the market that could also be used. Likewise, several options exist for interfacing IR cameras as USB webcams. Other electronic parts such as the Raspberry Pi, display, and all necessary cables are available on Amazon. Lastly, virtually any heating/cooling plate can be used and can be chosen based on the temperature range that needs to be considered based on the samples of interest. All design files are provided and available for modification to suit the needs of any future design modification.

EASE OF BUILD

Initial planning and design are necessary based on the hardware components that are chosen. In this example, the enclosure was designed and fitted for the Echotherm IC25 heating/cooling plate that was used. Producing the enclosures requires operation of a 3D printer and securing the enclosure to the Echotherm was straightforward and only required a series of screws based on our design, with similar ease for mounting the rest of the components. The most advanced portion of the build would require basic knowledge of CAM software (such as Fusion 360) along with operation of a CNC mill to design and machine the aluminum well plates. The flexibility of the components that can be chosen to integrate into the system allows for the build complexity to be tailored to the specific user's desire. After obtaining all the necessary materials, we estimate that the build could be completed comfortably in a day with proper planning and experience.

OPERATING SOFTWARE, PERIPHERALS, AND DEPENDENCIES

The hardware depended on the use of a Raspberry Pi and Lepton 3.5 IR camera with PureThermal 2 module.

The Raspberry Pi OS is required to initiate data collection on the all-in-one system. To capture thermal images using the FLIR Lepton 3.5 IR camera, the open-source image capture software purethermal1-uvc-capture was used (*https://github.com/Kheirlb/purethermal1-uvc-capture*) [10].

The PhasIR package was written in Python and depends on various common libraries (pandas, numpy, scipy, matplotlib and scikit-image). Additionally, the proposed data analysis requires the use of Jupyter Notebook.

HARDWARE DOCUMENTATION AND FILES LOCATION

Name: GitHub

Persistent identifier: *https://github.com/pozzo-research-group/phasIR*

Licence: MIT License

Publisher: Maria Politi

Date published: 13/08/2021

Software code repository GitHub

Name: PhasIR

Identifier: *https://github.com/pozzo-research-group/phasIR*

Licence: MIT License

Date published: 13/08/2021

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(5) DISCUSSION

CONCLUSIONS

We have demonstrated the successful use of an IR camera in combination with aluminum well plate systems to automatically detect and measure the phase transition temperature for both pure organic substances and binary mixtures such as deep eutectic solvents (DES). Comparing the results to the industry leading system, Differential Scanning Calorimetry (DSC), the PhasIR results agree with a maximum deviation that is below 10%. The unique capabilities of the system include obtaining results in under 15 minutes, for up to 96 samples being measured simultaneously in a single experiment. In comparison, a single DSC measurement requires upwards of one hour per sample for analysis. The open-source nature of the PhasIR system will allow for users to make modifications and to extend the package according to their specific needs. It now allows for a collaborative space to develop additional high-throughput techniques for thermal and physio-chemical analysis.

ADDITIONAL FILE

The additional file for this article can be found as follows:

- **Supplementary File.** Bill of materials for this project. DOI: *https://doi.org/10.5334/joh.39.s1*

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COMPETING INTERESTS

The authors have no competing interests to declare.

AUTHOR CONTRIBUTIONS

L.P. and J.R. conceived of the presented idea. M.P. functionalized and fully revised the code and software originally developed by S.S. and S.B. J.R developed hardware. M.P and J.R. tested device. M.P., J.R., S.S., L.P. discussed the results and contributed to the final manuscript.

Jaime Rodriguez and Maria Politi contributed to the work equally.

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