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Technology Report

# Extensible Interface for a Compact Spectrophotometer for Teaching Molecular Absorption in the Undergraduate Laboratory

Edward C. Navarre*

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**ABSTRACT:** A simple computer interface for controlling a compact spectrograph for use as a spectrophotometer in an undergraduate teaching laboratory was developed. The project was implemented on a Raspberry Pi computer which permits the integration of a light source into the software. The interface was written in Python to facilitate modification by the user and because of its compatibility with several computing platforms. An implementation of the project in Linux on a Raspberry Pi computer is described.

**KEYWORDS:** *First-Year Undergraduate/General, Second-Year Undergraduate, Laboratory Instruction, Hands-On Learning/Manipulatives, Spectroscopy, Laboratory Equipment/Apparatus*



## ■ INTRODUCTION

Absorbance spectrophotometry is widely used throughout the chemistry curriculum to the extent that it is described at least qualitatively in most introductory chemistry textbooks and often basic univariate quantitative methods are included.[1,2] The theoretical and quantitative aspects of absorbance spectrophotometry are often presented for the first time in a classical quantitative chemical analysis course[3,4] taken in an undergraduate student's second or third year at university.[5] As a result, simple and cost-effective equipment is essential to teaching this technique in a variety of university laboratory situations with levels of student sophistication from first-semester university students to students in their final semester of an undergraduate degree. Many commercial solutions are offered ranging from about $400 to $2000 for basic absorbance systems and considerably more for advanced features. Additionally, many publications in this *Journal* describe low-cost approaches to making absorbance spectrophotometry more accessible[6,7] and innovative ways to use low-cost instruments.[8,9]

The author was recently faced with the decision of how to replace a set of Bausch and Lomb Spectronic 20 instruments used in chemistry teaching laboratories. Although the ThermoScientific Spectronic 200 would be a "one-for-one" replacement, the author pursued a different premise: How could existing spectrophotometric resources be used to solve the replacement issue? The author's academic department possessed several compact spectrographs that were originally acquired for an upper-level teaching laboratory. The technical solution described below is the author's attempt to develop a compact, economical replacement to the functionality of the Spectronic 20 in a sophomore-level quantitative analysis laboratory. The project sought to replicate the features without adding complexity to the use of the instrument.

An additional motivation for the project was two limitations related to the manufacturer-provided software: space considerations and complexity. The laboratory into which this project would be deployed has limited space, and an earlier trial of the compact spectrographs with small form factor PCs proved too unwieldy for regular use. Additionally, the compact spectrograph manufacturer justifiably wants to offer all of the hardware features in the software interface. This wealth of options was more confusing than helpful to students in the early trial of the hardware.

The author pursued an interface design that presented all of the important spectrophotometric conditions to the student in one place. As a result, the student user would be able to focus on learning about spectrophotometry rather than spend time understanding a software interface. Presenting only the essential experimental conditions limits the available spectrometer functions by removing features like derivatives, smoothing, and event triggers. Additionally, convenience features, such as automatic plotting of calibration curves, detract from the pedagogical value of spectrophotometry. The project objective was a deliberately limited functionality that focused on students learning the experimental aspects of spectrophotometry.

Other manufacturers offer small format spectrophotometry equipment that can address the space considerations. For example, the Pasco wireless spectrometer (model PS-2600) is very small. However, it requires a connected computer for the software that records the data or the company's SPARK LXi Datalogger (model PS-3600). Likewise, Vernier has several compact options, the most appropriate of which is the Go Direct SpectroVis Plus Spectrophotometer. The spectrophotometer can be connected to a computer for recording data or to a Vernier LabQuest2 data-collection system. Approaching this

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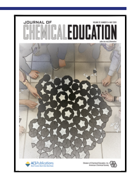

project with a Pasco or Vernier spectrophotometer connected to a computer does not change the space issues significantly and would have required purchasing the spectrophotometers. Using the SPARK LXi or LabQuest2 system would have been extremely space-efficient. Ultimately, this option was not selected, largely for economic considerations; the complete spectrometer and data-collection system would be several times more expensive than the chosen solution.

## ■ EQUIPMENT

The spectrograph used for recording visible spectra in this work was a StellarNet Black Comet C-25 (StellarNet Inc., Tampa, Florida). The particular model had a 2048-pixel CCD, 16-bit ADC, and a $\Delta\lambda_{effective}$ of about 1 nm across the spectral range 179–1016 nm. The project was also tested on an Ocean Optics HR4000 (Ocean Insights Inc., Largo, Florida). The software interface was developed in Python (version 2.7 and 3.7, Python Software Foundation) on a Pi-top CEED (Pi-top, London, UK). A wireless compact keyboard (model RT-MWK12+, Riitek Technology, Shenzhen, China) was selected to minimize space requirements.

There are two versions of the project. One simply controls the spectrograph and would require the use of existing light sources and cuvette holders. The second integrates a light source into the software and Raspberry Pi hardware. Two light sources were investigated: a "cool white" LED (LTW-2R3D7, Lite-On Inc.) and a "warm white" LED (334–15/X1C5-1QSA, Everlight Electronics Co Ltd.). The spectra of the two LEDs are shown in Figure 1 under conditions that place the maximum emission at

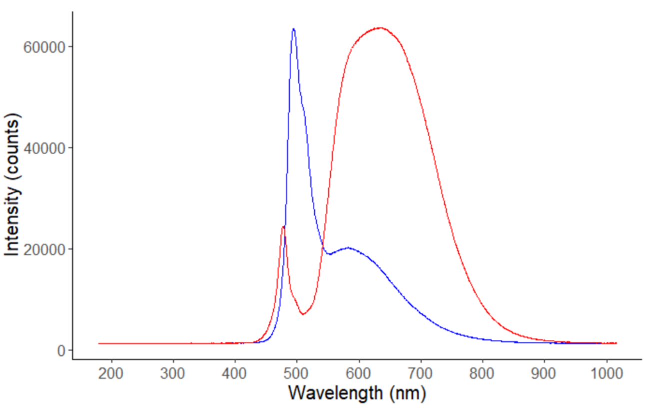


**Figure 1.** Emission spectra of the LEDs. The spectrum of the LTW-2R3D7 is drawn in blue, and that of the 334-15/X1C5-1QSA is drawn in red. The spectra were recorded with 5 ms integration time and an LED duty cycle of 99% (red trace) and 31% (blue trace) so that the maximum intensity values are equivalent and near the maximum of the spectrometer range.

the upper limit of the spectrometer range. The choice between the LEDs is up to the user depending on the spectral range in which they are interested. A cuvette holder was manufactured by the author from Delrin thermoplastic for direct attachment to the face of the spectrograph. The cuvette holder is designed for use with the integrated LED light source; other cuvette holders can be used if an external light source is used. Fabrication plans for the cuvette holder are available in the Supporting Information. In the project version with an integrated LED light source, the brightness of the LED is adjustable in the software interface via a pulse width modulation (PWM) circuit shown in Figure 2. The PWM frequency can be adjusted in the

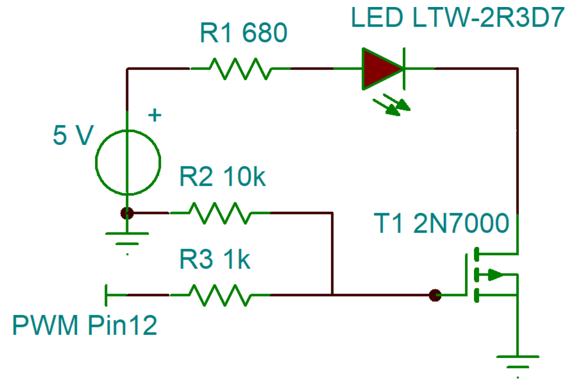


**Figure 2.** Pulse width modulation circuit for controlling the brightness of an LED light source. The pin number is relevant to a Raspberry Pi implementation of the circuit.

code but is set initially to 2000 Hz which is sufficiently fast to avoid the appearance of signal flickering at integration times greater than or equal to 3 ms (the spectrometer minimum integration time). The PWM duty cycle was tested from 1% to 100% and found to produce constant LED intensity at all values.

## ■ HAZARDS AND SAFETY PRECAUTIONS

There are not any inherent chemical hazards in the implementation of this project as a spectrophotometer. Its use in a teaching laboratory will need to respect the risks and hazards of the chemical system that is studied with the spectrophotometer.

## ■ RESULTS

The major product of the project is a simple software interface for performing spectrophotometry measurements. The software written for this project consists of a Python module that collects the physical parameters of the spectrograph at startup and provides an interactive interface for spectrophotometry. The code for the interface is located on GitHub (https://github.com/acpo/) with versions for StellarNet and Ocean Optics spectrographs. Instructions for installing the project are available in the Supporting Information. There are versions available with and without an integrated LED light source. The integration of the LED light source provides control of all parts of the spectrophotometry instrument within the interface. A description of the user interaction with the interface is shown in Table 1 for the cases in which most experimental conditions are preset in the code (e.g., for the least experienced users) and the case in which the user must work with all of the experimental conditions.

An example of the complete system hardware and software interface are shown in Figure 3. The Raspberry Pi-based system used in this project was useful to demonstrate that a very low-power computer was suitable. On the Pi-top system, the response times of the interface and spectrum redrawing were fast enough for most students to be comfortable using it. The project could readily be adapted to a small (3.5 or 5-in.) touch screen display to radically reduce the size of the device, including the elimination of the keyboard.

The project as implemented on a Pi-top computer and StellarNet spectrograph was tested with a quantitative analysis laboratory of 45 students divided into sections of about 12 each. Each student worked independently on a spectrophotometric determination of iron with *o*-phenanthroline by external


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**Table 1. User Interaction with for a Typical Spectrophotometric Measurement**

| | Case: Some Conditions Preset in Code | Case: All Conditions Set by User |
|---|---|---|
| Select integration time such that 100% $T$ signal is on scale[a] (text box) | Not required | Required |
| Select wavelength boundaries appropriate to the light source (text box) | Not required | Required |
| Select the number of spectra to average[b] (text box) | Not required | Required |
| Record 0% $T$ (button click) | Required | Required |
| Record 100% $T$ (button click) | Required | Required |
| Switch to Absorbance mode (button click) | Required | Required |
| Select wavelength to monitor (text box) | Required | Required |
| Observe absorbances | Required | Required |

[a]If the integrated LED is used, then the LED duty cycle and the integration time both must be adjusted to give an on-scale signal. [b]Averaging performs the arithmetic mean of the number of successive spectra indicated by this value, and acquisition requires a total time of the integration time × averages.

calibration.[10,11] Relative to the student results of prior years in which a Spectronic 20 was used in this experiment, the data showed similar linearity in the range of 0−0.6 absorbance units. Linearity of data above 0.6 absorbance was slightly better with the compact spectrograph. It should be noted that the spectrophotometric performance of the system is largely dependent upon the particular hardware that a user selects, so the author's experience may not be the same as other users. However, in the transition from a Spectronic 20 ($\Delta\lambda_{effective} \approx 20$ nm) to a modern compact spectrograph ($\Delta\lambda_{effective}$ typically less than 2 nm), it would be unusual to find poorer performance related to deviations from the Beer−Lambert law.

The student experience with this project was similar to the Spectronic 20, with some advantages. Both systems required the student to record a 0% and 100% transmittance measurement at the start of analysis. The Spectronic 20 accomplished this task via two analog dials whereas in this project students clicked two buttons on the interface; effectively, the student experience is identical. Once the prerequisites were recorded, the absorbance at the selected monitor wavelength was continuously displayed on the spectrum window (see Figure 3). Selection of the monitored wavelength was done via a numerical entry box on the interface. An important advantage in this project was that the absorbance spectrum was displayed continuously during use. The continuous display of the complete absorbance spectrum offers the instructor an opportunity to have students easily explore the concept of $\lambda_{max}$ and other properties of the Beer−Lambert law.

A pedagogical advantage to this project is that the Python code for this project is available to be edited and customized to an instructor's needs. The distributed version sets the wavelength range to the range reported by the spectrograph firmware. An instructor has the choice to modify two lines of code to preset the boundaries or to ask students to select with the interface the appropriate boundaries for the light source that they are using. For example, if a white light LED is used, the range can be restricted to 450−850 nm. Likewise, the integration time of the detector can be preset in the code by the instructor to appropriately utilize the dynamic range of the detector, or students can be asked to explore how the integration time can be used to make best use of the available light. Additionally, the interface developed in this project gives the user access to the raw signal from the spectrograph and can be used for emission

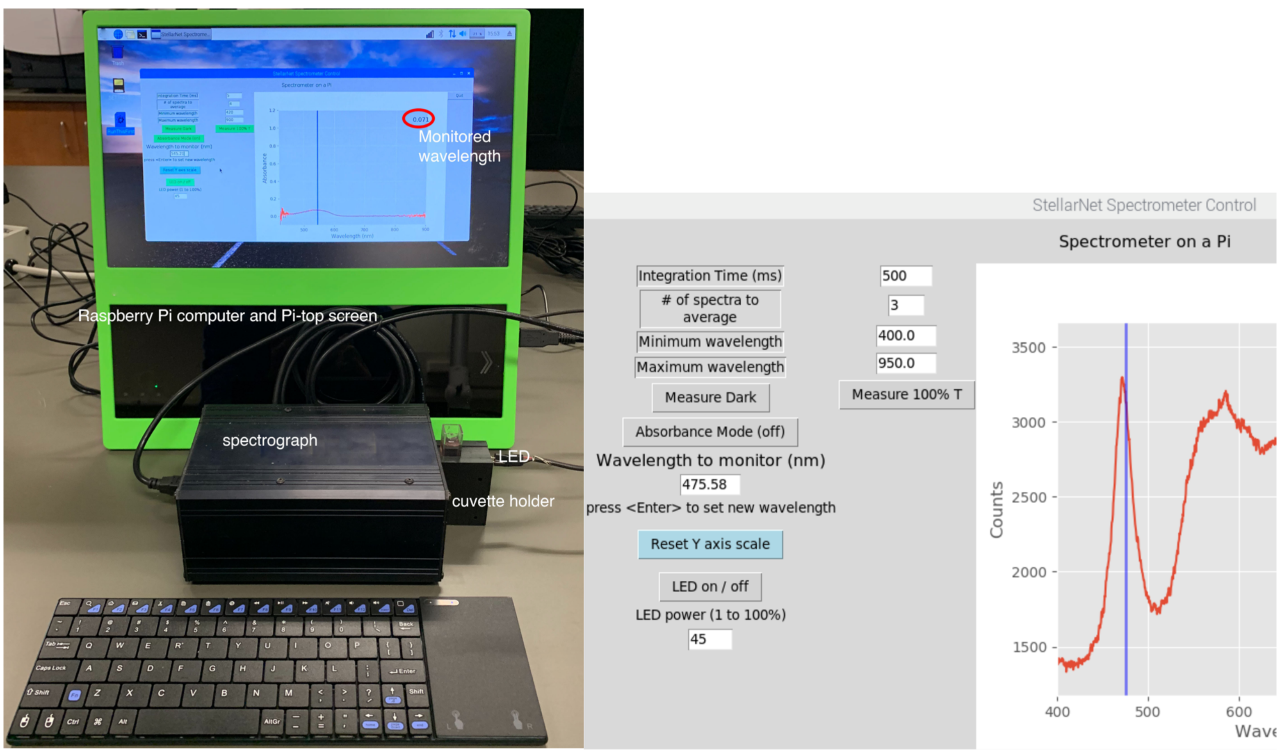


**Figure 3.** Complete spectrophotometer implementation (left) and the Python interface (right).



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(e.g., fluorescence or chemiluminescence) measurements which were never part of the Spectronic 20 scope of functions.

Last, to the author's knowledge, the interface developed in this project is the first free spectrophotometry interface for StellarNet spectrometers on the Linux platform. While this project was being tested, the company introduced Mac OS compatible software, but there are not currently any solutions for the Raspberry Pi or other Linux distributions. This project also offers a free, open-source Linux interface to Ocean Optics instruments which the company does not currently provide.

## ■ ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.9b01023.

Cuvette holder fabrication plans (PDF)

Notes to guide the installation of the project (PDF)

Description of each functional unit in the software (PDF)

Description of the hardware requirements for Raspberry PI, Windows, and Apple systems (PDF)

## ■ AUTHOR INFORMATION

### Corresponding Author

**Edward C. Navarre** – *Department of Chemistry, Southern Illinois University Edwardsville, Edwardsville, Illinois 62026-1652, United States;* orcid.org/0000-0001-5727-8052; Email: enavarr@siue.edu

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.9b01023

### Notes

The author declares no competing financial interest.

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