

Cell Phone Spectrophotometer
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Background: To really understand instrumentation, one must build and characterize an instrument. Seeing how an instrument behaves in reality as opposed to how it should behave theoretically is eye-opening. The instrument you will build has all the components of a "real" spectrophotometer, but is made from readily-available, inexpensive parts. It will be able to measure absorbance in the visible region of the spectrum, but it will not be able to do so very well. In seeing where it fails, you will learn how one must engineer a laboratory-grade instrument. You will gain appreciation for how well those instruments work – while understanding that they, too, are imperfect.

Kathleen Kelley, graduate student at Illinois, made major contributions to designing the instrument, suggesting samples, and designing the laboratory activities.

THIS IS A FIRST DRAFT DOCUMENT. MORE DIAGRAMS AND PICTURES WILL BE ADDED
LATER. STUDENT SUGGESTIONS FOR IMPROVEMENTS WOULD BE MOST WELCOME

I. Why build a spectrophotometer as opposed to anything else

Given that there are thousands of different analytical instruments, why build a spectrophotometer? Aside from those who are blind, eyesight is one of the richest paths humans have for learning about the world. Color is one of the earliest stimuli we can identify, even before faces (my youngest daughter turned her head to track the bright blue screen of a PC when she was one day old). We thus develop intuition most quickly when we can see how data are formed rather than simply trusting equations or our other senses.

Visual spectrometric instruments date from at least the time of Newton. Since the middle of the 19th century, with the development of photographic plates, and then in the 20th century with the development of photomultipliers and photodiodes, it was ludicrous to think that reasonable measurements could be made with nearly-free equipment. When digital cameras first appeared, they were not only expensive, but also had such limited dynamic range that most spectroscopists dismissed their utility out of hand. Since 2007, however, two things have changed. The first is that over 1/6 of humanity has access to a cellular telephone, and a large fraction of those phones have built-in cameras. Thus, what was previously the most expensive, least easily obtained component of a spectrometer, is now in wide circulation. The second change has been the realization that, if an instrument works too well, it is hard to grasp the ideas about the instruments foibles. Having an instrument whose flaws are clearly displayed is an asset in teaching. So let's go build a (really bad!) spectrophotometer.

II. Why home-built instruments are becoming practical

The same insights that led to this experiment are being exploited to develop inexpensive medical and water quality test devices. The best known person in the US working on these ideas is George Whitesides at Harvard University, who is using microcontact printing to make 96 well test plates that use a cell phone and the internet to send data to a central lab for analysis. Pre-printed color panels, analogous to color reference panels used on spacecraft for camera calibration, are used to standardize the data. Everyone recognizes that, as cell phones get smarter, the data will not be sent to a central facility. Rather, the results of the tests, processed with software on the cell phone, will report a diagnosis, send the diagnosis to an appropriate node on the net, and then alert the phone's owner of the doctor's medical advice. In the distant future (at least a few years!), there may be a sufficiently reliable database in many phones that the MD will only be consulted in unusual, confusing situations.

III. Components of a spectrophotometer

List the components of a spectrophotometer in the order they are typically laid out for single wavelength measurement:

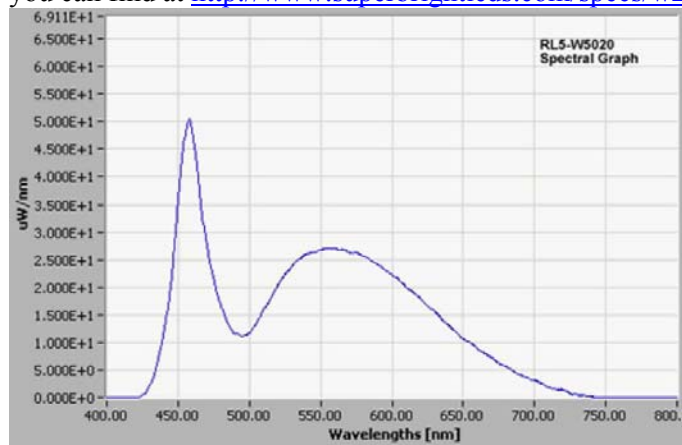
_____ → _____ → _____ → _____ (after which the signal is transduced to a number)

Now list the components in the order they are typically laid out for full spectral observation in parallel:

_____ → _____ → _____ → _____ (after which the signals from the multiple elements in the final component are transduced to a number)

There are many variations on each component.

The light source with which you will work is an RL-5-W5020 white LED, the specifications for which you can find at http://www.superbrightleds.com/specs/w2_specs.htm. Here's the spectral output:



The output power is specified for a current of 20 mA which requires a drive voltage of 3.8 V. Our 3V batteries barely provide 2 mA, so output is only about 1/10 of the full power rating (based on reading the specifications. Would you trust the specifications? How would you measure if the estimate of current from the battery is correct?)

You will be supplied with a plastic 1 cm pathlength cuvette to hold a liquid sample. These are regarded as "disposable" because they are inexpensive. However, there is no reason not to use them many times provided

samples don't stick to the polystyrene surface, leading to cross-contamination, solvents don't cause the plastic to deteriorate, and the outside stays free of scratches.

The diffraction grating is a holographic transmission grating, 12700 lines/inch or 500 lines/mm. These gratings are not blazed.

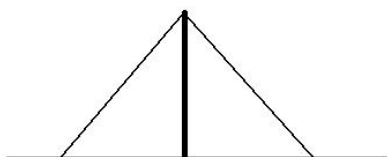
What is the detector? Only you know that. Any device that can generate a JPG picture can act as the array detector for this spectrophotometer! Do you have a digital camera? A cell phone with a camera? A webcam? If you don't have one, find a friend who does.

My detector is: _____

IV. Layout of home-built instrument

Clearly, for there to be any hope of having this work, the components have to be aligned reproducibly. *While a paper "baseplate" is provided, you should use ingenuity to devise something better.* Kathleen Kelley found a piece of Styrofoam and linked everything to that base, which is much sturdier than folded paper. What will you use?

The LED leads are the right spacing so that the battery slides between them and the LED immediately turns on. Which leg goes on top? The LED must be forward biased (anode on the + side of the battery). In theory, the battery should be able to illuminate the LED for a total of 80 hours before burning out. *This has not been tested.* If you aren't using the LED, slip it off the battery to conserve power. The baseplate folds in such a way that the LED is at the right height to be centered along the grating. Should the LED shine along the center axis of the grating? Should the grating be offset at some angle?



Side View. Grating perpendicular to paper, tape bracing grating.

Should the LED shine directly in line with the grating or be aimed to one side? The specification is that the LED emits most of its light $\pm 10^\circ$ from the diode's axis. Play with this – see what alignment makes sense. How can the grating be kept upright? Tape it in place with a hinge at the bottom and two pieces of tape making right triangles.

Where will the detector go? Where will the cuvette go? Are there ambiguities? Do you see multiple diffraction orders?

Which order will you use? Why? Once you see what angle you want to use, how far from the grating will you want to be with the camera lens (approximately)? How did you reach this estimate? What will happen if the distance varies by 10%?

V. If it works right, how would we obtain and process data?

Suppose we get everything put together just right. What relationship between measurement and concentration will be used with this instrument? Beer's Law, $A(\lambda) = \epsilon(\lambda) b C$. Can we measure A directly? No. What can we measure? Transmittance, T ? No. All we can measure is light intensity.

$$\epsilon(\lambda) b C = \log_{10}(I_0(\lambda)/I(\lambda))$$

How do you know $\epsilon(\lambda)$? You don't – for each compound and solvent, it must be measured. How do you know b , and what is its value?

At minimum, how many intensity measurements must be made to determine $\epsilon(\lambda)$?

"How will we get from a picture to an intensity? Your fearless instructor is writing software, to be described in §XIII below. Software can manipulate JPG files, but YOU will have to provide valid files with meaningful intensity measurements for the software to work.

VI. What isn't ideal about the current layout?

Compared to a commercial spectrophotometer, what do you see (even before you collect any data) as non-ideal about this instrument? Discuss what would work well for a real instrument, what you have here, and how the two compare. Incidentally, there are at least a few things about this instrument that are superior to any commercial spectrophotometer, so look for positive points as well as negative!

VII. Build it!

Put the components together.

VIII. Play with it!

Look at the spectra without a cuvette in place. Put in a cuvette and see what changes. See the various diffraction orders. If you don't like having the spectrum dispersed left/right, try rotating the grating and disperse the light at some other angle. Take pictures of the spectrum with your camera. See how you can vary the fraction of the frame that the spectrum fills. Is the spectrum too bright? Too dim? Is the room too bright? Can you tell where any particular wavelength is in the spectrum (the spectral plot suggests 460 nm and 560 nm should be discernable. Are they?)? Does the spectrum look anything like what you'd expect from the plot in §IV?

What will we use for a sample? Sitting in Urbana, I have no idea! We will need to find something that has a distinctive visible spectrum and that we can easily dilute to give transmittance between 10% and 95%. In our testing, we have found food coloring or sugary drinks with food coloring work well, but pH indicators or colored metal ions should be OK. We'll figure it out "on the fly."

IX. Trial: see how well 100% T can be reproduced

Either with no cuvette present or with just water in the cuvette, take 3 or 4 spectra. Later, we'll see how reproducible these data are.

X. Trial: see what 0% T looks like

0% T is what one measures when the light source is blocked (or turned off). So either turn off the LED or block its light and take 3 or 4 spectra to get the signal when there is "infinite absorbance."

Is there a problem here? Yes, as a matter of fact, there is. In a "real" spectrophotometer, when the light source is turned off, there really is very little light in the instrument (just leaks from the outside world, phosphorescence of any long-lived species, and any glow from semi-conductors or heated surfaces). But in this instrument? In a lighted room, there is a HUGE amount of light from the environment. If you take the instrument into a darkened room, the camera wants to use flash, another source of stray light. If you convince the camera not to use the flash, how can it focus if there's no light?

How will you deal with this stray light problem? Argue with your neighbor and see if you can figure out an equation to use with raw camera measurements to compensate for stray light.

XI. Get photometric data

Obtain a spectrum useful for measuring $I_0(\lambda)$. Then for each of 3 (or more) dilutions of the sample, obtain spectra from which you can measure $I(\lambda)$. Name the pictures/files so you'll know which is which later.

Sample compound: _____

Reference spectrum filename: _____

Sample Spectrum 1: _____ Concentration _____

Sample Spectrum 2: _____ Concentration _____

Sample Spectrum 3: _____ Concentration _____

Will we have an unknown to analyze? I don't know IF we have an unknown, run it:

Unknown Spectrum: _____ Concentration _____

You might want to take multiple exposures in case some are blurry, badly exposed, or some such.

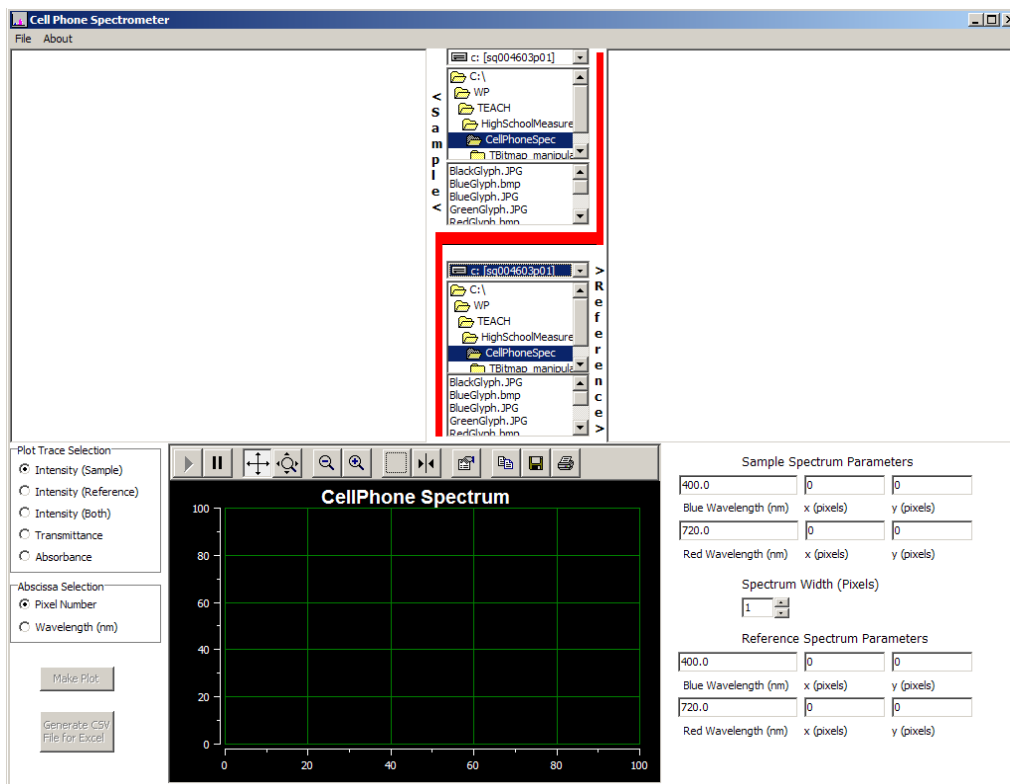
XII. The Software

As with most modern instruments, software is used to convert raw signals to useful results. As this lab is being written, the software is incomplete. Rather than write pages and pages of documentation (which, if everything's written correctly, should be needed anyway!), let me outline what's there. You can play with it, let me know what does not work (or what works badly), and then we'll rewrite it.

There are 3 graphical insets and 2 control sections. In the upper LEFT of the screen, put the JPG for the SAMPLE (the picture from which you want to find $I(\lambda)$). In the upper RIGHT of the screen, put the JPG for the REFERENCE (the picture from which you want to find $I_0(\lambda)$). I have not designed this for "drag and drop." You must use the directory functions in the middle of the screen to select the files by name. If you regard this as a serious limitation, let me know, and after we make sure the science parts of the software are error-free, I'll try to install that capability.

After the JPGs are in place, you have to tell the software where the spectrum is. Point to either the red or blue end of the spectrum with the mouse. When you click, you'll get to choose whether it's the red or blue end. Once you have both ends marked, you can use the data fields in the lower right of the screen to tell the software what wavelengths correspond to your clicks. You won't know exactly, but give the machine your best estimate. As long as you are consistent between the two frames, your results will be precise, though perhaps not accurate.

"Spectrum width" lets you use more than one row of pixels at a time. How does this influence signal-to-noise ratio? Experiment and find out! Does it influence resolution?



Once you've marked where the spectral data is, you can plot it. In addition, you can export the data as a comma-separated variable (.CSV) file, readable by most spreadsheets. That way, you can improve on the very limited data processing that the software performs (when it computes absorbance, it only ratios intensities without correcting for any of the problems that you have found in looking at the data).

Notice that plots can be as a function of pixel number (bluest pixel, corresponding to the blue wavelength in the lower right of the screen, is numbered 0) or wavelength (interpolated from knowing the dispersion implicit in the data in the lower right entries). Also notice that the graphics window, while fairly small, has the ability, independent of the rest of the program, to save data to a file or print.

XIII. Reprocessing data in *Excel* or some other spreadsheet

The software described in the previous section will export the red, green, and blue intensity values for each wavelength setting, identifying each wavelength with a pixel number as well. What if you want to get information about a part of the image that isn't really spectral data? Just click into the software a line along which to report intensity values and export those lines of numbers. The software is dumb – it will believe that ANY line of pixels corresponds to a spectrum, whether it does or not! Once the lines of data are in the spreadsheet, you get to take over and figure out how to combine intensity values, subtract background, and so on, to get transmittance or absorbance. From these, you can make a working curve.

XIV. Attempt to make a working curve

Choose a wavelength where absorbance seems to be a strong function of concentration. Make a working curve. Is it a straight line? If not, can you figure out why? Can you obtain data that allow you to combine your extra information with the raw $I(\lambda)$ and $I_0(\lambda)$ to make it straight (or, at least, straighter)? If you have an unknown, determine its concentration. CHALLENGE: how in the world do we determine precision or accuracy with this system?

XV. Evaluation of the instrument

There are two ways to write this section of the exercise. I could list the parameters I want you to have measured. If I do that, I am sure you will measure all those properties, but you won't ask yourself "what characteristics matter?" One goal of having you build this system is to work out for yourself what parameters are important, to figure out how to measure them, and then to decide how to improve them. So here is what I will do: when the class comes up with at least 6 parameters to evaluate, I will be willing to suggest an additional parameter or suggest what you may wish to consider in figuring out an additional parameter. I'll even start you with a hint: did everyone use the same camera? If not, did all the numbers for intensity at a particular wavelength come out to be the same? If not, why not?

XVI. Evaluation of the experiment

There are many ways to evaluate what you have done. Here are some of them.

1. Did you succeed in building a working spectrophotometer? If so, how well did it work? If not, what did you see about components, instructions, software, or other circumstances that prevented it from working?
2. Did you learn anything about designing and building instruments from working on this device? If so, what did you learn? If not, can you identify why you learned little or nothing? Would better instructions have helped? Better software? If you can see ways to improve the software, describe how it should function.
3. There are only 30 contact hours for American faculty when teaching at HUS. This spectrometer consumed at least 2 hours of that time. Was this a good use of that time? If not, what would you suggest would be a better use of that time?

XVII. If you want to do more

There are many questions we haven't answered. Here are some of them, in no particular order.

1. What is the theoretical resolution of this instrument, and what sets that resolution?
2. What is the ideal distance from the LED to the grating? How did you decide this number?
3. What limits photometric precision – shot noise, digitization noise, stray light, detector saturation, too much adaptability in the camera (making photometry impossible because of ever-adjusting exposure times), or something else?
4. Is there some other component arrangement that would be just as inexpensive but work better?
5. Could these components be used to develop a fluorimeter?
6. Given how much of a problem stray light and digitization noise are, is this spectrometer worth using for anything but teaching purposes?

In addition, it is obvious that having the data processed the way it is now is quite awkward. Future plans for the software include:

1. Recast the current software so it runs in a browser. That way, the processing can occur on any computer, not just a Windows machine.
2. Rewrite it a second time so that it runs natively in a cell phone. That way, the whole data processing cycle can be done in the palm of the hand of anyone with a camera phone.