Inexpensive, Open Source Spectrophotometers That Use Part of a CD or DVD as a Diffraction Grating

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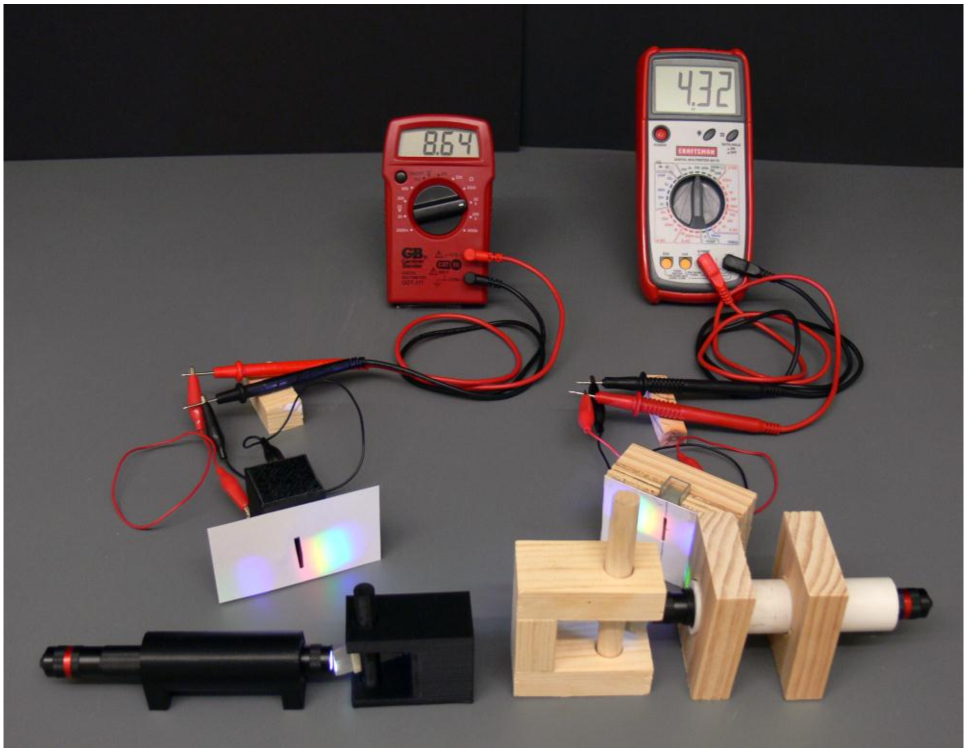
ABSTRACT

Building upon the work of others, we describe two different open source designs for inexpensive, single-beam spectrophotometers that use part of a CD or DVD as a diffraction grating to generate their transmission spectrum. Like other instruments that we have designed, one model can be 3D printed, and the other can be built from supplies available at most hardware stores or online. Both versions use an LED flashlight with a convex lens as their light source as well as a light dependent resistor (LDR) connected to a digital multimeter as their detector. We tested these models in two ways. First, we used them to create a simple Absorption spectrum for a dilute Methylene Blue solution, taking readings for the seven colors in the visible spectrum (i.e., violet, indigo, blue, green, yellow, orange, and red). Second, we used these designs to conduct a simple assay to measure the Absorbance of increasing concentrations of Methylene Blue in solution. In both instances, we found that the instruments generated results and trends that were similar to those of a commercial spectrophotometer (although at roughly half the magnitude). As a result, we believe that these devices could easily be incorporated into a classroom or teaching lab to demonstrate basic principles of spectroscopy or conduct various spectroscopic assays for educational purposes. Finally, because the designs and parts for these devices are all open source, we have named them "OPN Spectrophotometers" (or "OPN Specs" for short), and we include instructions on how to 3D print or build these instruments in the Supporting Information (along with the underlying computer design and 3D printing files), so that others can use or modify them to fit their needs.

ABSTRACT GRAPHIC



KEYWORDS

General Public, Analytical Chemistry, Biochemistry, Laboratory Instruction, Hands-On Learning / Manipulatives, Laboratory Equipment / Apparatus, Spectroscopy

INTRODUCTION

Recently, we described how to make a set of inexpensive colorimeters for educational or other purposes, using 3D printing technology or materials available online or at most hardware stores.[1] We called these instruments "OPN Colorimeters" because, like other open source instruments we have developed,[2] their plans and parts are freely and widely available, so that others can use or modify them as need be. However, because these colorimeters tend to generate a fairly broad spectrum given the cellophane filters that they use, these devices are not as sensitive as various commercial (and even some educational) instruments.[3] Thus, building upon the work of other teams,[4-13] we explain here how to make a set of relatively inexpensive spectrophotometers that generate their spectrum using part of a CD or DVD as a diffraction grating. As such, these devices are more sensitive than the OPN Colorimeters that we previously described (although still not as sensitive as a commercial device). Nevertheless, given the ease with which these instruments can be built and operated, they are ideal for conducting various educational experiments or other instructional activities in the classroom or teaching lab.

Similar to a colorimeter, a spectrophotometer can measure the amount of light absorbed by an opaque or translucent substance, such as one or more chemicals in solution.[14-17] However, instead of being limited to a specific color (or colors) of light as often occurs with a colorimeter, a spectrophotometer is able to break up light into a spectrum (e.g., all wavelengths in the visible range and, in some cases, infra-red or ultra-violet light as well). The device then selects one or more wavelengths from this broad spectrum to send into the sample to determine how much of this light was transmitted or absorbed.

To accomplish this task, a spectrophotometer typically generates an intense beam of white light, which it sends through a monochromator (such as a prism or a diffraction grating) to create its spectrum – e.g., all the colors in the rainbow (Fig. 1, left). The instrument then has an aperture that selects a specific wavelength from this spectrum to send into a sample (Fig. 1, middle). That incident light (I) then passes through the solution, whose particles absorb some of that light (Fig. 1, right). The remaining transmitted light (T), which passes through the solution, eventually reaches a detector that calculates an Absorbance value (A) based on the proportion of light that the sample has absorbed – i.e., the ratio of the transmitted light T to the incident light I (Fig. 1, far right).

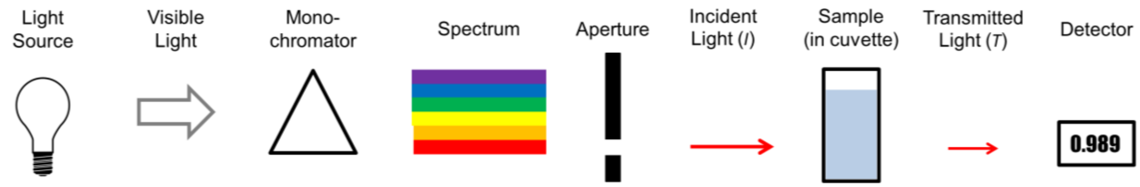


Figure 1. The workings of a basic single-beam spectrophotometer.

As explained in our OPN Colorimeter paper,[1] there is a negative logarithmic relationship between the intensity of the light transmitted through the sample (T) compared to the intensity of the incident light initially striking the sample (I), and this relationship is further proportional to specific qualities of the sample. Specifically, as expressed in the Beer-Lambert law,

$$A = -\log_{10}\left({}^{T}/_{I} \right) = \varepsilon c l,$$

where ε denotes the molar extinction coefficient of the sample under investigation $[L/mol{\cdot}cm]$, c denotes the concentration of that sample in solution $[mol/L]$, and l denotes the path length of the sample $[cm]$, which is typically the length of the cuvette containing the sample (i.e., 1 cm).[14-19]

Even though colorimeters and spectrophotometers are important analytical and diagnostic tools, these instruments are often too costly to use in an educational setting, especially given the constrained budgets of many schools.[20-22] In addition, due to the way in which many colorimeters and spectrophotometers are built, students often see these devices as “black boxes” that provide little insight into how they actually work.[23-26] In an effort to address these and other issues, numerous groups of scientists, engineers, and educations have developed various low-cost and user-friendly colorimeters and spectrophotometers, which teachers and students can use in the classroom or teaching lab.[3, 20-38]

These designs include models that use a CD or DVD as a diffraction grating to generate a visible spectrum (i.e., the colors of the rainbow).[4, 6, 7, 9-13] Building upon these ideas, we have developed two fairly inexpensive, single-beam spectrophotometers for the classroom or teaching lab. As with other OPN instruments that we have developed,[1, 2] readers can 3D print the components for one version (Fig. 2A), and they can build the other model using parts available at most hardware stores or online (Fig. 2B). Like the OPN Colorimeter,[1] both designs are easy to use and understand, and they require no specialized knowledge of (or experience with) electrical circuits or soldering techniques (unlike some more sophisticated designs). Finally, as with other OPN instruments that we have created,[1, 2] the instructions and supplies needed to make these spectrophotometers (as well as the underlying computer files) are all open source. As a result, we have named this general design “the OPN Spectrophotometer” (or “OPN Spec” for short), and we hope that these devices can help expand the use of spectroscopy in the classroom, teaching lab, or wherever else they might be useful.

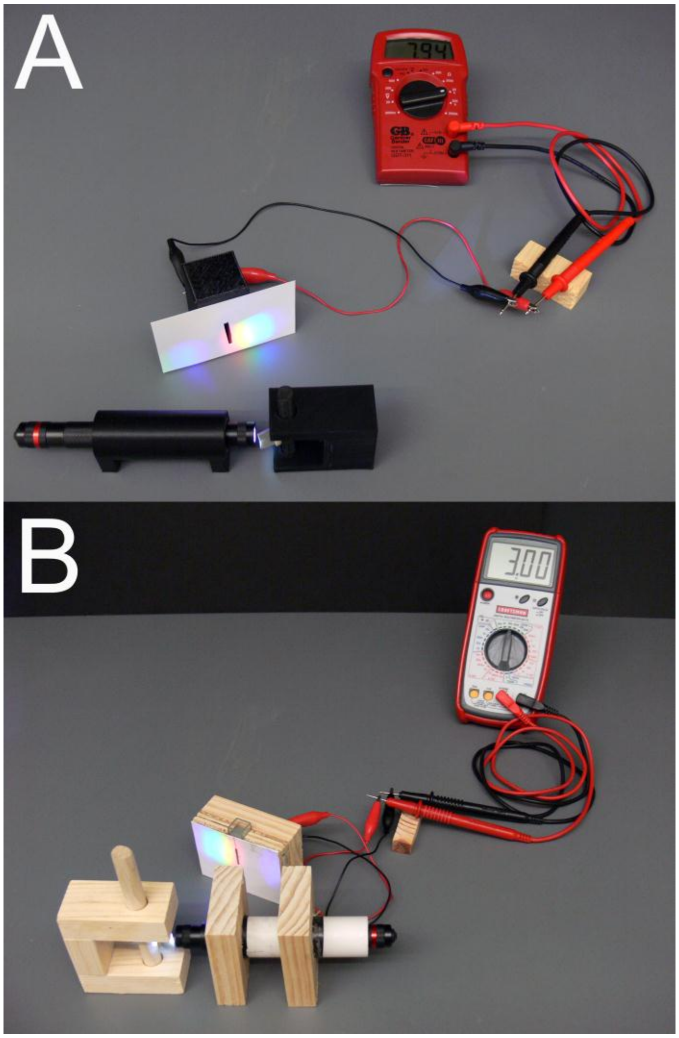


Figure 2. The OPN Spec. (A) 3D-printed version. (B) Wooden version.

MATERIALS AND METHODS

The 3D-printed version of the OPN Spec consists of six parts: (i) a holder for a standard plastic cuvette, (ii) a lid to cover the cuvette, (iii) a plug that fits into the back of the cuvette holder and contains a light dependent resistor (LDR), (iv) a tube that holds the light source (an LED flashlight), (v) a holder for the diffraction grating, and (vi) a small post that holds part of a CD or DVD, which serves as a diffraction grating to generate a visible spectrum (Fig. 3). As with other OPN instruments that we have designed,[1, 2] we have included the underlying Computer Aided Design (CAD) files (S2) and related STereoLithographic (STL) files (S3) for these parts in the Supporting Information, so that readers can print or modify them to fit their needs. Again, we used the free version of DesignSpark Mechanical (RS Components, Corby, Northhamptonshite, U.K.) to create these files (S1, S2, S3).

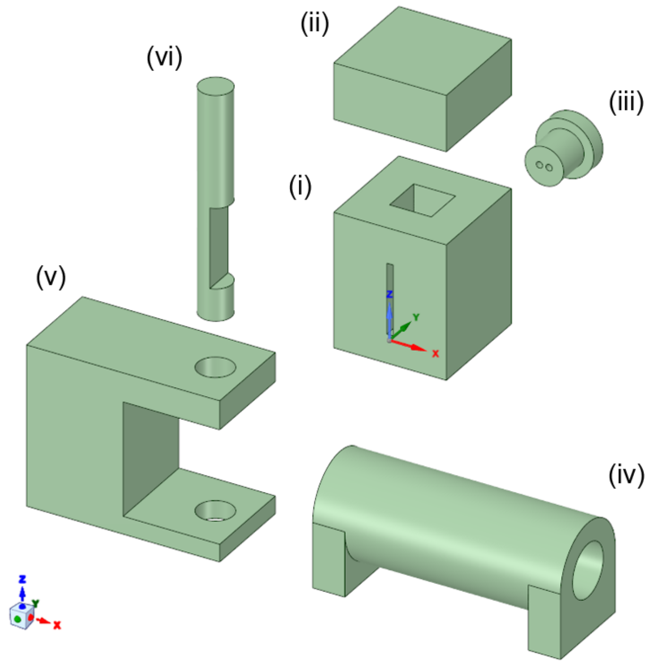


Figure 3. Schematic of the 3D-printed version of the OPN Spec, which contains a (i) holder for a standard plastic cuvette, (ii) lid to cover the cuvette, (iii) plug that holds a light dependent resistor (LDR), (iv) tube for the light source, (v) holder for the diffraction grating, and (iv) post that holds part of a CD or DVD that serves as a diffraction grating to generate a visible spectrum.

We further include in the Supporting Information instructions on how to build a wooden or PVC version of the OPN Spec using parts available at most hardware stores or online (S4). We made this version of the OPN Spec (Fig. 2B) using ¾-inch thick board, ½-inch thick plywood, ¾-inch Schedule 40 PVC pipe, and other materials, such as super glue and electrical tape (S4).

Like the OPN Colorimeter,[1] both versions of the OPN Spec can hold a standard cuvette (external dimensions: 1.25 cm x 1.25 cm x 4.5 cm), and we again use a Coast G20 LED inspection light as our light source in these models (Fig. 2; S1 and S4).

However, other LED flashlights will suffice (S1, S4). As our detector, we use the same inexpensive (85-cent) LDR that we use with the OPN Colorimeter – specifically, a PDV-P8103 (Advanced Photonix, Inc.; Ann Arbor, MI), which has a 500-kOhm "dark" resistance.[1] We then connect this LDR to a digital multimeter to take our readings. Alternatively, readers can build a wooden or PVC version of the OPN Spec that uses a commercial light meter as its detector (similar to the OPN Colorimeter).[1]

To test these designs, we first used the OPN Spec to create a simple Absorbance spectrum for 40 µL of a dilute Methylene Blue solution (100 mg/L) added to 3 mL of deionized water (DI H2O) (S5). We then used this information to identify the color of the peak Absorbance wavelength for Methylene Blue (Fig. 4), and we subsequently used that setting on the OPN Spec to conduct the same Methylene Blue assay described in the Supporting Information for our OPN Colorimeter paper.[1] In particular, we added increasing concentrations of our Methylene Blue solution (100 mg/L) to 3 mL of DI H_2O contained in a standard plastic cuvette. We then calculated the corresponding Absorbance values for each sample, and we repeated the experiment in triplicate to ensure that our results could be replicated (S5). For comparison purposes, we also used a 3D-printed version of the OPN Colorimeter with a red cellophane filter in it, and we further used a commercial spectrophotometer (a Hitachi U-1100) in this assay as a control instrument (S5).

After completing our experiments, we entered our data into Microsoft Excel and calculated an Absorbance value for each entry. As with the OPN Colorimeter, for both versions of the OPN Spec, we used the formula $A = \log_{10}(T / I)$ in our calculations (omitting the negative sign from the Beer-Lambert equation) because the resistance of the LDR is inversely proportional to the intensity of the light striking it.[1] We also treated the "dark" value as zero, which did not create any noticeable irregularities in or inconsistencies with our Absorbance calculations.

We then generated our graphs by subtracting the initial absorbance value from each reading to account for the absorbance of the cuvette and DI H_2O in each assay, and we displayed our results as either column graphs to show the simple Absorbance spectrum for Methylene Blue (Fig. 4) or as scatter plots to show how Absorbance changed as the concentration of Methylene Blue increased (Fig. 5). We also fit lines to the linear region of our scatter plots, and we displayed the equations for these lines (as well as their R^2 values) on the graph (Figs. 5B).

Hazards

Please review each supplement in the Supporting Information (S1, S4, S5, and S6) for a discussion of the hazards associated with making the 3D-printed and wooden versions of the OPN Spec and conducting the related Methylene Blue assays since some of the risks are significant (as would be expected when working with power or other tools or performing many chemistry experiments).

RESULTS

The simple Absorbance spectrum for Methylene Blue that we generated with the OPN Spec followed the general trend of similar graphs created using more sophisticated instruments.[39, 40] In particular, at relatively short wavelengths (i.e., in the violet, indigo, and blue spectrums), our Methylene Blue sample demonstrated a fairly low Absorbance (Fig. 4). However, beginning in the green spectrum, the Absorbance of our Methylene Blue sample began to increase dramatically, with its peak Absorbance wavelength occurring in the red spectrum (Fig. 4). We did, however, find that the wooden version of the OPN Spec tended to generate higher Absorbance readings than the 3D-printed version, especially in the “lower” Absorbance wavelengths (i.e., violet, indigo, and blue) during our Methylene Blue assays (S4, S5). We believe that this discrepancy may result from more ambient light striking the cuvette in the wooden version (S4), and we have found that including a thicker wooden face and a cuvette lid with this version of the instrument can help to address the situation (S4, S5).

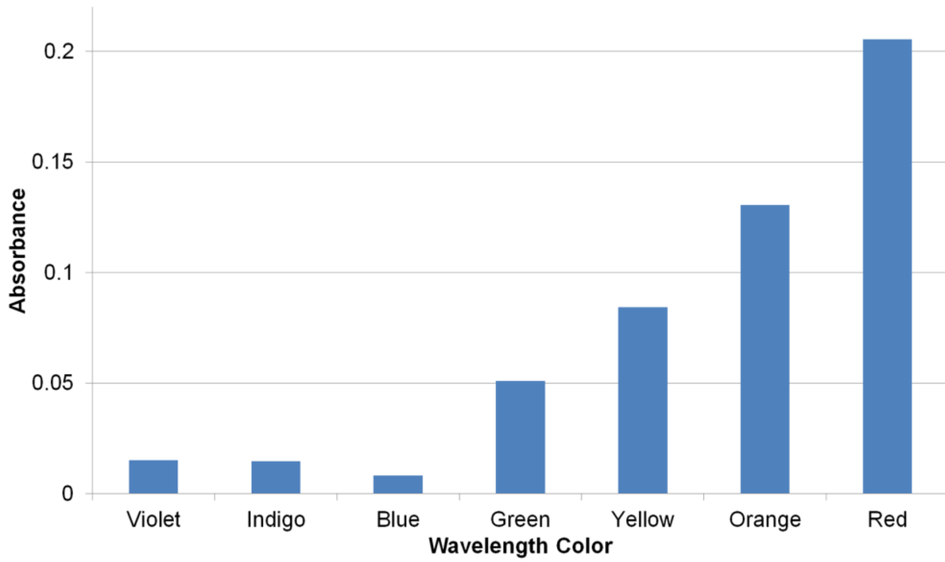


Figure 4. A simple Absorbance spectrum for 40 µL of Methylene Blue (100 mg/L) suspended in 3 mL of deionized water (DI H_2O) generated using the 3D-printed version OPN Spec.

In the concentration assay that we performed, both versions of the OPN Spec generated Absorbance readings that were consistent with the trends that one would expect in this type of experiment and similar to (albeit lower than) those of a commercial spectrophotometer (Figs. 5A and 5B). In particular, we found that Absorbance increased linearly at relatively low concentrations of Methylene Blue (Fig. 5B), but this linear relationship began to break down as the concentration of Methylene Blue increased (Fig. 5A). We also found that the OPN Spec results were consistently higher than those of an OPN Colorimeter by 51% to 72% on average (with standard deviations of 31% and 19%) for the 3D-printed and wooden models, respectively (n = 18). This improvement is likely due to the more specific wavelength that can be generated by the DVD that we use as our diffraction grating in the OPN Spec (compared to the red cellophane filter that we use in the OPN Colorimeter).[1]

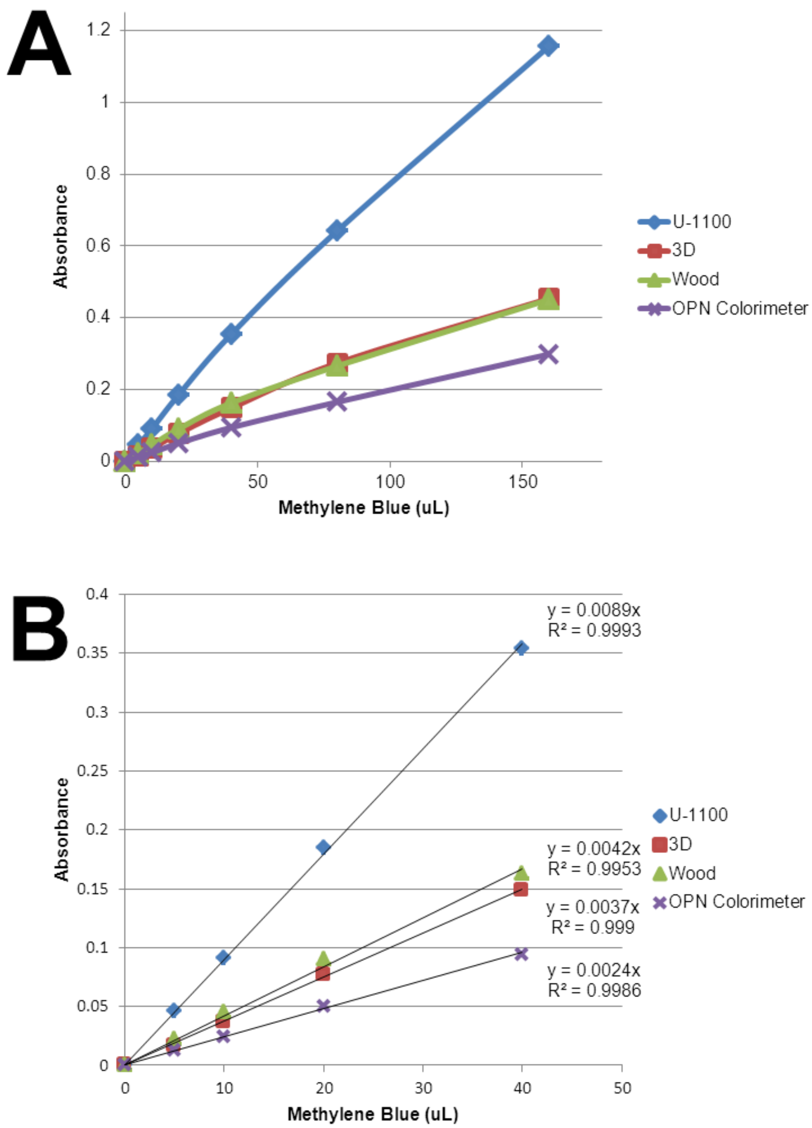


Figure 5. Results from our Methylene Blue assay. (A) Scatterplots showing the Absorbance of 0 to 160 µL of Methylene Blue solution (100 mg/L) added to 3 mL of deionized water in a standard plastic cuvette placed into the OPN Spec or OPN Colorimeter compared to the results from a commercial (Hitachi U-1100) spectrophotometer. (B) Scatterplots showing the linear range of this data with accompanying best-fit lines and R^2 values.

Nevertheless, the Absorbance readings generated by both models of the OPN Spec were still substantially lower than those of a commercial spectrophotometer (Fig. 5). Thus, like the OPN Colorimeter,[1] students could not use published molar extinction coefficients with the instrument, but they could calculate their own extinction coefficients given their data as an academic exercise (e.g., $A = \varepsilon cl \rightarrow \varepsilon = {}^{A}/_{cl}$). Students could further compare their results to published values and discuss reasons for these differences, which might provide a better understanding of how these coefficients are calculated and what they actually mean.

DISCUSSION

As with other "homemade" spectrophotometers that use a CD or DVD as a diffraction grating,[4, 7, 9-13] the OPN Spec is rather simple to make and easy to use. For example, the parts fit together intuitively, and students can further see firsthand the spectrum that they generate as well as the specific band of light that falls onto the LDR. Thus, by using an OPN Spec, students can hopefully gain a deeper insight into how these (and, thus, more sophisticated) instruments actually work, which may remove the mystery that often surrounds these devices.[21, 23, 25, 26]

Moreover, because the OPN Spec (like the OPN Colorimeter) uses an LED flashlight as a light source and a commercial multimeter as a detector, teachers and students do not need to have any advanced knowledge of electronic circuits or experience with electrical soldering in order to assemble the instrument.[1] As a result, the device could be used in classrooms or teaching labs at many different levels. Plus, because students can generate the entire visible spectrum using the OPN Spec, the device is more versatile than the OPN Colorimeter and other similar devices that use fixed optical filters or specific LEDs, which often limits the set of experiments that can be conducted with these devices (since they can only transmit a limited set of wavelengths into a given sample). Thus, even though the OPN Spec may not be as sensitive as some other educational spectrophotometers or colorimeters described in the literature,[3] the instrument is still rather versatile and fairly inexpensive to make.

For example, as explained in the Supporting Information (S1), we estimate that 3D printing the basic parts for the OPN Spec on either the MakeXYZ[41] or 3DprintUK[42] websites would cost approximately $55 at October 2016 prices (not including any taxes or shipping). As a result, with a basic LDR ($1), a reasonably priced multimeter ($13), and an LED flashlight ($11), the entire set-up should cost around $80 or much less for readers who already have a 3D printer (e.g., a 2.2-kg or roughly 400-m long spool of black ABS filament typically costs about $25 online and will print the parts for at least five OPN Specs, so a set of ten could be 3D printed for roughly $50). Similarly, buying the raw materials to make a wooden or PVC version of the OPN Spec should generally cost between $34 and $100 depending on the specific materials used (S4), not including the price of tools. Thus, readers could outfit a classroom or teaching lab with several working models at a relatively low cost, creating a variety of educational opportunities for students.

By way of illustration, if used in a chemistry, biology, or physics course, the OPN Spec (like the OPN Colorimeter) could help demonstrate many basic spectroscopic principles, such as how these instruments are designed and built, how they can be used to generate a simple Absorbance spectrum or to collect other readings, what those results mean given the sample(s) under investigation, and what role those values play in the Beer-Lambert equation.[1]

Instructors could further have their students create a standard (i.e., calibration) curve using the OPN Spec to determine the concentration of a given substance in solution. In the process, students could observe how Absorbance varies linearly with concentration at low levels and how, at higher concentrations, this linear relationship begins to break down (Fig. 5; S6). Instructors could also have their students use their linear data to estimate the concentration of one or more "unknown" samples – a common practice in many teaching labs. For even more ideas, we encourage readers to review our OPN Colorimeter paper, which contains numerous references for additional educational experiments that can be conducted with the OPN Spec (such as running

Bradford, Benedict, or Lowry assays or conducting experiments to examine enzyme activity and the related Michaelis-Menten kinetic parameters).[1]

Given the possibilities, we hope that the OPN Spec (like other OPN instruments that we have designed)[1, 2] will help students develop a better understanding of the chemical and physical principles involved in these types of experiments while also gaining deeper insights into how scientific instruments like spectrophotometers actually work. As a result, we hope that the OPN Spec will help contribute to the impressive work that others have done (and are continuing to do) in developing useful and user-friendly scientific equipment for educational and other purposes.

CONCLUSION

As with other OPN Spec and OPN Colorimeter,[1, 2] we hope that the 3D-printed and wooden versions of the OPN Spec will help to make learning about science and engaging in the process of scientific inquiry more accessible and understandable for others, particularly those who may lack the funds for more expensive devices. We further invite teachers, students, and others to use or adapt these designs to fit their particular needs, and we look forward to learning about the results.

ASSOCIATED CONTENT

Supporting Information

The following materials are available on our web page http://pages.stolaf.edu/opn-lab/equipment/: our protocols for 3D printing the parts for the OPN Spec (S1), the underlying CAD and STL files for the components of the 3D-printed version of the OPN Spec (S2 and S3, respectively), instructions for building a wooden or PVC version of the OPN Spec (S4), and our protocols for the Methylene Blue assays described above (S5 and S6).

AUTHOR INFORMATION

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Notes

The authors declare no competing financial interest.

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