Construction and Evaluation of a LEGO Spectrophotometer for Student Use

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Abstract: A simple visible-wavelength spectrophotometer has been constructed for educational purposes. The spectrophotometer contains simple, inexpensive components students can easily work with (small flashlight bulbs, batteries, etc.) and uses LEGO pieces for construction of the optical support elements. The spectrophotometer was designed to give students hands-on experience with typical spectrophotometer modules so that they may understand the important stages in the design of a scientific instrument. The spectrophotometer was characterized by examining an absorption spectrum and calibration curves of potassium permanganate.

Introduction

Chemical instrumentation is a key element in standard analytical chemistry curricula. Senior-level undergraduate or first-year graduate-level analytical chemical instrumentation laboratory courses often focus on either the use of such instrumentation or the theory of its operation rather than analytical instrument design; however, comprehension of the different modules and engineering aspects that go into any chemical instrument is a key element in designing and improving chemical instrumentation. A valuable aid to students in the process of understanding instrumentation is the opportunity to dissect a simple instrument into its component modules; however, cost can be a deterrent to using a modern commercial instrument for this purpose. A few examples of simple instruments built either by faculty for easy student use or constructed by the students themselves have been reported, including micro-Raman [1], mass spectrometry [2], NMR [3], and UV–visible spectrophotometry [4–6].

Previous reports of UV–visible spectrophotometers have involved inexpensive designs for student use or designs that can be built by students at the circuit level or at a more modular level. Of these, only one was designed to be built by students at the component level [5]. Bernazzani and Paquin used an Ocean Optics modular spectrophotometer that could obtain a true spectrum as well as kinetic information [6]. They reported that, in comparison to the standard Spectronic 20 that is commonly used to teach students the basics of spectrophotometry, the implementation of an Ocean Optics modular spectrophotometer was useful in teaching the students about data acquisition and analysis [6].

In this article, we introduce a simple and inexpensive LEGO-based UV/vis spectrophotometer with wavelength scanning capabilities designed for student construction. The present instrument uses LEGO to provide inexpensive and stable optical supports. This approach was motivated by a recent report [7] on the use of LEGO blocks as optical mounts. The spectrophotometer was designed for a graduate-level course entitled Spectrochemical Instrumentation in the Department of Chemistry at Purdue University. Implementation of this instrument in senior-level undergraduate courses should be straightforward and may also be considered. In class, students learned about spectrophotometer instrument components, optics, and electronic circuitry, all of which are applied to the spectrophotometer. The spectrophotometer discussed below was built by the instructors of the course; however, in the future, this instrument may be completely constructed by the students. Data were then collected on the instrument and compared to data obtained from two commercial instruments.

Spectrophotometer

The spectrophotometer contains the five basic modules of a typical UV–visible transmission instrument. It has a light source, optical elements including a grating and an adjustable mirror for wavelength selection, a sample holder made of LEGO pieces, a silicon photodetector, and a readout module containing an amplifier circuit and digital multimeter for data display. A block diagram of the instrument may be seen in Figure 1 and photographs are shown in Figure 2 and Figure 3. All modules were constructed from inexpensive materials and designed to be as cost effective as possible. The price of the overall spectrophotometer was estimated to be approximately $200, and the price of each of the individual components is listed in Table 1.

Optical mounts are designed to ensure high mechanical stability. Because of their size, weight, and precision manufacturing, they are often expensive. LEGO is a highly modular construction system of acrylonitrile-butadiene-styrene pieces with a patented stud-and-tube coupling system. LEGO pieces provide the necessary stability of optical components in order to limit the effects of jostling of the instrument during use or movement [7]. Precise tolerances are applied during the production process (pieces are created so that they are no more than two hundredths of a millimeter from the nominal size) resulting in a force of 1.5 to 3.5 N needed to separate the pieces [7]. This creates the high level of stability necessary for optical components. Finally, because LEGO pieces undergo standardized production, all similar LEGO pieces are almost identical in size. This makes vertical and horizontal positioning of optical elements straightforward. The base of the instrument

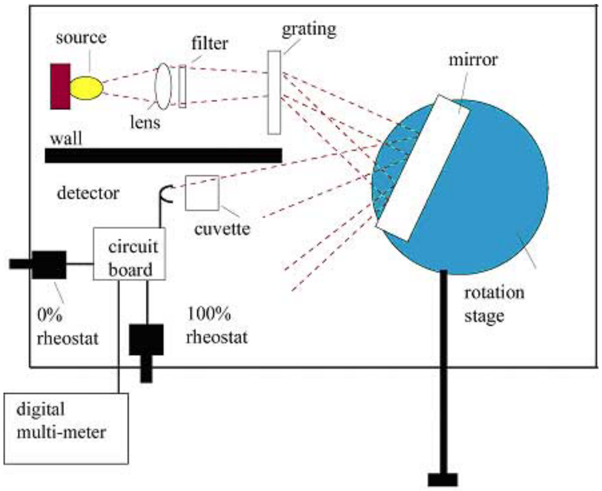

Figure 1. Schematic diagram of the home-built LEGO spectrophotometer. Dotted lines represent light paths through the instrument. The entire instrument was placed in a 20-cm-by-30-cm box with the exception of the multimeter.

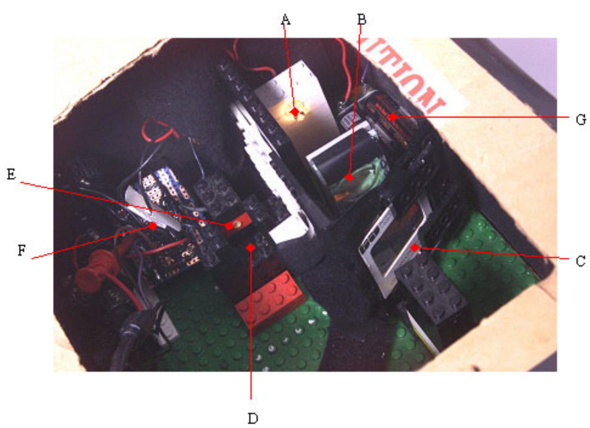

Figure 2. Photograph of the inside of the instrument. The photograph shows the (A) source, (B) lens and IR filter, (C) grating, (D) sample holder, (E) detector, (F) amplifier circuit, and (G) battery and power supply.

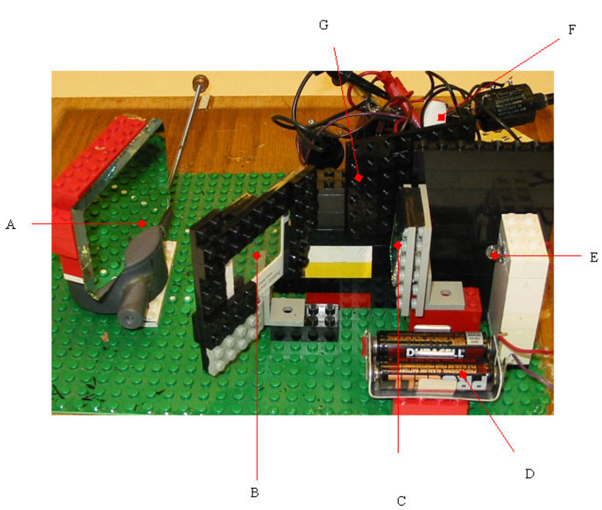

Figure 3. Photograph of a side view of the instrument. The photograph shows (A) the mirror, (B) grating, (C) lens and IR filter, (D) light power source, (E) light source, (F) circuit and amplifier power source, and (G) detector location.

was a flat LEGO board, making horizontal positioning and aligning of optical elements simple. The entire instrument was encased in a cardboard box painted black on the inside to limit light reflection and stray light reaching the detector. Wood or another material could also be used for durability.

The light source for the instrument was a Sylvania miniature-lamp light bulb, which was powered by two 1.5-V batteries. The batteries were electrically connected to a two-position double-throw switch to allow for light activation. The light source was stabilized in position by placing it between two connected 2 × 4 LEGO bricks that had a ¼-in hole drilled between them to hold the light bulb in place. These LEGO bricks were then placed atop two other standard 2 × 4 LEGO bricks for proper vertical positioning. As the miniature bulb was a filament light source, it mainly produced visible light (though some NIR and IR light was also produced). The filament had dimensions approximately 0.5 by 4 mm and was oriented vertically to take advantage of its small size, thereby eliminating the need for an entrance slit.

The wavelength selector module consisted of a lens, an IR filter, a transmission grating, and a rotating mirror. Approximately 4.5 cm from the light source a convex lens (focal length 5 cm) was placed to focus the light from the source. An IR filter was placed on the opposite side of the lens to cut out any NIR light, which would otherwise reach and be detected by the photo-diode detector. It was noticed that second-order diffracted light caused a large background signal before the IR filter was added. The source, lens, and filter were sheltered from the detector by a LEGO wall and covered with black felt to further limit stray light. The light was then passed through a linear transmission diffraction grating (1000 lines/mm, Edmund Scientific) mounted on a frame constructed of flat LEGO pieces. The diffracted light pattern then intersected a silver mirror (5.5 cm by 7.5 cm), which was used to increase the focal length of the spectrophotometer. There are few LEGO components available with good stability and consistent rotation; therefore, the mirror was mounted on a spring-loaded rotation stage roughly based on a similar device described in Quercioli, et al. [7] and constructed by the Purdue Chemistry Department machine shop. This rotation stage contained a flat rotating piece on top of which the mirror was mounted. The bottom piece contained a spring-loaded piston that allowed for smooth rotation of the mirror. A schematic of this piece may be seen in Figure 4. This piece was then glued to a flat LEGO brick and positioned on the large LEGO base of the instrument. The rotation stage was placed in a position where it would allow for scanning through the light spectrum with reasonable resolution while maintaining a satisfactory amount of light intensity. The optimal location placed the mirror at a distance of 7.0 cm from the diffraction grating and 13.5 cm from the detector. The wavelength selector was calibrated such that one turn of the screw on the rotation stage corresponds to an approximate wavelength change of 32 nm in the light reflected onto the detector. Calibration of the wavelength selector was performed using a holmium oxide sample (NIST). The resolution of the spectrophotometer was determined to be approximately 8 nm, or ¼ turn of the adjusting screw, a value that is based on our ability to reproducibly turn the rotation stage.

The detector was an Edmund Scientific silicon photodetector with a borosilicate window and a detector area of 3.2 mm^2. Due to its small detection area, an exit slit was considered unnecessary. A LEGO sample holder designed to

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Table 1. Instrument Pricing

Component	Source	Price
Lamp	Sylvania	$8.00
Lens	Edmund Scientific	$21.00
IR filter	Edmund Scientific	$29.00
Grating	Edmund Scientific	$1.00
Mirror	Edmund Scientific	$9.00
Mirror mount	Purdue Univ. Machine Shop	$15.00
Detector	Edmund Scientific	$15.00
Operational Amplifiers	Newark	$3.00
Resistors	Newark	$1.00
Rheostats	Newark	$32.00
Switches	Newark	$5.00
Batteries	Dura-Cell	$9.00
Multi-meter		$15.00
Lego bricks	LEGO	$30.00
Cardboard Box and Paint	Rust-Oleum	$2.00
Total		$195

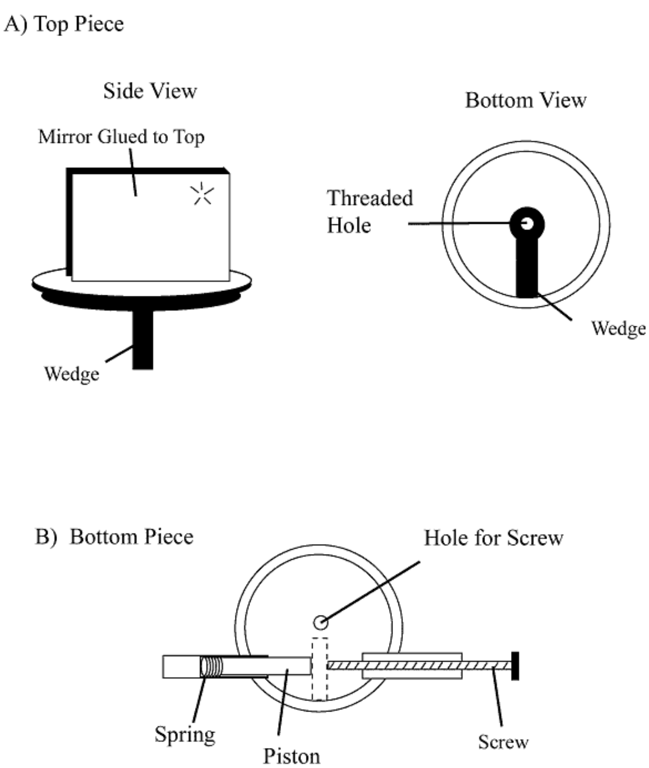

Figure 4. Diagram of the mirror rotation device. The device is divided into a top piece (Figure 3A) and bottom piece (Figure 3B). The device works by turning a screw attached to the bottom piece. The screw pushes against a solid wedge of the top piece, causing this piece to rotate relative to the bottom piece. The mirror is attached to the top piece and the bottom piece is fastened to the instrument; therefore, the mirror rotates relative to the instrument. The side of the wedge opposite the screw is in contact with a spring-loaded piston to give smoother rotation. The piston is associated with the bottom piece.

hold 1-cm plastic cuvettes (Sigma) was placed in front of the detector.

The signal from the detector was passed through an amplifier circuit [8], which is shown in Figure 5. The circuit contained two operational amplifiers, one to introduce variable gain and a second to act as a voltage offset controller. The operational amplifiers in the circuit were powered by two 9-V alkaline batteries. The batteries were attached to a double position–double throw switch to allow for deactivation of the circuit. The two variable resistors were placed in the circuit to control the zero and 100% transmittance of the spectrophotometer. The signal was then transmitted from this amplifier circuit to an external multimeter where the readout of the spectrophotometer was obtained. In the experiments discussed below, a Tektronix digital multimeter was used; however, a less expensive multimeter (Sperry DM-350A, $15) may be implemented into the design to reduce cost.

Experimental

Three procedures were used to characterize the home-built instrument. These tasks were and can be adapted by students to evaluate the spectrophotometer. First, an absorption spectrum of $KMnO_4$ was obtained and then used to determine the wavelength of maximum absorption for $KMnO_4$. The concentration of potassium permanganate for these experiments was 8.3×10^{-5} M. Two separate calibration curves, one for the home-built spectrophotometer and one for a Spectronic 20 instrument (Bausch and Lomb, Inc.) were determined. Calibration curves for potassium permanganate solutions were obtained at the wavelength of strongest absorption with concentrations varying from 1.6×10^{-5} M to 1.0×10^{-2} M. Solutions were obtained by placing a predetermined mass of $KMnO_4$ into a 100-mL volumetric flask and filling to the mark with distilled water. This solution was subsequently diluted using other volumetric flasks. Solutions were wrapped in aluminum foil and stored in the dark to limit photodecomposition.

A standard procedure was followed for acquiring the measurement data using the home-built spectrophotometer. First, the zero of the instrument was set with the light bulb turned off. Then the light bulb was activated and allowed to warm up for approximately five minutes, and a measurement was obtained using water as the blank. The voltage readout of this measurement was considered to be 100% transmittance and could be adjusted by the experimenter. The transmittance of the sample was then recorded. The wavelength was then changed by some predetermined amount using the wavelength selector. Alternatively, a new solution of different concentration was placed in the spectrophotometer for the calibration curve determination. A blank measurement was obtained before each measurement of any sample. This procedure was performed for two reasons. First, the light-bulb intensity drifted over time, and this procedure limited the effects of drift. A regulated power supply would greatly reduce this problem while adding some cost and decreasing portability of the spectrophotometer. Second, the output intensity of the light bulb was highly wavelength dependent. In modern spectrometers, it is possible to perform only one blank measurement prior to recording an entire wavelength absorption spectrum; however, in our spectrophotometer we saw as much as a 70% decrease in light intensity over the entire visible wavelength spectrum (the lamp produced lower light intensities at smaller wavelengths). This made it important to take a new blank measurement prior to each sample measurement. All solutions were placed in 1-cm plastic cuvettes (Sigma). For measurements using the Spectronic 20, 1 cm diameter glass test tubes were used. The same solutions were used for Spectronic 20 measurements; however, a blank measurement was only taken prior to the first of a series of measurements (the Spectronic 20 is considered to have less drift than the home-built spectrometer due to its electronic power supply). All results were obtained using potassium permanganate solutions.

Results and Discussion

An absorption spectrum using a solution of 8.3×10^{-5} M $KMnO_4$ is shown in Figure 6 for the home-built spectrophotometer, a Spectronic 20 instrument (Bausch and Lomb, Inc.), and a Cary 300 (Varian, Inc.). The intensities of

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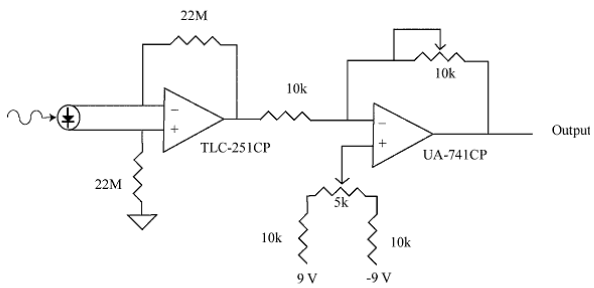

Figure 5. Amplifier circuit diagram. The variable 5k resistor controls the zero of the instrument and the 10k resistor in the feedback loop controls the gain and is used to set the 100% value.

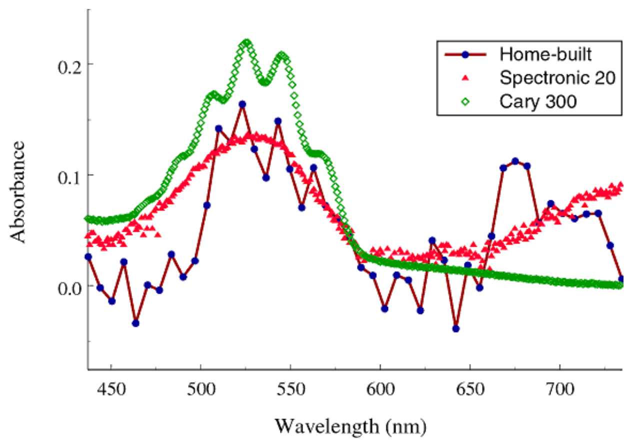

Figure 6. Absorption spectra of an 8.3×10^{-5} M potassium permanganate solution obtained with the Cary 300, the home-built spectrophotometer, and the Spectronic 20 spectrophotometer. Spectra were taken at room temperature using square plastic cuvettes.

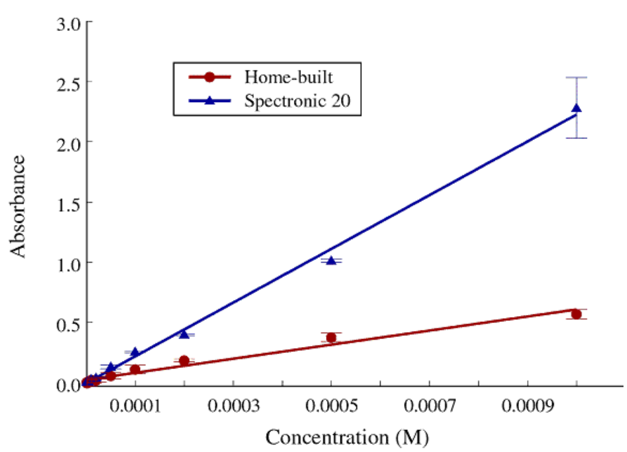

Figure 7. Calibration plots for potassium permanganate using the home-built spectrophotometer and the Spectronic 20. Both plots are an average of three data points at each concentration.

all three spectra are comparable at this low concentration (see below). In the spectrum obtained with the LEGO spectrophotometer, two major absorption peaks that appear at approximately 523 and 543 nm are evident in Figure 6. The spectrum is reasonably similar to that of the Cary 300, which has maxima at 526 and 545 nm, along with some other, minor peaks and shoulders. In contrast, the spectrum for the Spectronic 20 shows only a single broad absorption peak with a maximum around 530 nm. The reason for the wavelength discrepancy is likely related to the wavelength scale estimation of the home-built instrument. The home-built instrument covers the visible range estimated to be from 420 nm to 780 nm (comparable to Spectronic 20 range of 340 nm to 950 nm). Due to possible error in the wavelength selector calibration, the range may be off by a few nanometers in either direction.

The wavelength is adjusted by a spring-loaded screw device (see Figure 4). This device was calibrated using holmium oxide and it was determined that a greater change in wavelength occurred for each turn at higher wavelengths. A calibration curve was constructed by comparing wavelengths of absorption peaks of the holmium oxide [9] for the home-built instrument and used to estimate this nonlinearity. The following equation for the wavelength calibration was obtained:

$$\lambda_{\text{calib}} = \lambda_{\text{lin}} + (\lambda_{\text{lin}}/14)$$

Here, λ_{lin} is the wavelength assuming a linear response in wavelength for the mirror turning. The above equation was used to adjust the wavelengths in the absorption spectrum for the home-built instrument shown in Figure 6. The home-built instrument has a wavelength resolution of approximately 8 nm, which corresponded to approximately one quarter turn of the wavelength-selector screw. This resolution is compatible with that displayed in the spectrum. Possible resolution limitations may be due to the lack of entrance and exit slits, finite filament width, or poor quality of the diffraction grating in the home-built spectrophotometer. In contrast, the Spectronic 20 had a reported wavelength resolution of 1 nm, although according to the observed spectrum, the resolution was far poorer. We note that miniature UV/vis spectrophotometers are commercially available with resolution as low as 2 to 5 nm [10]. The home-built spectrophotometer also has a broad absorption peak at approximately 680 nm. This peak is most likely a result of poor mirror geometry leading to residual light from a high order reflection or a result of residual stray light. The actual source is unknown; however, it did not appear in all absorption spectra taken, making it a probable source of random error.

Calibration curves for both the home-built spectrophotometer and the Spectronic 20 were made using a variety of potassium permanganate solutions. Two representative calibration curves are shown in Figure 7. Both of these calibration curves were taken at a wavelength of 528 nm and used an average of three data points. The sensitivity of the two instruments was determined to be 580 ± 20 M^{-1} for the home built spectrophotometer, and 2130 ± 30 M^{-1} for the Spectronic 20. The reason for this large discrepancy was most likely due to considerably more stray light in the home-built spectrophotometer. The home-built spectrophotometer had a limit of linearity of approximately 0.001 M, while limit of linearity of the Spectronic 20 was approximately 0.002 M (estimated by finding concentration values where linear fit R^2 values were greater than 0.95). Deviation from linearity of the home-built spectrophotometer and the Spectronic 20 may be seen in Figure 8. In the home-built instrument, the source was shielded with black felt in an attempt to limit this stray light, but it could not be completely eliminated. The concentration limit of detection of the home-built spectrophotometer was 6×10^{-5} M while the limit of detection of the Spectronic 20

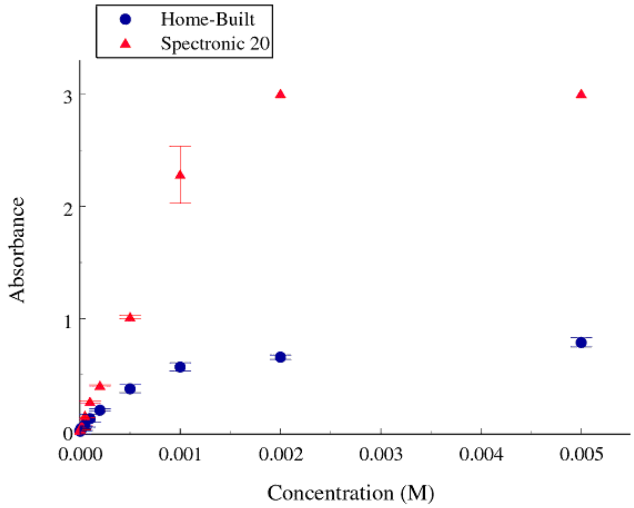

Figure 8. Calibration plots of potassium permanganate at higher concentrations showing nonlinear characteristics of the home-built spectrophotometer and Spectronic 20. Data were taken under the same conditions as in Figure 7.

was 3×10^{-6} M, which were determined using a value three times the standard error of a blank measurement. The two major reasons for the higher limit of detection in the home-built spectrometer were resolution of the multimeter used for data analysis and source drift. Drift problems were especially noticeable if the light-bulb source was not given a proper warm-up period. This drift made accurate readings at high transmittance difficult. Students can benefit from a demonstration and discussion of the origin of the various errors encountered above.

Conclusions

An inexpensive, easily constructed visible-wavelength spectrophotometer was designed for student use. The spectrophotometer was used to obtain spectra and create calibration curves. Absorption spectra acquired with the instrument demonstrate similar features to spectra obtained from a high quality commercial instrument, although the resolution is inferior to that instrument, but comparable to other, inexpensive spectrophotmeters. Calibration plots obtained from the home-built instrument had similar deviations from linearity as plots obtained from an inexpensive commercial instrument (Spectronic 20). The home-built instrument demonstrated low output at short wavelengths and was subject to more performance difficulties from stray light being introduced to the detector and drift than the commercial instruments; however, effective procedures were introduced to counter these difficulties, and therefore decent spectra and calibration data were successfully acquired.

There are several benefits of the spectrophotometer described above. The instrument is inexpensive (approximately $200) and easy to construct for (or by) students. The spectrophotometer provides wavelength-scanning abilities. It is believed that such a spectrometer can be successfully used for instruction in a chemical instrumentation laboratory because students can construct such an instrument with minimal help. It is also believed that the students may learn a great deal from the actual construction of this instrument, including the electronic and optical modules important for its function. It should be noted that the instrument went through several iterations in the construction phase, including the construction of optical mounting elements from wood, which were unsuccessful for a variety of reasons. The various problems encountered with constructing such an inexpensive spectrophotometer could also be explored and analyzed by students, as well as a number of possible future improvements. Finally, the sources of error present within the instrument can be used to demonstrate commonly observed problems in spectrophotometry. Students may obtain absorption and calibration spectra as well as calculate the limit of linearity, limit of detection, and resolution of the instrument. A number of applications are readily available in the literature to allow students to gain practical experience with the instrument. The ability to break a scientific instrument down to its components and reassemble it into a functional condition is a highly useful skill for an analytical chemistry student. Inexpensive construction of such an instrument as the one described here gives students a hands-on opportunity to learn and demonstrate this analytical ability.

Finally, several improvements can still be made to the home-built spectrophotometer described above. A regulated power supply could be added to stabilize the light source. Another lens may be used to collimate light onto the detector after it has been diffracted by the grating. A better grating and slits could be used to improve the spectral resolution. Also, a more precise, possibly motorized rotation stage could replace the current manual mirror-rotating device. The instrument could even be made into a dual-beam instrument to help eliminate drift problems. All of these are issues that can be tackled by students in an educational environment.

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