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UV-Vis spectrometer from scratch: a budget do-it-yourself solution to a growing problem

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UV-Vis spectrophotometry is one of the most commonly applied spectral methods for quantitative analysis. Its concept, meaning and applicability are an important part of the specialized chemistry course *Methods for control and compound analysis*. As most schools lack UV-Vis spectrophotometers, there is a tendency to skip the laboratory exercises dedicated to this topic. Our work presents a simple and practical way to remedy the present problem. A methodology is proposed that allows students to perform simple spectrophotometric experiments using low-cost equipment. A sample experimental protocol for conducting a successful lab exercise is developed and further data processing is demonstrated. The results are promising, showing that UV-Vis spectrophotometry can be successfully taught in practice with low cost, minimal preparatory time and without specialized equipment.

Keywords: low-cost spectrophotometric teaching equipment; inquiry-based learning; self-led exercise, chemistry education.

INTRODUCTION

In the past years, the Bulgarian curriculum and high-school system were changed in a way that allows students to choose and pick up to four specialized subjects during their last two years of education, called second high-school level (similar to A level). Those who choose chemistry are taught in much more detail including aspects of applied science, which broadens their knowledge and prepares them for further scientific work and academia. The curriculum in chemistry is divided into four separate parts that are taught in the following order:

1. Theoretical foundations of chemistry (11th grade)
2. Inorganic chemistry (11th grade)
3. Organic chemistry (12th grade)
4. Methods for control and compound analysis (12th grade)

The present work focuses on the fourth, last part, because it appears to be the most challenging one for high-school teachers. Common reasons why they face difficulties are: (i) reduced number of hours due to the shorter semester for 12th-graders; (ii) insufficient time for preparation and conducting laboratory exercises; (iii) lack of equipment for students to conduct any spectroscopic analysis.

This article presents a simple and low-cost, yet effective experiment for quantitative analysis of colored aqueous solutions. The analysis is quite suitable for a 2- or 3-h laboratory exercise, as outlined in the Experimental part. Its main advantage is that students can experiment almost without any input from the teacher (self-led exercise). The presented approach for quantitative analysis has already given excellent results among other students worldwide [1-8] with simple 3d printed devices and use of smartphones, moreover, such low-cost approach has merit in real life applications [9]. While the experimental setup suggested in this work does not significantly differ from other examples, the mathematical methods for data processing do. Depending on the students' mathematical knowledge, one of two approaches should be utilized to process experimental data (e.g., excluding or including logarithms).

Aims and research purpose

This article suggests a low-cost, multi-aspect, practical lab experiment dedicated to quantitative UV-Vis spectroscopic analysis. It could be easily conducted by high-school students during their chemistry lessons. The authors aim to prove that including a reliable and accurate spectroscopic experiment at school is achievable even provided limited financial and material resources.

Problem statement

The current task is to analyze two sets of freshly prepared standard solutions of copper (II) sulfate ($CuSO_4$) and nickel (II) sulfate ($NiSO_4$), as well as

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to derive calibration curves (Beer's law). Additionally, the results obtained with the presented spectrometer are compared to those measured with a reference PASCO spectrometer. The questions to be answered are; - is the accuracy of our measurement tool comparable to that of a professional spectrometer, and how to best process the obtained experimental data.

EXPERIMENTAL

Setup

The experimental setup includes the following:

- Small cardboard box;
- Duct tape, glue, ruler and scissors;
- Aluminum foil;
- Cuvette;
- Two smartphones (or a smartphone and a laptop);
- Purified water and standard solutions of Cu(II); and Ni(II) (chosen because their absorbance is in the visible spectrum);
- Weighting scale Kern TGD 50-3C;
- PASCO PS-2600A spectrometer (used as reference).

A small 50×50 mm box is made of cardboard (box size could be modified). A circular hole is made on one side of the box so it can accommodate a smartphone camera. Then, another bigger rectangular hole is made on the opposite side to place a smartphone or laptop screen as a red-green-blue (RGB) light source. A small square hole is made at the top of the box so that a standard cuvette could be placed inside (Figures 1, 2). The outside of the constructed spectrometer is covered with aluminum foil, so it blocks light entering the box thus reducing error.

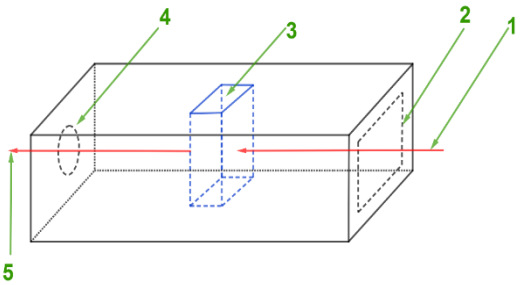


Fig. 1. Sample scheme of the constructed spectrometer: 1 – input light ray; 2 – rectangular hole for the light source; 3 – cuvette space; 4 – small circular hole for a camera; 5 – output light ray

Procedure

A set of $CuSO_4$ aqueous solutions with concentrations of 0.025 M; 0.050 M; 0.10 M; 0.20 M and 0.30 M are prepared by weighing an exact mass of stock $CuSO_4.5H_2O$ and dissolving it with purified water in a 100 mL volumetric flask. The mixture is homogenized, then an aliquot is taken and diluted with water in a 50 mL volumetric flask. The procedure is then repeated to prepare the rest of the solutions. All aliquots are measured with a burette to ensure that exact volumes are transferred to the volumetric flasks. The solutions of $CuSO_4$ should be measured at a wavelength $\boldsymbol{\lambda_{max}} \sim 635$ nm ($\varepsilon = 2.8\ \mathrm{L \cdot mol^{-1} \cdot cm^{-1}}$) [10, 11] and the solutions of $NiSO_4$ - at $\boldsymbol{\lambda_{max}} = 393$ nm ($\varepsilon = 5.1\ \mathrm{L \cdot mol^{-1} \cdot cm^{-1}}$) [12]. Given the educational focus of this work, our aim is to emphasize the key aspects of spectrophotometry, as well as to facilitate the experiment itself and make it more suitable for students. Therefore, analyte solutions with higher concentration are preferred, which justifies the choice of the absorption bands for $CuSO_4$ and $NiSO_4$ corresponding to low intensity $d \rightarrow d$ transitions. Light sources with continuous spectra allow a free choice of wavelength. However, students do not often come to school with such light emitters. In contrast, they never miss the opportunity to bring their smartphones and laptops to school every day. So, the main question is: can they use digital screens as light sources, given the obstruction that they only emit a linear RGB spectrum? The answer is — yes, however, a slight change in results interpretation is required. Digital screens emit red, green, and blue light, and thus each sample is measured by the color it absorbs the most. For example — blue samples like $CuSO_4$ and methylene blue absorb most intensely red light. Red compounds like Co(II) salts or the $[Fe(SCN)_6]^{3-}$ complex absorb mostly in blue. Therefore, the classic concept for absorption at a fixed wavelength is substituted by absorbing red, green, or blue light.

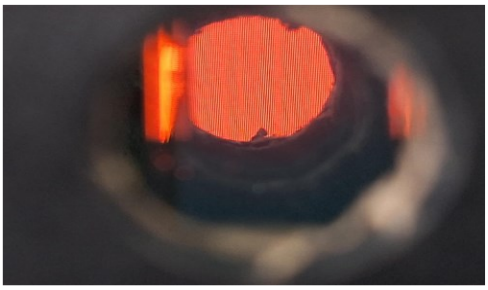


Fig. 2. Picture made with a smartphone camera placed in front of the spectrometer circular hole

RESULTS AND DISCUSSION

Although professional spectrophotometers directly display the absorbance A of a sample at certain λ, the presented tool can only measure RGB light components. For green and blue solutions, the most significantcomponent is $[R]$ while for red

solutions it is the green one [G] [13]. It is essential to note the correlation between numerical values for [R] light and sample concentration c. Suppose a purely red screen is a light source, the measured [R] should be proportional to the light intensity I passed through the cuvette. Although each smartphone camera introduces transformations to the measured light, for this article's aims the correlation between [R] and I could be assumed linear without an intercept: $I = \alpha \cdot [\mathrm{R}]$, where α is a coefficient specific for each camera and depends on the surrounding light, screen brightness and parameters that are specific for each individual measurement set. The constructed educational measurement tool should be calibrated before changing the surrounding light, the sample color, the screen/its brightness and the detecting camera. Given all the assumptions are requirements, we do not propose, nor do we claim that this is a universal calibration protocol. The calibration of the spectrometer only consists of obtaining a linear correlation between the sample concentration and the specific function of [R], representing the absorbance A. Thus, for concentrations in the linear section of Beer's law, the following relation is obtained:

$$A = \lg\left(\frac{I_0}{I}\right) \sim \lg\left(\frac{[R]_0}{[R]}\right),$$

where $[R]_0$ is the absolute [R] value of the red screen. Ideally, $[R]_0 = 2^8 = 256$. Given that we work with line light spectrum, no wavelength could be specified. At first glance, this might seem to be a limitation, however the entire spectral analysis regards only one of the spectral components present in the emitted light – [R], [G] or [B] [14, 15]. Therefore, samples are analyzed, based on their general sensitivity to red, green, or blue light.



Fig. 3. Front view of the constructed spectrometer

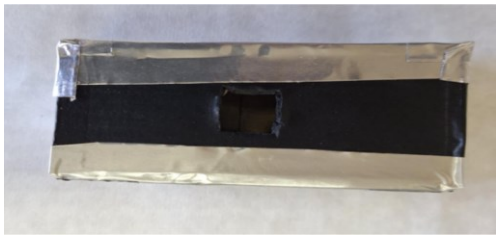


Fig. 4. Top view of the constructed spectrometer

The working protocol presented below is followed. It is useful, but not the only one, so it could be optimized depending on the teacher's goals and the students' preparation level.

Protocol

1. Samples preparation;
2. Spectrometer calibration against purified or distilled water;
3. Measurements with the constructed spectrometer;
   Data processing as:
   a. [R] *vs.* c plot and $c = \alpha[R]$ fit;
   b. lg [R] *vs.* c plot and $c = \beta - \alpha.\lg[R]$ fit;
4. Comparison between both methods and data analysis methods.

Analysis with reference PASCO spectrometer

For each solution set, all samples are analyzed starting from the most dilute one. The spectrometer is calibrated using its built-in functions against a cuvette filled with purified water. Samples are then transferred to the cuvette, and the absorbance is read and written down. All data gathered for both compounds are summarized in Table 1.

Table 1. Experimental data for the absorbance A of all samples obtained with the reference PASCO spectrometer

№	c_1($CuSO_4$), M	A_1, -	c_2($NiSO_4$), M	A_2, -
1	0.025	0.06 ± 0.02	0.019	0.03 ± 0.02
2	0.050	0.09 ± 0.02	0.038	0.10 ± 0.02
3	0.100	0.21 ± 0.02	0.075	0.21 ± 0.02
4	0.200	0.43 ± 0.02	0.150	0.43 ± 0.02
5	0.300	0.70 ± 0.02	0.300	0.93 ± 0.02

The absorbance is plotted against solution concentration – $A(c)$, and correlation coefficients R^2 of 0.9990 and 0.9959 are obtained.

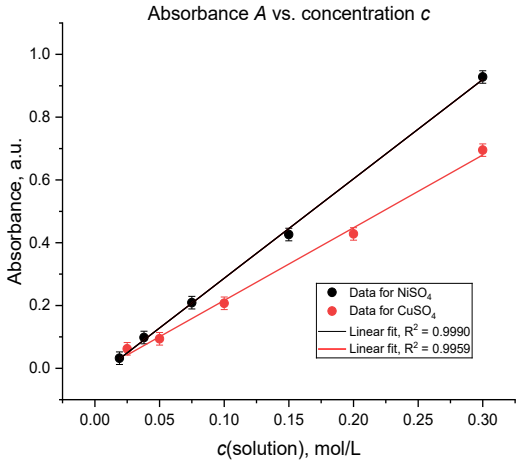


Fig. 5. Absorbance results for both sets of analyzed solutions using the PASCO spectrometer

Analysis with the constructed spectrometer and the linear data model

New samples from the already prepared standard solutions are taken and analyzed against a bright laptop screen which emits light in the discrete RGB range of the spectrum. The measurement procedure is the following: a laptop screen is set on a specific color and is put right next to the large rectangular hole of the constructed spectrometer. A cuvette containing a colored sample is put in the spectrometer, and then a smartphone is used to take a picture of the sample through the smaller circular hole. Preferably, the pictures should focus in the cuvette's center. All pictures are carefully analyzed using *Color Analyzer* mobile app. Its main advantage is that it displays RGB values both quickly and accurately. In addition, RGB values are available for each point of the analyzed picture. That means one could easily specify the desired spot for investigation and could potentially conduct multiple sample analyses if more samples are present in the picture.

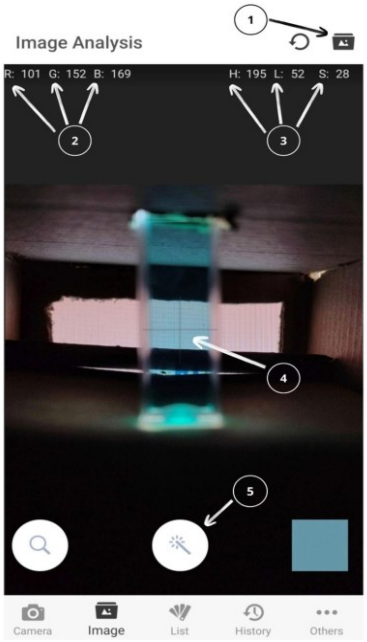


Fig. 6. Screenshot showing the interface of the RGB analyzing software

Main criteria for linearity of the results is assumed to be the numerical value of the correlation coefficient R^2. The obtained experimental data are summarized in Table 2. The results in Figure 7 confirm the hypothesis that a linear correlation analogous to Beer's law can be derived for a certain RGB spectral component.

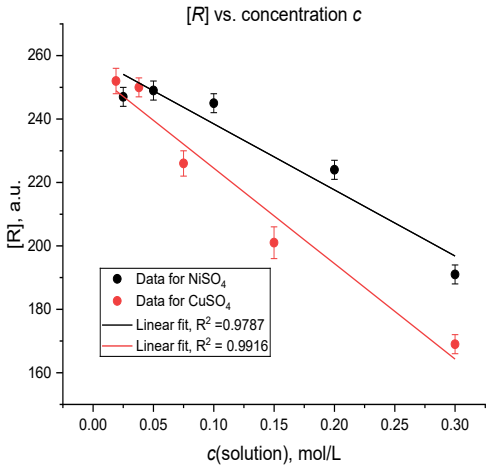


Fig. 7. Experimental results for all samples + spectrophotometer + linear data model

Table 2. Absolute [*R*] spectral value vs. samples concentration *c* for measurements with the constructed spectrometer

№	c_1(CuSO4), M	[*R*], -	c_2(NiSO4), M	[*R*], -
1	0.025	247 ± 3	0.019	252 ± 4
2	0.050	249 ± 3	0.038	250 ± 3
3	0.100	245 ± 3	0.075	226 ± 4
4	0.200	224 ± 3	0.150	201 ± 5
5	0.300	191 ± 3	0.300	169 ± 3

Analysis with constructed spectrometer and logarithmic model

The previously gathered data for [*R*] are logarithmized, and a linear regression is fitted.

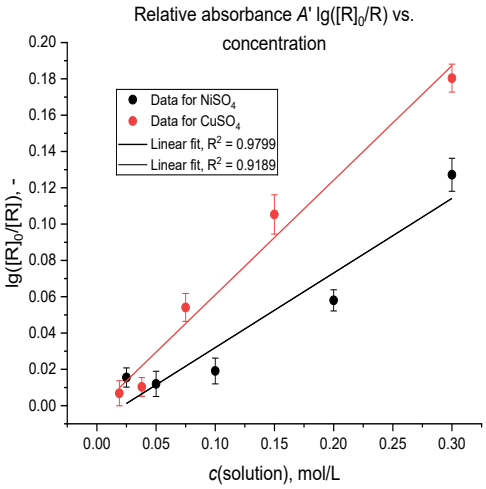


Fig. 8. Experimental results for all samples + spectrophotometer + logarithmic data model

Table 3. Logarithmized [*R*] spectral value *vs*. concentration *c* for measurements with the constructed spectrometer

№	$c_1(CuSO_4)$, M	$\lg([R]_0/[R])$, -	$c_2(NiSO_4)$, M	$\lg([R]_0/[R])$, -
1	0.025	0.016 ± 0.005	0.019	0.007 ± 0.005
2	0.050	0.012 ± 0.007	0.038	0.010 ± 0.005
3	0.100	0.019 ± 0.007	0.075	0.054 ± 0.008
4	0.200	0.058 ± 0.006	0.150	0.105 ± 0.011
5	0.300	0.127 ± 0.009	0.300	0.180 ± 0.008

CONCLUSION

Although the proposed spectrometer does not reach the same precision as a professional instrument, its accuracy is fully adequate for educational use. Moreover, the do-it-yourself version is very low-cost, easy to construct and flexible in its operation. It succeeds in demonstrating key spectroscopic phenomena and measurement techniques, which makes it a powerful tool for teaching. In this sense, the advantages of the proposed instrument far outweigh its small loss of accuracy.

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