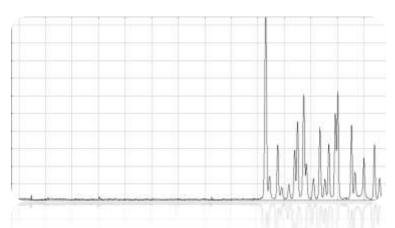
High resolution DIY spectrometer







Chemistry4all, a physical chemist.

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Introduction

Spectroscopy is a branch of science (chemistry and physics in particular) which relies on the interaction between matter and radiation. Spectroscopic techniques such as NMR, IR, Gamma spectroscopy, Raman, OES .. provide a huge amount of information about the chemical and physical nature of a studied sample, and hence they have been a key part of scientific development. Nowadays, modern spectroscopic techniques are employed in a large variety of fields including quantum physics and chemistry, astronomy, physics or analytical chemistry.

Within those techniques, **optical spectroscopy** could be defined as the branch of spectroscopy that deals with photons (and their interaction with matter) within the visible (400-700 nm) and near visible region. The applications of optical spectroscopy in particular may extend anywhere from the determination of the chemical composition of a star to the study of the excited state chemistry and physicochemical properties of different molecules. Thus, an optical spectrometer is a very versatile instrument which helps us achieve a better knowledge of the properties and characteristic of our surroundings. Unfortunately, these instruments are usually very expensive and hence, usually inaccessible for the home scientist or undergraduate student. Therefore, in this project, a DIY optical spectrometer is constructed and evaluated.

Objectives

The main objective of this project is to construct a fully functional high resolution optical spectrometer with the lowest budget possible.

Design

The proposed design of the current spectrometer is relatively simple as represented in the following figure:

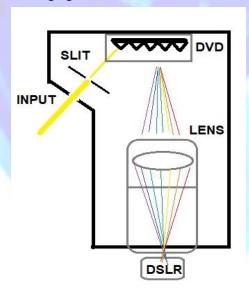




Figure 1. General scheme of the DIY spectrometer.

As shown in **Figure 1**, the spectrometer consists of 4 main different parts: the optical input, a slit, a diffraction grating, a focusing lens and a high resolution CCD detector (DSLR¹).

Working principle

The working principle of the spectrometer relies on the well known diffraction phenomenon, The light to be analyzed enters the spectrometer unit through the optical input, where it reaches an entrance slit of a defined slit width (**below 1 mm**). The majority of the light is then blocked and the remaining light passes through the slit and hits the diffraction grating.

A diffraction grating is an optical component exhibiting a periodic, well defined and regular pattern in its structure.

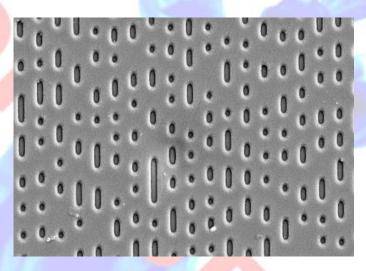


Figure 2. Electron micrograph of a regular DVD²

Since the size of such pattern is of the same order of magnitude than the wavelengths of the light interacting with it, the diffraction phenomena can take place. The diffracted light undergoes then a series of constructive and destructive interference phenomena which leads to a so-called optical spectrum, in which the studied light is separated in its constituent photons. The diffracted light passes then through the objective lens, where it's centered and focused towards the CCD detector of the DSLR camera, generating the final spectrum.

This design is actually similar to the one of a professional equipment, however professional spectrometers often employ a collimator and a focusing mirror to achieve good spectral resolution. In our case, we are using the objective lens to properly focus the photons towards the detector.

¹ Digital single lens reflex camera.

² Source: http://www9.open.ac.uk/emsuite/research/metallography

Components

-Optical Input: the "entrance" of the spectrometer was designed using the FreeCad software³ and 3D printed using a Wanhao 3D printer⁴. The general design is oriented towards the construction of a highly tunable spectrometer and therefore different accessories such as an entrance slit or a SMA connector were also designed and printed.



Figure 3. Image of the Optical input of the spectrometer

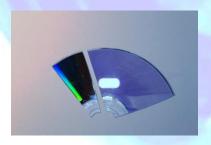
-Optical Slit: the slits employed to focus the light towards the diffraction grating were designed and 3D printed as mentioned before. Three different slits were printed having a slit size of 1000 um, 750 um and 500 um.





Figure 4. Image showing the 3D printed entrance slit and the current slit installed in the spectrometer.

-Diffraction grating: As a source of a diffraction grating a regular DVD was employed. The diffraction grating was obtained cutting in half the DVD and separating the two thick plastic sheets, the "reflective" sheet was then cut and glued in a 3D printed support.



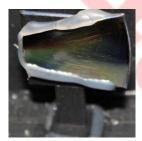


Figure 5. Image showing the two sheets of the DVD and the actual diffraction grating of the spectrometer

³ https://www.freecadweb.org/

⁴ Wanhao duplicator i3 mini.

-Lens: As a focusing lens an old 28-80 mm Canon objective lens was employed. The focusing lens was secured in a 3D printed platform.



Figure 6. Image showing the focusing lens of the spectrometer.

-Detector: the detector is actually a used Canon EOS 1100D (Rebel T3) DSLR camera. In this case, the infrared filter of the CCD detector was removed, which increases slightly the detection range of the spectrometer. However an unmodified camera will also work for this project.



Figure 7. Canon EOS 1100D camera.

Budget

The individual cost of each component as well as the total cost of the DIY spectrometer is shown in the following table:

Component	Price (€)
3D printed components (entrance slit, supports, platforms)	~1*
Diffraction grating	~1
Focusing lens (used)	35
Detector (used)	150
Total Cost of the spectrometer	187

Table 1. Table showing the components, and their respective costs, employed for the construction of the high resolution spectrometer. Components shown in blue are a fixed part of the spectrometer and cannot be removed, on the other hand, components in red are not a "permanent" component of the spectrometer. *The cost also accounts for the additional tests and failures.

The total cost of the spectrometer turned out to be below 200 €, and therefore can be considered to be indeed a low cost spectrometer. Furthermore, a cheaper DSLR camera could be employed which would reduced even more the total cost of the spectrometer.

Calibration of the spectrometer

Considering that there are several components in the spectrometer which can be tuned, replaced and removed, the spectrometer must be calibrated each time that one of these modifications is performed.

The calibration of the spectrometer is performed using two different regular light sources: a neon light bulb and a compact fluorescent lamp.

Calibration source	Calibration point (nm)	Calibration source	Calibration point (nm)
Neon lamp	585.25	Neon lamp	630.479
Neon lamp	588.19	Neon lamp	633.443
Neon lamp	594.48	Neon lamp	638.299
Neon lamp	597.55	Neon lamp	640.225
Neon lamp	603	Neon lamp	650.653
Neon lamp	607.434	Neon lamp	653.288
Neon lamp	609.616	Neon lamp	659.895
Neon lamp	614.306	Neon lamp	667.828
Neon lamp	616.359	Neon lamp	671.704
Neon lamp	621.728	Fluorescent light bulb	436.6
Neon lamp	626.649	Fluorescent light bulb	487.7

Table 2. Table showing the light source and the corresponding calibration points employed for the calibration of the spectrometer.

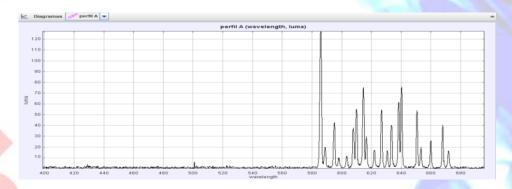


Figure 8. Spectrum of a neon light bulb taken with the DIY spectrometer.

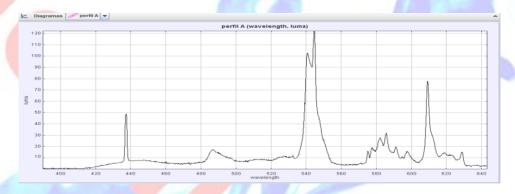


Figure 9. Spectrum of a compact fluorescent light source taken with the DIY spectrometer.

Additional calibration sources might include different LASER pointers such as the regular 650 nm and 532 nm LASER diodes or even the more unusual 405 nm LASER source.

As it can be seen in the following graph, the calibration of the spectrometer is almost ideal, having a goodness coefficient of 0.9998, indicating an ideal linear dependence between the wavelength and the pixel position.

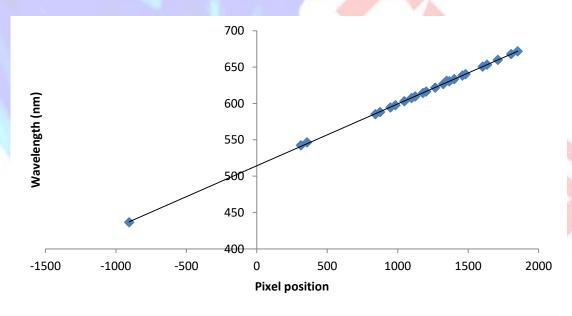


Figure 10. Calibration curve of the spectrometer.

Operation modes of the spectrometer

The spectrometer can be operated in two different modes:

-Raw mode: In this mode, no additional components are attached to the optical input and an entrance slit is placed between the light input and the diffraction grating. In general, this mode offers higher signal intensity, reducing the total acquisition time required and the noise of the final spectrum. On the other hand, when working in this mode the spectrometer cannot be coupled to other units (raman spectrometer, UV-VIS spectrophotometer...).

Notes:

- -When working in this mode, the use of a **light diffuser film** is highly recommended to achieve a nice and homogeneous spectrum.
- -The total resolution achieved depends on the slit width employed, the smaller the slit width the greater the resolution.
- -SMA mode: In this mode, a SMA905 connector is attached to the main optical input of the spectrometer, which allows a fiber optic cable (200 um) to be connected to the spectrometer. Additionally, when working in this mode, the entrance slit is removed from the spectrometer and the light goes directly from the fiber optic cable to the diffraction grating. In general, this

mode offers slightly greater resolution than that obtained with the Raw mode. Furthermore, the spectrometer can be coupled to other units for more specific measurements. On the other hand, this mode leads to lower signal intensities which involves higher acquisition times and results in higher noise.

Figure 11. Image showing the 3D printed SMA connector.

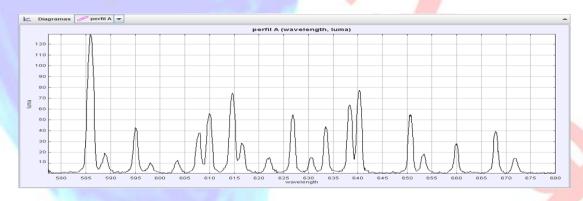


Figure 12. Neon spectrum taken with the spectrometer in the **SMA mode**. Range from 580 to 680 nm.

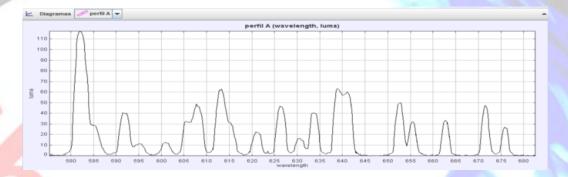


Figure 13. Neon spectrum taken with the spectrometer in the **RAW mode**. Range from 580 to 680 nm.

As it can be seen in the spectra shown above, the SMA mode offers indeed a net better resolution (about 1 nm) than the RAW mode.

Data acquisition and signal processing

Data acquisition

The data is acquired directly through the DSLR display. Each spectrum is taken in the "manual" mode, the acquisition time and the ISO value of the DSLR are selected depending on the intensity of the light source to be analyzed. The data is stored as a JPG image and then it is transferred to the computer where it is finally analyzed.

Alternatively, the DSLR can be directly controlled through the usage of a micro-USB by the computer.

Signal processing



The JPG files are then loaded in the Tracker⁵ Physics software (freeware), the spectrum is then obtained through a linear profile analysis of the sample image. Additionally, the proper pixel to wavelength calibration

can be loaded directly through the software as a mathematical function. Finally the spectrum can be exported as a plot or as a csv file.

⁵ Tracker software webpage: https://physlets.org/tracker/

Results and some examples

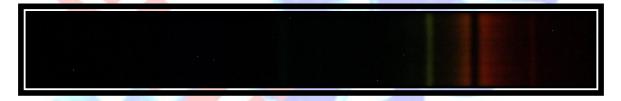
Raw data

In the current section some raw spectra taken with the DIY spectrometer are presented:

Neon spectrum (SMA mode)



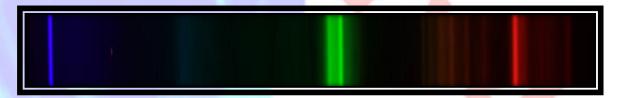
High pressure sodium lamp (30 meters away from the light source, RAW mode)



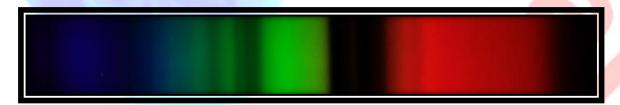
Fraunhofer lines (solar spectrum, SMA mode)



Compact fluorescent light bulb (SMA mode)



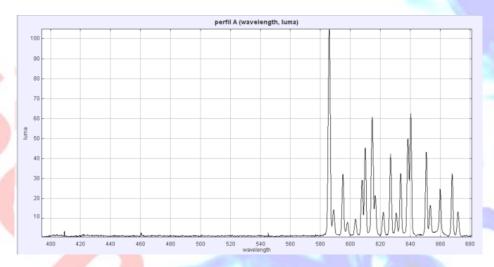
Didymium filter (transmition spectra using an incadescent light bulb as light source, SMA mode)



Processed data

In the current section some already processed spectra are shown and compared with the corresponding reference data:

Neon spectrum (SMA mode)



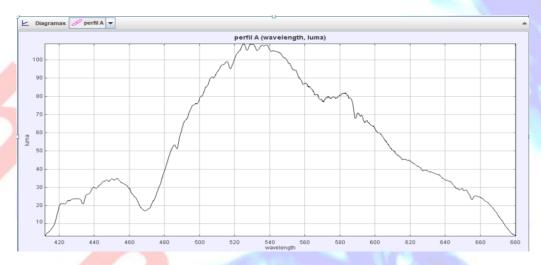
Experimental peak (nm)	Reference peak (nm)	Absolute difference (nm)
585.8	5 85.25	0.55
588.8	58 8.19	0.61
594.9	594.48	0.42
598	597.55	0.45
603.4	603.00	0.40
607.7	607.43	0.27
609.9	609.62	0.28
614.5	<mark>614</mark> .31	0.19
616.5	616.36	0.14
621.9	621.73	0.17
Mean di	fference	0.35

Table 3. Comparison of the experimentally obtained Neon spectrum and the reference data.

High pressure sodium lamp (RAW mode) (30 meters away from the source)



Solar spectrum (SMA mode)



Line	Experimental (nm)	Reference (nm)	Absolute difference (nm)
G (Fe)	433.5	434.1	0.6
d (Fe)	468.5	466.8	1.7
F (H)	486.8	486.1	0.7
b ₄ (Mg)	517.5	516.7	0.8
E ₂ (Fe)	527.0	527.0	0.0
D lines (Na)	588.8	589.0	0.2
a (O ₂)	627.0	627.7	0.7
C (H)	655.5	656.3	0.8
Mean difference			0.68

Table 4. Comparison of the experimentally obtained Fraunhofer lines with the reference data.

As it can be seen in the previous tables, the experimentally obtained values are in good agreement with the reference data showing a total discrepancy of less than 1 nm.

Further development

Currently, the spectrometer could be further improved mainly through the development of different accessories for specific applications or purposes. A good example of one of these accessories might be a UV-VIS spectrophotometer unit:

UV-VIS absorption accessory (Still being developed)

A fully portable, battery powered and 3D printed UV-VIS absorption accessory was designed to be coupled to the DIY spectrometer.

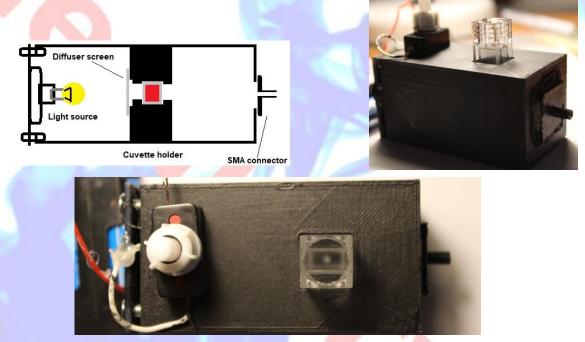


Figure 14. UV-VIS spectrophometer unit.

As shown in the previous image, the design of this accessory is pretty simple. A small 3.00 V light bulb serves as a continues light source within the visible range (400-700 nm). The light is then diffused and "homogenized" by a diffuser screen and after that it reaches the cuvette holder, where a standard glass or plastic cuvette is placed. The incoming photons interact with the molecules present in the solution, and some of them are absorbed promoting electronic excitations associated with the chromophoric groups of the species present in the solution. A fiber optic cable, connected to the unit through the SMA connector, collects the remaining photons and redirects them to the spectrometer, where the spectrum is taken.

This accessory is especially oriented towards chemistry, and its range of applicability may extend from the determination of the concentration of a solution to the study of the absorption bands of a molecule within the UV-VIS range.

Plasma-induced optical emission spectroscopy unit (Still being developed)

In addition to the previously mentioned accessory, some other accessories are currently being developed. One of them is a DIY plasma induced optical emission spectroscopy unit. This unit, is designed for the study of certain kinds of gaseous sample though the analysis of the spectral lines emitted by the corresponding plasma.

The working principle can be described as follows:

- -A glass test tube, equipped with a rubber septum is purged with the gaseous sample to be analyzed (usually a pure substance such as CO_2 , H_2O or a noble gas).
- -The tube is then evacuated several times (manually), using a regular medical syringe, until the tube is partially evacuated.
- -The tube is then placed and secured in the unit, where it is surrounded by two copper electrodes connected to a bipolar Tesla coil.



Figure 15 . Electric discharge generated by the bipolar Tesla coil.

-The Tesla coil is then turned on and a stream of electrons passes between the electrodes and through the evacuated tube. This stream of electrons causes the rapid formation of plasma, in which the atoms get rapidly excited to higher electronic states. When the excited atoms get relaxed to their ground state through different electronic transitions, energy is released as photons, which can be detected by the spectrometer. The frequency of the emitted photons depends on the electronic levels involved in the electronic transitions taking place, and hence on the chemical nature of the sample.

This unit is particularly useful for physics experiments, as it can be used as a regular discharge tube, generating the characteristic emission spectra of a given gaseous molecule or atom.

Despite the fact that it is not fully developed yet, here there are some examples of the plasma created by the unit:

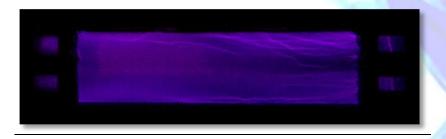


Figure 16. Plasma of regular air generated by the unit.



Figure 17. Plasma of pure Argon generated by the unit

Conclusions

Overall, a fully functional, low cost and high resolution DIY DSLR based spectrometer has been designed and constructed. The resolution of the spectrometer is about 1 nm and the total mean discrepancy with the reference data turned out to be below 1 nm. Additionally, the spectrometer has been designed to be fully versatile through the development of different accessories which can be coupled to it.

Contact and Support

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The 3D models may also be available if required.