



Chemistry workshops and investigations

Make a DVD
smartphone
spectrometer

Teacher Guide

CfE Advanced Higher
Inorganic and Physical Chemistry
Electromagnetic radiation and atomic spectra

Background

Spectroscopy is an important analytical tool in several areas of science. In the classroom, however, spectroscopy is not used as much as we would like due to the relatively high cost of the equipment.

A diffraction grating is an optical device with a structure which splits light into several beams travelling in different directions. They can do so either by reflection or transmission. The directions of these beams depends on the spacing of the grating and the wavelength of the light. If you shine white light on a diffraction grating, the grating will cause the white light to spread out into a spectrum.

In a CD or DVD, the tracks containing the data spiral in to the centre, resulting in an array of parallel lines which can work as a diffraction grating. This is what produces the array of colours you see when you look at the reflections in a CD or DVD. (Figure 1)

You will need

Blank DVDr	Scissors
Template printed on black card	Sticky tape or glue
Scalpel or craft knife	Methylated spirits and cotton wool (or a clean, soft cloth)
Black electrical tape	Phone or tablet

Making the spectroscope

The design here was developed by the Public Laboratory for Open Technology and Science (www.publiclab.org). *In order to access this site, you will need to register (free).*

1) Preparing the diffraction grating.

You will need a recordable DVD (DVD-R).

Cut the DVD-R into halves or quarters with a pair of scissors and then you should be able to get a fingernail in separate it into two layers: the metallic layer with the label a clear plastic layer with a purple sheen. (Figure 1)

You need the clear layer. Try to handle the surface as little possible to avoid marking it.

You can remove the purple colouring using some ethanol (methylated spirit works well) and cotton wool. (Figure 2) Cut a piece from the edge of the now clear plastic, approximately 1cm x 1cm. This is your diffraction grating.



Figure 1: DVD layers

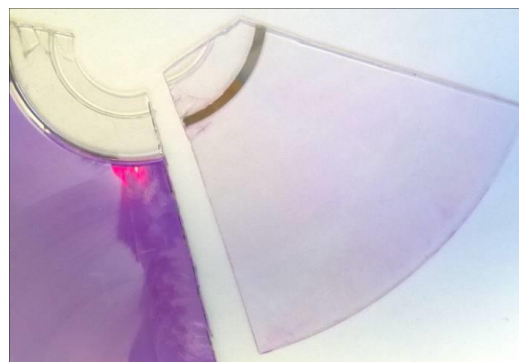


Figure 2: Cleaning the dye off

and
on and
as

2) Getting and preparing the template

You can find the template on the publiclab website (but a copy is on the back page of this document) It refers to printing on 11" x 8" paper but A4 seems to work fine. (<http://publiclab.org/sites/default/files/8.5x11mini-spec3.8.pdf>)

You need to print this out onto black card: card so it is stiff enough black to reduce internal reflection. might think printing black lines onto black card is a daft thing to do but it still possible to see the design clearly enough to cut it out.

Cut round the outside, scissors are probably easiest.

Use a scalpel or sharp craft knife to cut out the square (top right of the diagram) where the grating goes. use the scalpel/knife to cut a narrow slit (lower left of the diagram) - the narrower the better.

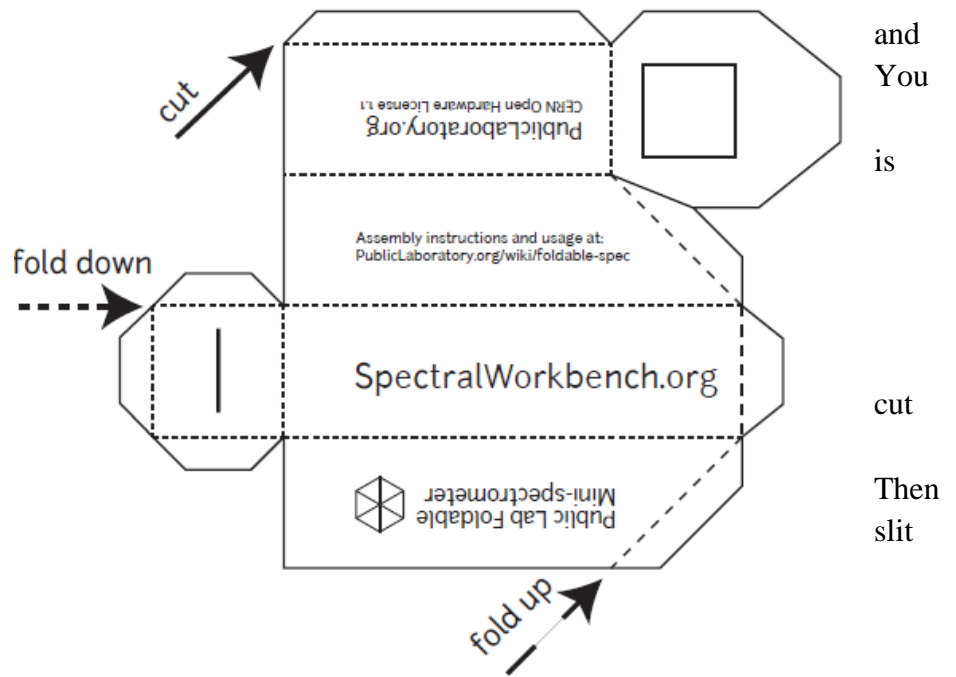


Figure 3: The template (not actual size)

3) Assembling the spectrometer

Use tape or glue to fix your 1 cm x 1 cm piece of diffraction grating on the inside of the 'door', over the square hole you cut out for it. The lines need to be horizontal so make sure that the edge of the DVD-R is at the top or bottom rather than to one side. Then fold the device as shown in the diagram and tape or glue it shut (tape is probably easier and black electrical tape is best).

You will now have a rectangular box, approximately 10 cm long with a slit at one end (Figure 4) and a slope at the other end with a window containing the diffraction grating (Figure 5)



Figure 4: The slit

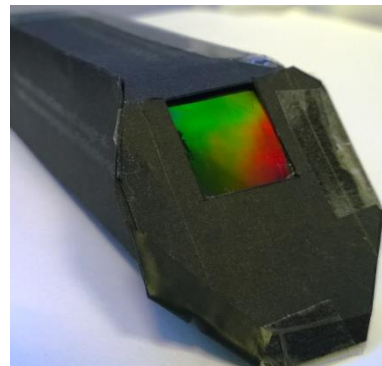


Figure 5: The diffraction grating

4) Attaching the spectrometer to your phone

You can simply do this using tape (again, black electrical tape is best). Launch the camera app. Place the 'window' with the diffraction grating against the lens, check that you are getting a pattern and then tape it in place. This is a bit tricky with an iPhone as the camera lens is stuck away in the top left hand corner. It is possible, however, to get it in place with a bit of



care.

(For more than a one off use, it is worthwhile making a mount if your camera lens is awkwardly placed. This can be done relatively easily using Corriflute or similar material).

Figure 6: Spectrometer attached to an iPhone

Once in place, launch the camera app (if you closed it) and then you can point it at various light sources and get photographs of their spectra. (Figures 7, 8 & 9)



Figure 7: spectrum of a compact fluorescent lamp



Figure8: spectrum from a sodium flame test

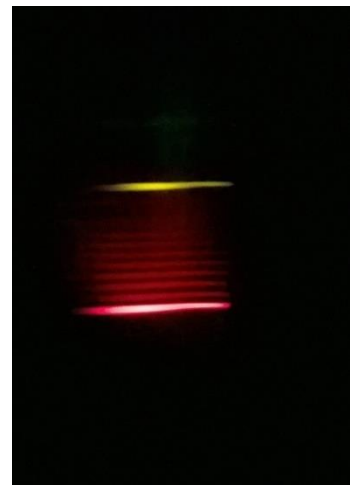


Figure 9: spectrum from a strontium flame test

5) Tips

Make sure the flash is switched off.

If you are getting light leakage, use more black electrical tape to block these off.

Pointing directly at a light source can lead to problems: The images can be excessively bright but you are also more prone to internal light leakage.

Exposure can be tricky so try several shots at different settings. Too bright and the software might have trouble analysing it, too dark and there will be too much background noise for a good spectrum.

Improving your images

One of the problems is that the spectrum is only a relatively small portion of the screen. This can give extraneous noise when you analyse it.

You could zoom in on the camera but there are a couple of problems with this:

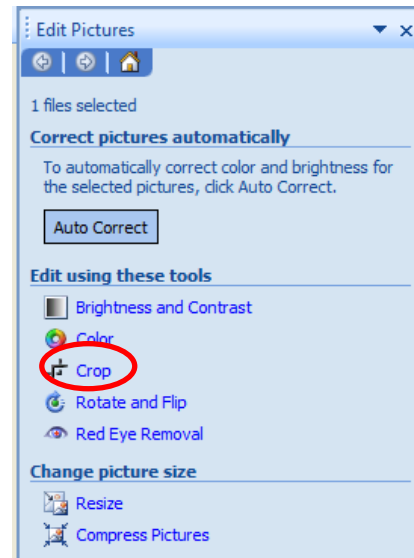
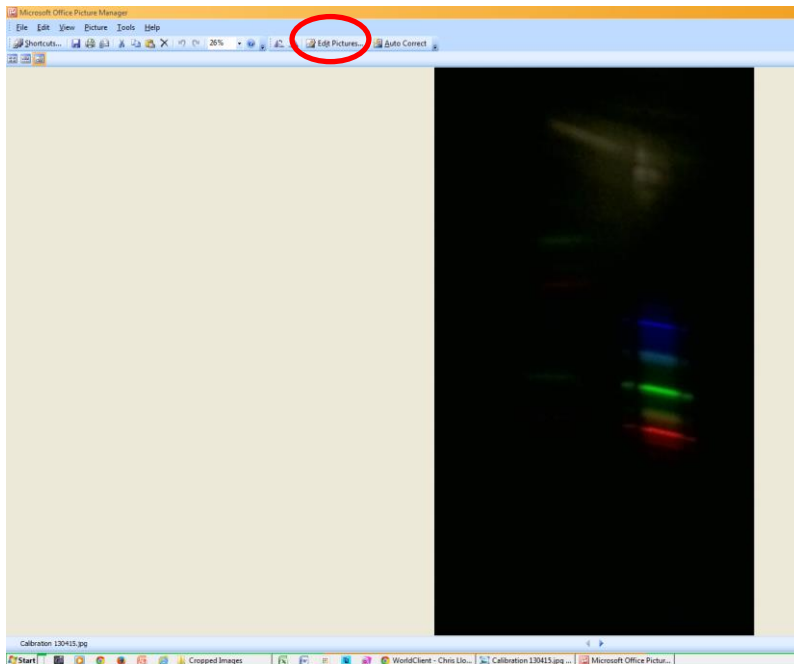
- 1) you might accidentally alter the zoom between shots.
- 2) Most (if not all) camera apps re-set when they close so if your phone switches off between shots you have lost the zoom setting.

This is a problem because the software uses the exact positioning of the bands within the image to work out its wavelength.

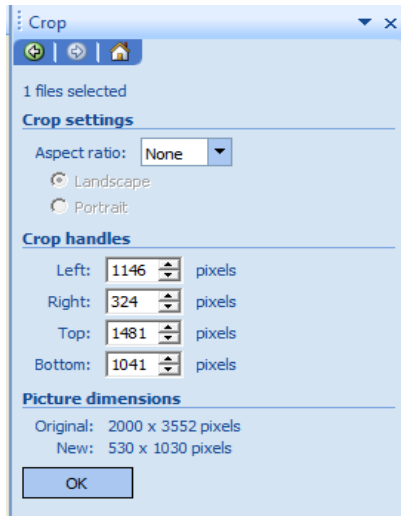
You can solve this by cropping the photographs afterwards. As long as you do it carefully.

Using Microsoft Windows Picture Manager.

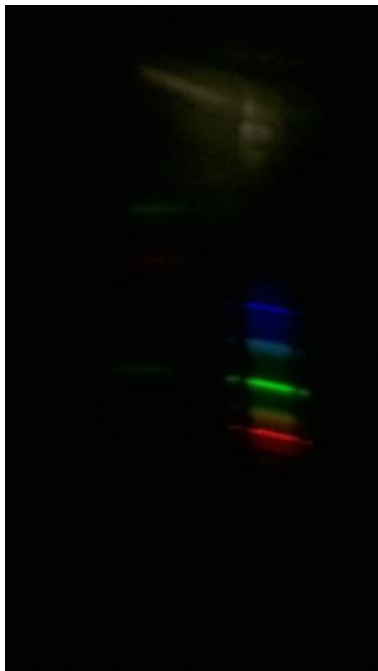
- 1) Open the reference file
- 2) Select the 'Edit Picture' option and then crop.



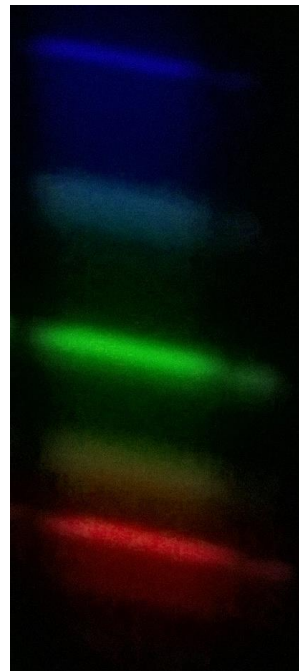
- 3) Move the cropping handles to give you a good spectrum.
- 4) You will notice on the right of the image in the section labelled 'crop handles' there are 4 numbers. These tell you the exact positioning of the cropping lines. Make a note of them.



- 5) Open up your next spectrum image, as before go to 'edit picture' and 'crop'.
- 6) This time type the numbers you wrote down into the boxes.
- 7) When you press OK, the image will be cropped to exactly the same section as the previous one and so can be accurately compared.
- 8) Repeat this with your other images.



Before



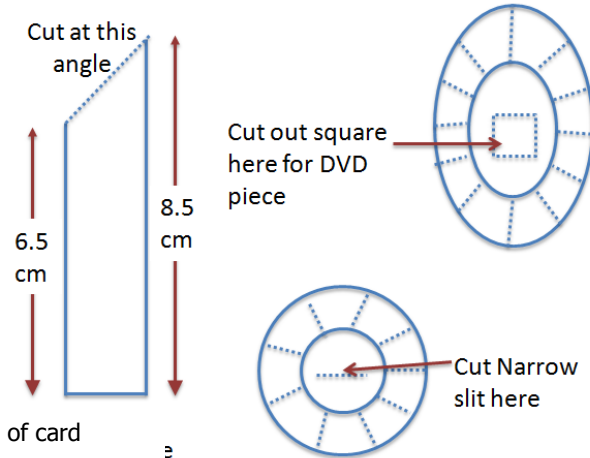
After

6) Improvements

The device works pretty well and it is possible to get some decent pictures of spectra. It is, however, a bit fragile.

It is possible to improve the construction by using a piece of plastic tubing as the body. 19 mm plumbing overflow pipe is ideal. You can cut it easily with a hacksaw and use a file or craft knife to smooth it off. (Figure 10) The pipe is white so you will need to either spray paint it black on the inside or line the inside with black paper or card.

It is easy to cut card for the ends and if you make a series of cuts round the edge, you can fold it down and tape it.



need to make sure that you tape the spectrometer to your well – you want to make there is no light leaking that will decrease the contrast of your image.

Figure 10: Using pipe instead of card

You phone sure that in as

Resolution – at present the resolution is not quite good enough to separate the two sodium bands. A narrower slit does improve resolution but then it also reduces the light level which is not good for photography.

Cuvette adaptor

At present this is only available for the card version. Again using card, it is relatively easy to place an adaptor on the front so that the light passes through a cuvette en route to the slit. Doing this allows you to photograph the spectrum obtained when full-spectrum light passes through a coloured solution and thus obtain an absorption spectrum.

Here is the template. Again, cut the solid lines and fold the dotted ones. All of them fold up this time.

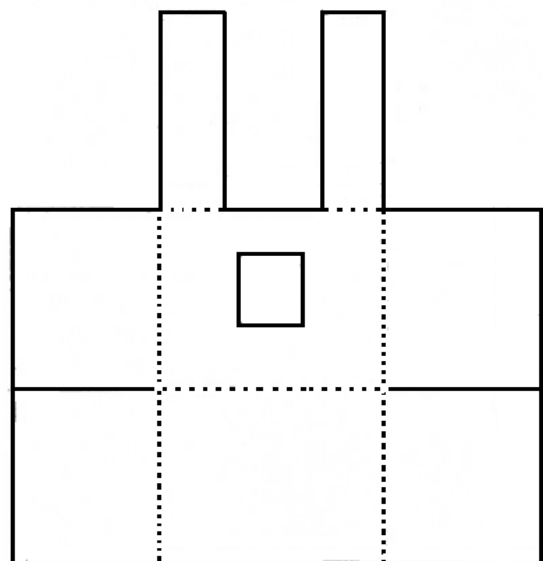


Figure 11: Cuvette adaptor template

You then slip this over the front of the spectroscope and secure it with tape again.

AS the spectrometer works at an angle, you will need to put lids on your cuvettes (or seal them in some other way) to make sure you don't spill it.

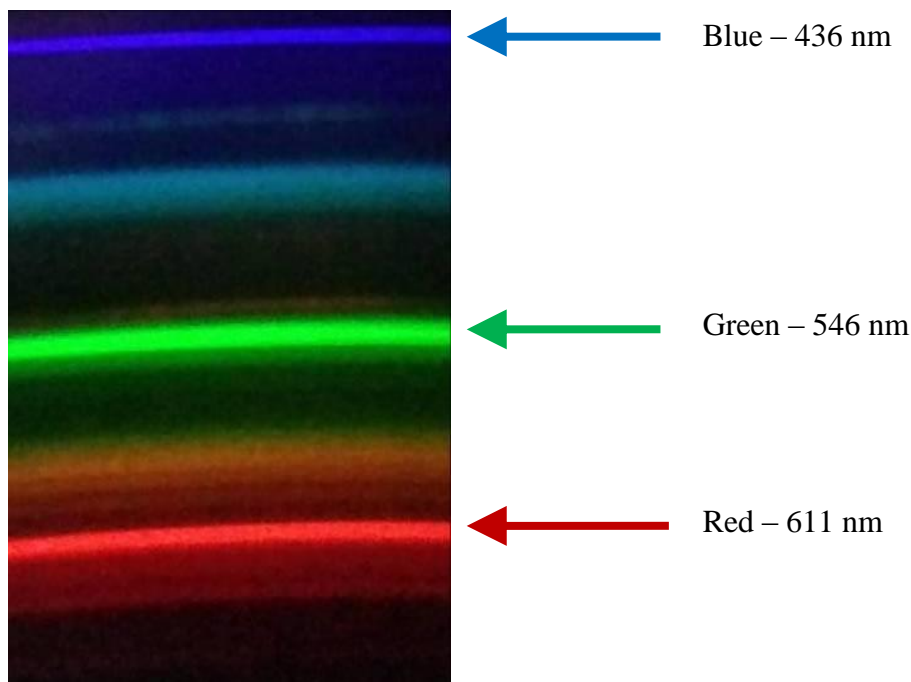


Figure 12: Cuvette adaptor fitted

Analysing the spectrum

This can be tricky but it is easier than it used to be.

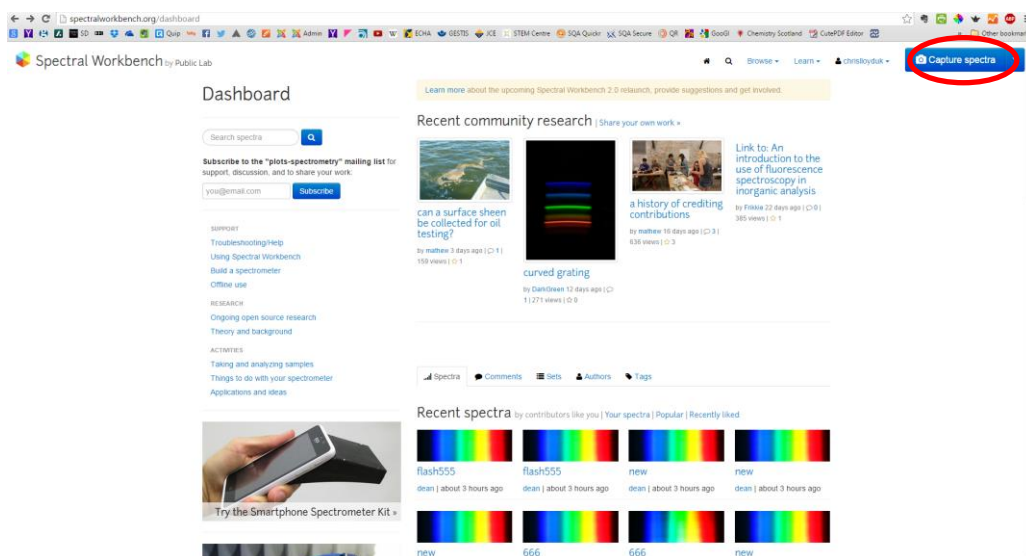
In order to analyse the spectrum and actually get a graph of it, you need to have some reference points. Fortunately, we have these in the form of the spectrum of a fluorescent tube (ideally a compact fluorescent). They do, unfortunately, vary a little but most CFLs have some notable spectral lines that can be used for calibration



So the first thing to do is to take a photograph of your CFL source.

In order for your reference to be valid, make sure you use the same spectroscope/phone assembly each time and do not zoom in on any of the photographs. (If you want to zoom in for better pictures to show then that is fine as long as the ones for analysis are all taken full-frame).

The easiest way to analyse your spectrum is to use the Spectral Workbench website (<http://spectralworkbench.org/>).



This is part of the Public Lab project (and the source of the spectrometer design). You need to register (for free) with Public Lab but that is all.

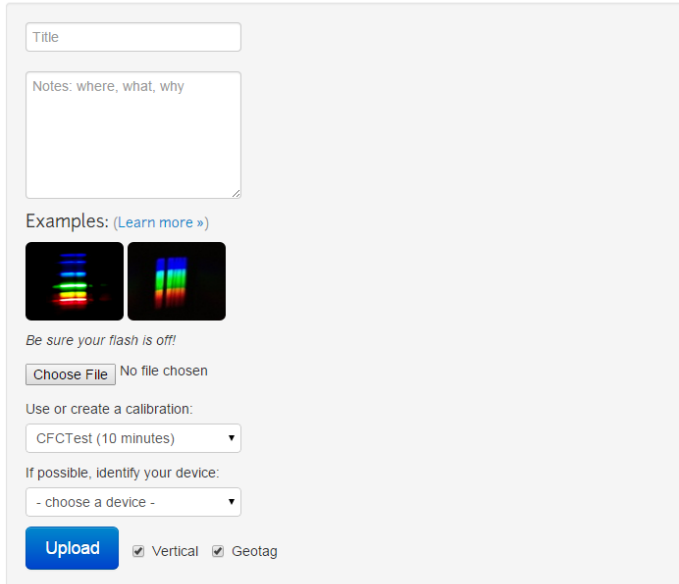
Annoyingly, even if you have logged into the Public Lab website, you still need to log in to Spectral workbench – using the same log in details as before though.

 Spectral Workbench by Public Lab

Upload a spectrum

Take a picture through [your spectrometer](#) and upload it. (Android or iOS 6+)

By uploading your data, you agree to release it under the [Creative Commons Zero license](#)



The screenshot shows the 'Upload a spectrum' form. It includes a 'Title' text input field, a 'Notes: where, what, why' text area, and two example spectrum images. Below the examples, there is a warning 'Be sure your flash is off!' and a 'Choose File' button with the text 'No file chosen'. There are two dropdown menus: 'Use or create a calibration:' set to 'CFCTest (10 minutes)' and 'If possible, identify your device:' set to '- choose a device -'. At the bottom, there is a blue 'Upload' button and two checked checkboxes: 'Vertical' and 'Geotag'.

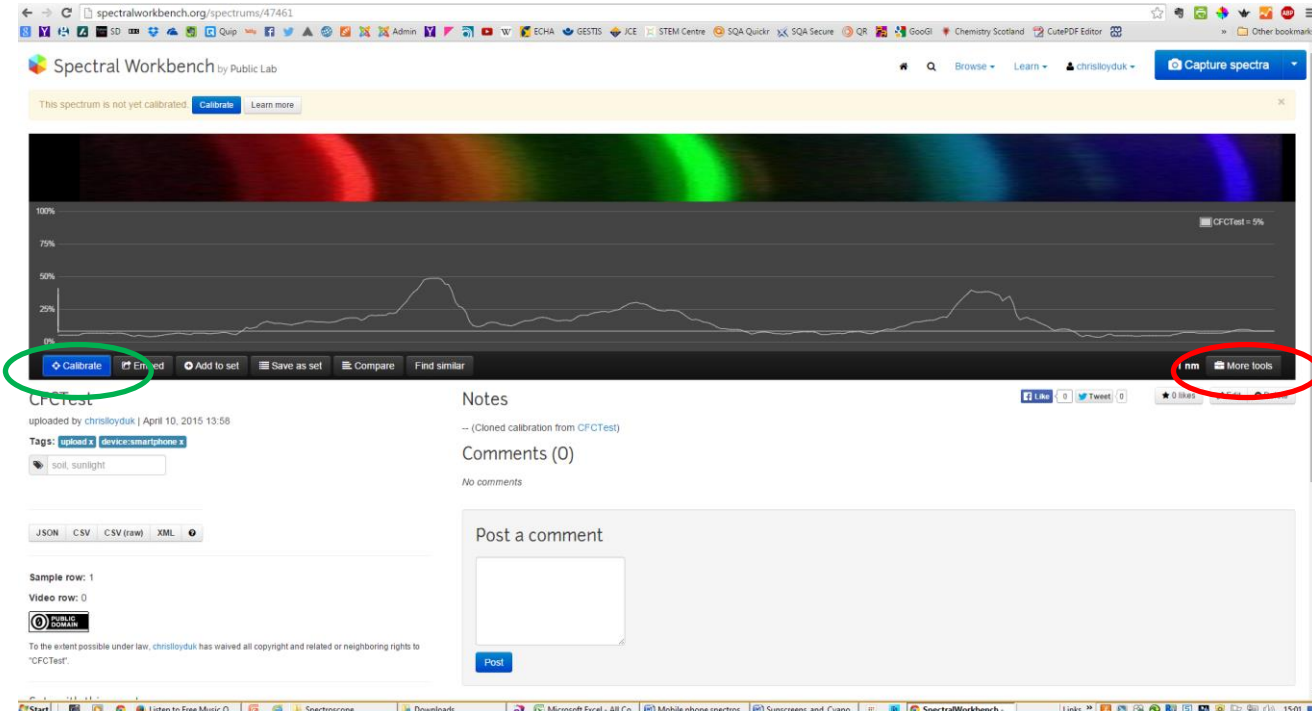
Once in, you will need to upload your image.

Click on 'Capture Spectra' (In blue at the top right – circled in red on the diagram above) and the drop down menu gives you the option to upload from file. Selecting this gives you this screen.

There is a tick box saying 'vertical' but as far as I can tell this makes no difference to how the software analyses your picture.

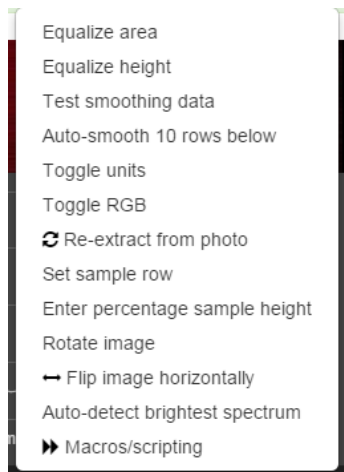
Enter a name and any other data you need and click the 'upload button'.

After a few seconds, your spectrum will appear – as shown below.



The screenshot shows the Spectral Workbench interface. At the top, there is a navigation bar with 'Capture spectra' circled in red. Below it, a message says 'This spectrum is not yet calibrated.' The main area displays a spectrum plot with a red-to-blue gradient background and a white line graph. The plot has a y-axis from 0% to 100% and an x-axis. Below the plot, there is a toolbar with buttons: 'Calibrate' (circled in green), 'Embed', 'Add to set', 'Save as set', 'Compare', and 'Find similar'. On the right side of the toolbar, there is a 'nm' label and a 'More tools' button (circled in red). Below the plot, there is a 'Notes' section with a 'CFCTest' title, a note about the calibration, and a 'Comments (0)' section. At the bottom, there is a 'Post a comment' form with a 'Post' button. The browser's address bar shows 'spectralworkbench.org/spectrums/47461'.

If you see a series of horizontal coloured lines rather than a spectrum similar to that above, click on the ‘more tools’ button. (Circled in red)



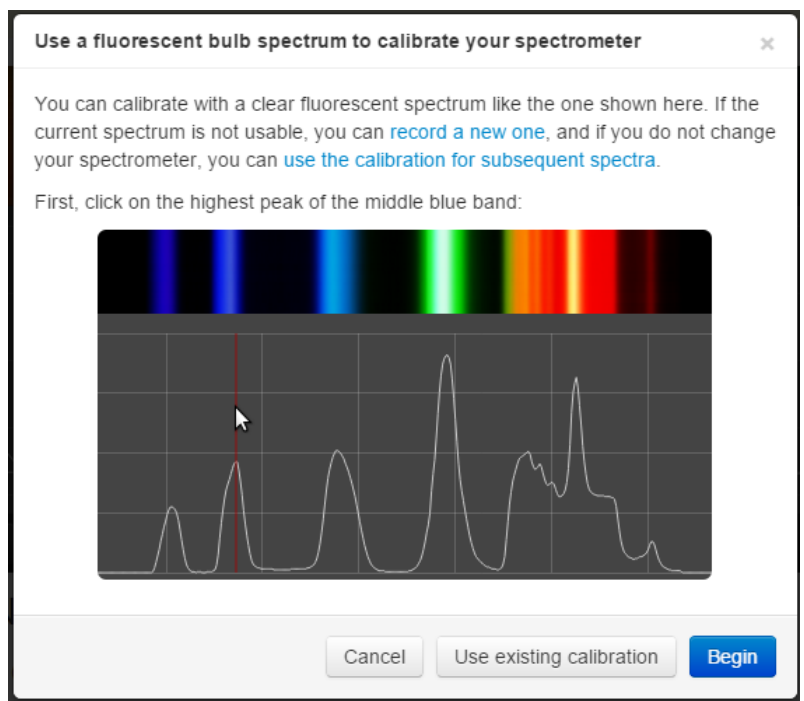
That will bring up the menu on the left.

Click on ‘rotate image’ and you should soon see something vaguely like the one above.

Another point you need to be aware of is that the analysis software only works if the blue lines are at the left. If, like in the illustration above, they are on the right, you need to click on ‘Flip image horizontally’.

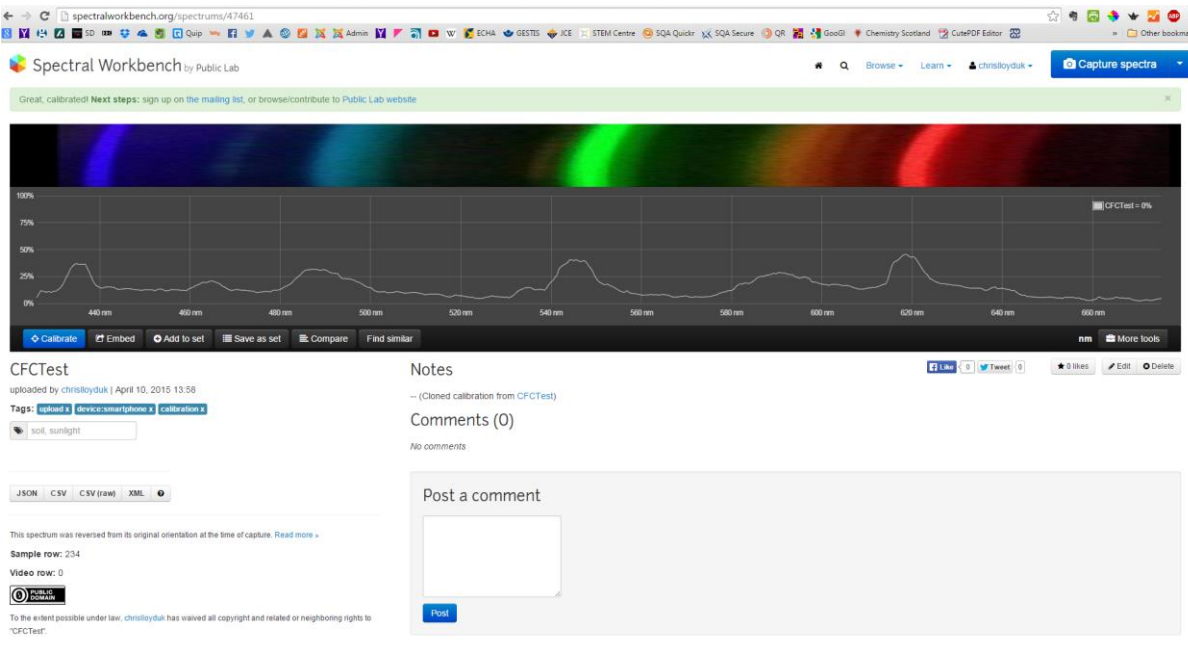
Now you have your spectrum loaded, you need to set it to be your reference sample.

Click on ‘Calibrate’ (the blue button on the left below the spectrum, circled in green, and you will see this screen appear.



Click ‘begin’ and then, as it says, find the brightest part of the appropriate blue band on your spectrum and click on it. That brings the screen back, this time telling you to find the brightest part of the **green** band. As before, find the brightest part of the green band this time and click.

After a few seconds your spectrum will reappear with the wavelengths along the bottom

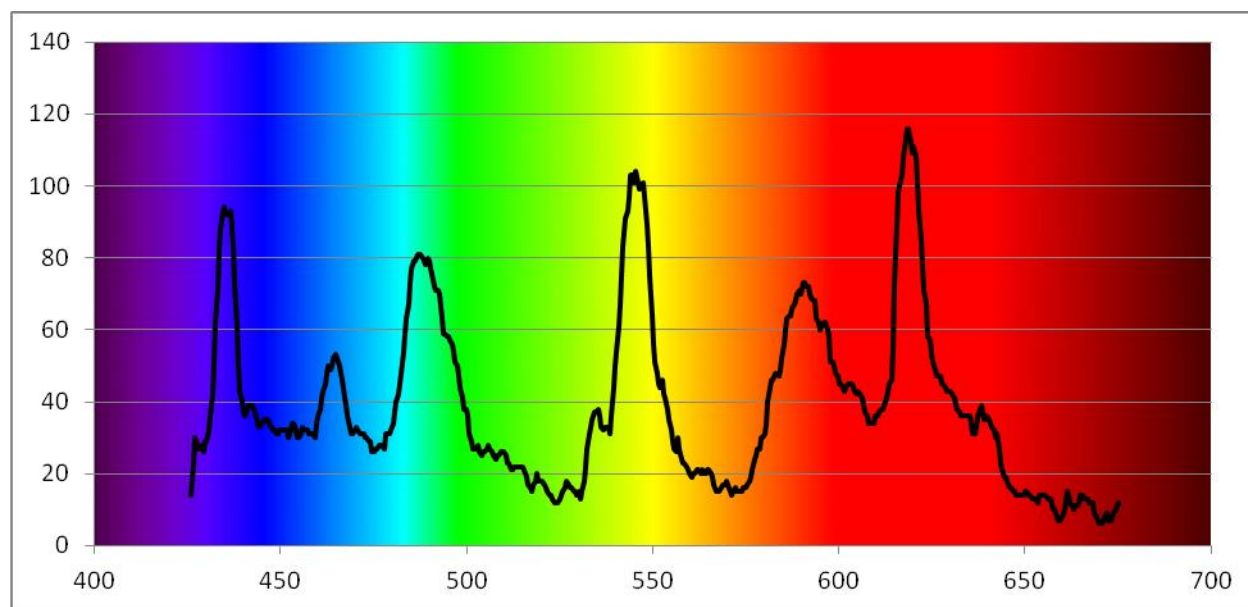


It is quite possible at this stage that the graph along the bottom will look rather unimpressive. This is likely due to the line being sampled across your spectrum not being in the best place. To fix this, click on the 'more tools' button again and this time select 'auto-detect brightest spectrum'.

There will again be a short delay and your spectrum should come up with a much better sample.

If you want to get a graph you can print off or otherwise manipulate (to look a bit more impressive), you can export the data. .csv is the best format to choose as it will open directly in Excel.

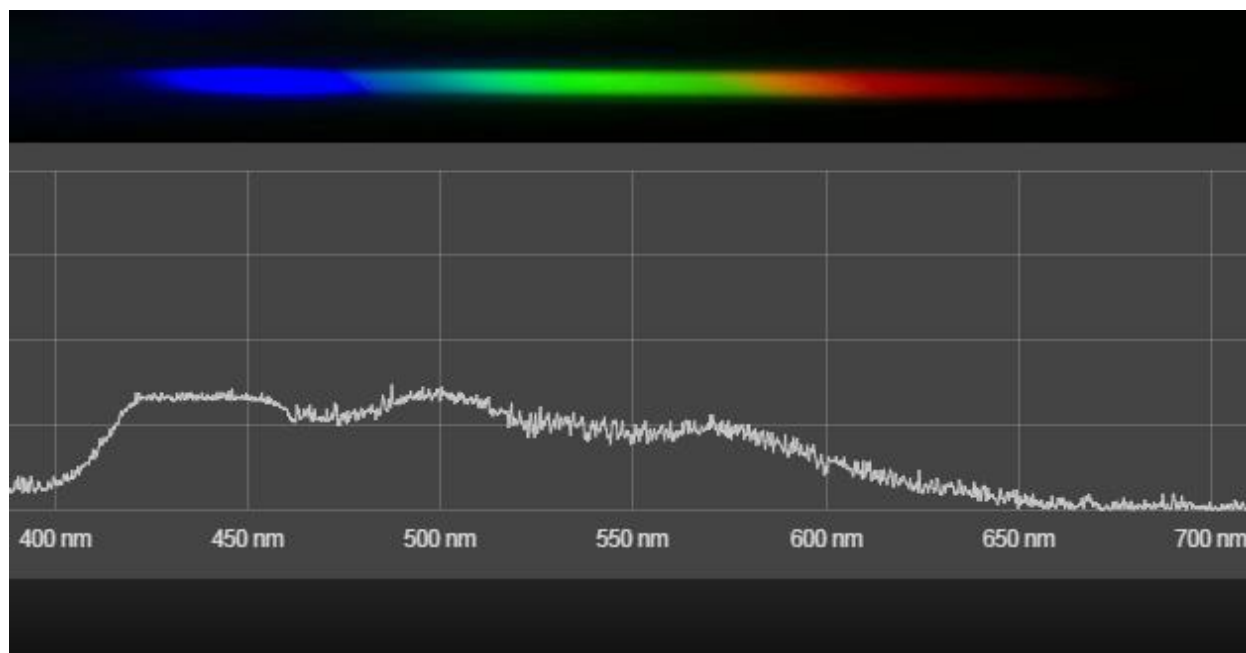
Here is an excel version of the same graph: still with the wavelength along the bottom. (I just used a picture of a spectrum as a background to make it look prettier!)



Now you have your calibration graph, things are much simpler.

Upload another image (rotating and flipping it as before if you need to) and the software will automatically interpret it using your reference spectrum.

So the graph will appear with the wavelengths along the bottom. The same will be true of all the other spectra you photographed in this session. Here is one of a white LED (Section shown only).



Using Excel to get better graphs

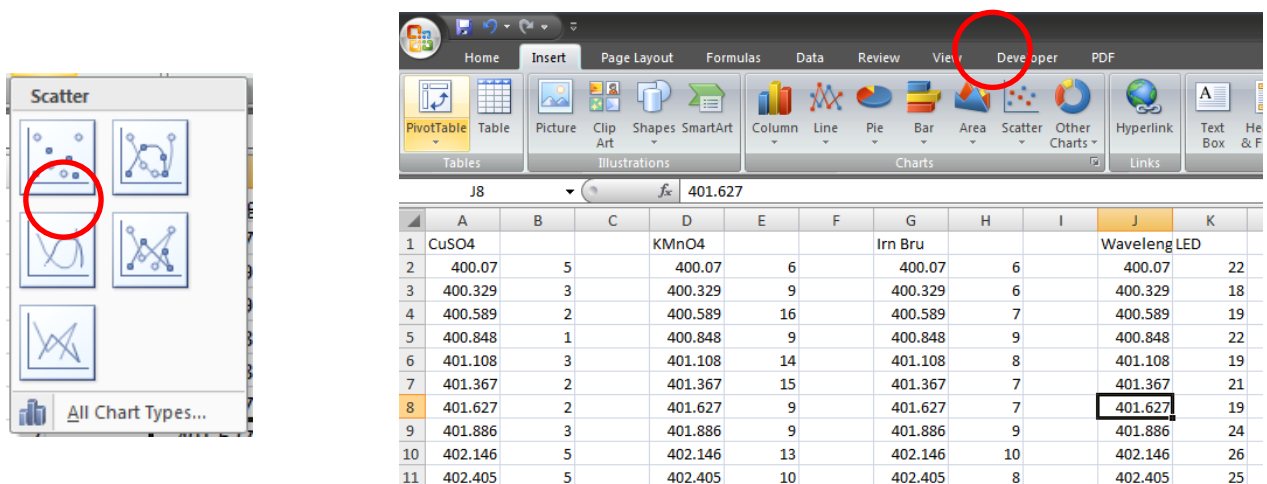
When you open up your csv file (it automatically opens in Excel) you will notice a couple of things.

- 1) There are two columns: column 1 is the wavelength in nm, column 2 is a reading of intensity in arbitrary units)
- 2) There are a lot of points. The file gives you readings at about 4-5 per nm.

To plot a graph of the readings, first insert a row at the top and enter the column headings; 'wavelength' and the name of your source.

Then select both columns and on the insert tab, go to Scatter.

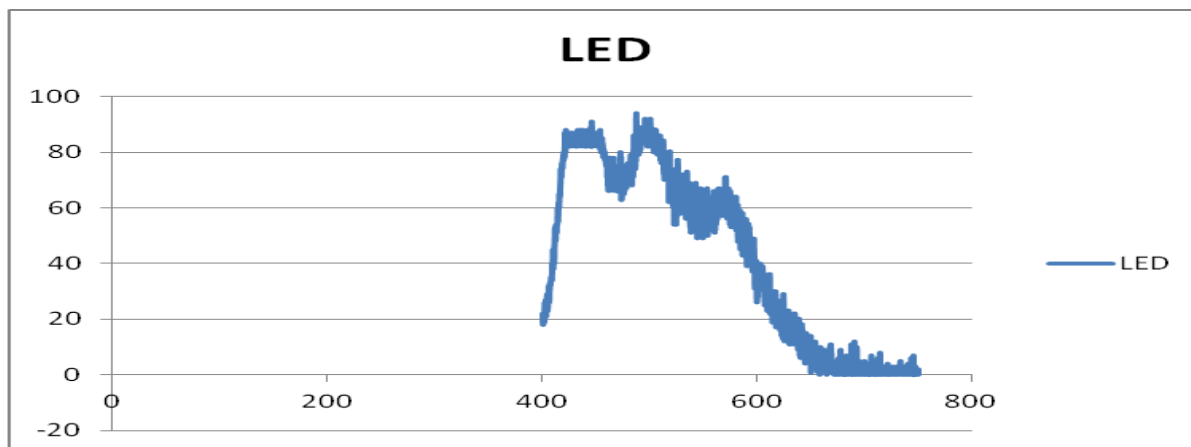
From here, select the option for smoothed lines.



The image shows two parts of the Excel interface. On the left is the 'Scatter' chart type selection menu, with the 'Smoothed Lines' option circled in red. On the right is the Excel ribbon, with the 'Developer' tab highlighted in red. Below the ribbon is a spreadsheet with the following data:

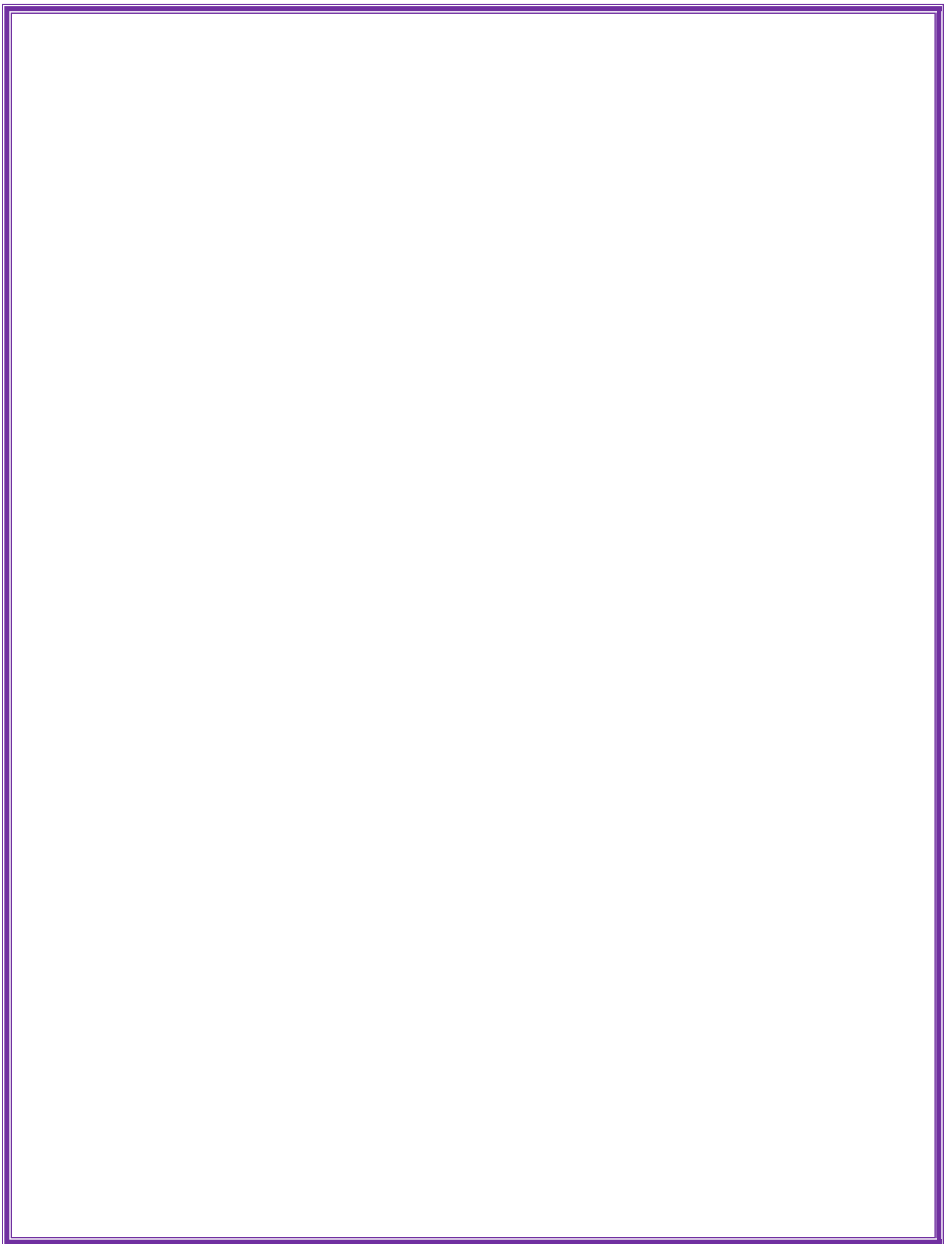
	A	B	C	D	E	F	G	H	I	J	K
1	CuSO4			KMnO4			Irn Bru			Wavelength	LED
2	400.07	5		400.07	6		400.07	6		400.07	22
3	400.329	3		400.329	9		400.329	6		400.329	18
4	400.589	2		400.589	16		400.589	7		400.589	19
5	400.848	1		400.848	9		400.848	9		400.848	22
6	401.108	3		401.108	14		401.108	8		401.108	19
7	401.367	2		401.367	15		401.367	7		401.367	21
8	401.627	2		401.627	9		401.627	7		401.627	19
9	401.886	3		401.886	9		401.886	9		401.886	24
10	402.146	5		402.146	13		402.146	10		402.146	26
11	402.405	5		402.405	10		402.405	8		402.405	25

You will get something like this.

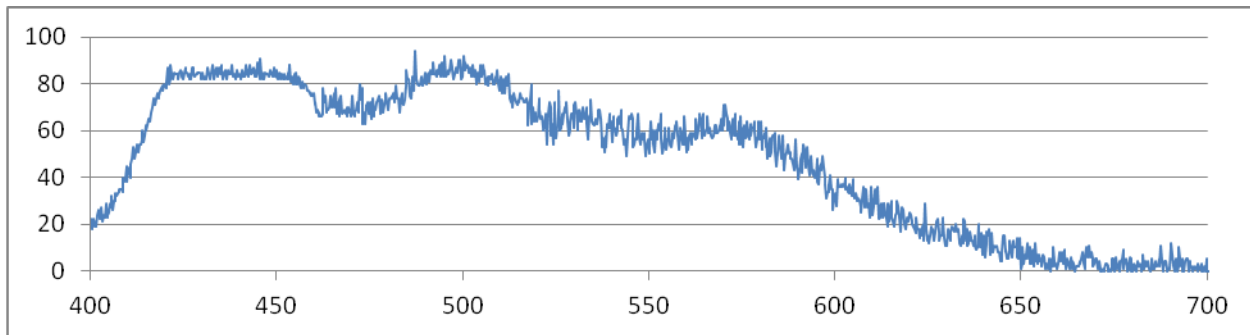


It still does not look right. By default, Excel starts both axes at 0. You want your x-axis to run from about 400 to 700 (You decide exactly by looking at your data).

Right click on the x-axis and select format horizontal axis. On this screen, set the minimum and maximum values. Your graph will immediately seem much better.



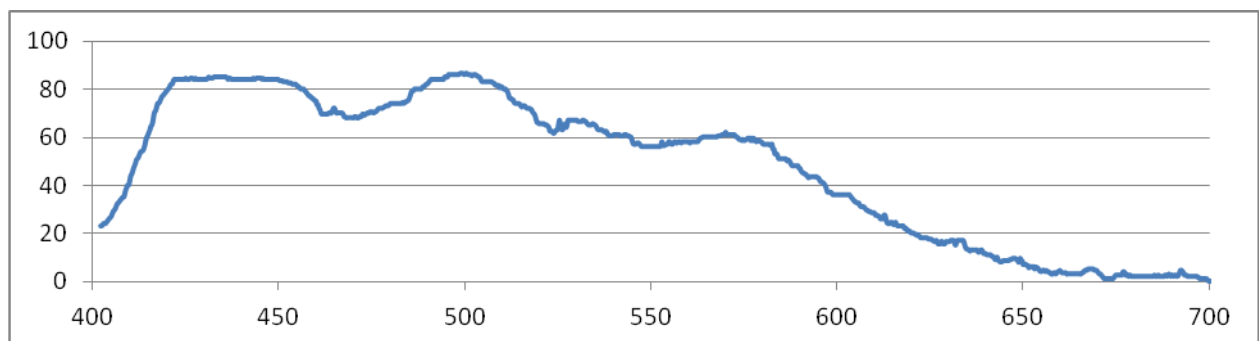
Smoothing



You can see, however, that the graph is a bit 'rough'. There is quite a lot of variability in the data. To make the graph better, you can smooth the data.

A well-known statistical technique is called 3-median smoothing. Basically, you replace every point with the median value of the point itself and those above and below it.

Given that we have such a lot of points, however, you can get a more satisfactory effect by taking the median of 10 points above and below (20-median smoothing). Here is the graph above smoothed in this way.

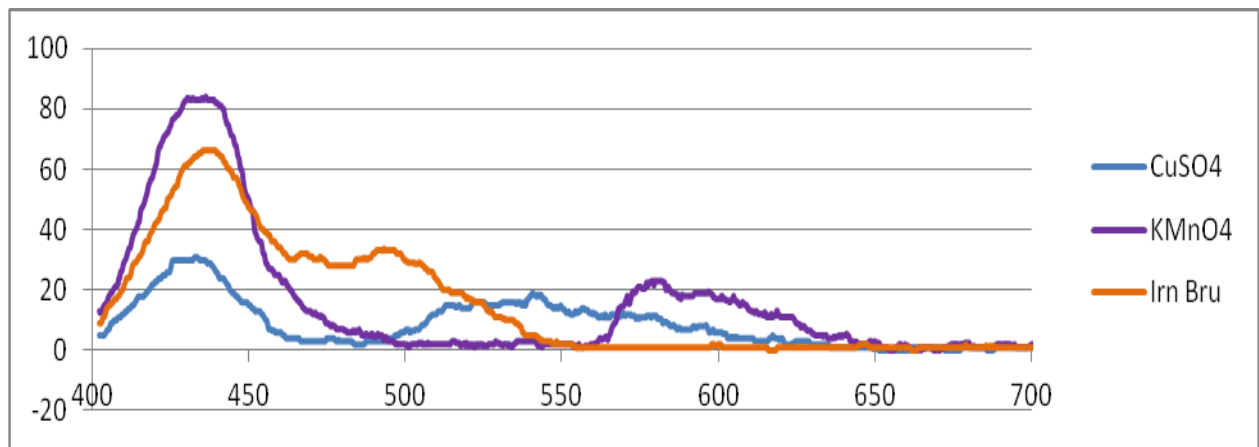
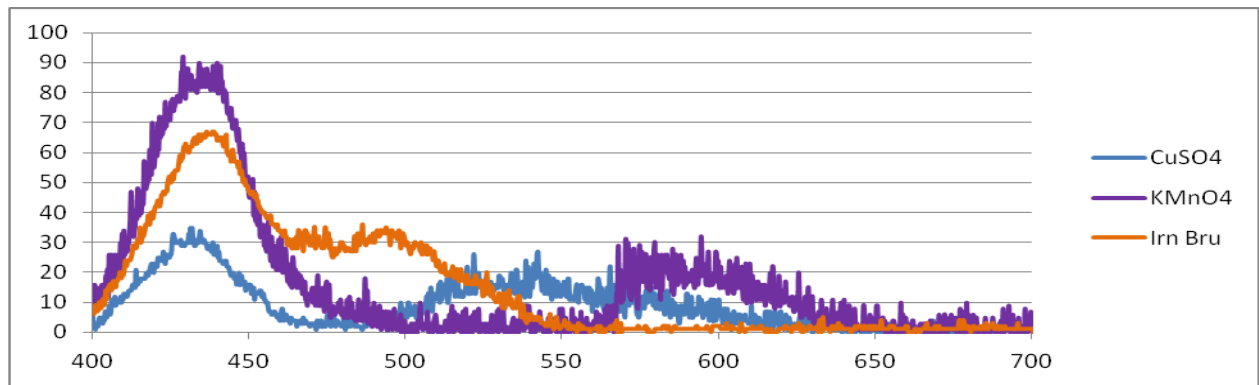


The excel formula is `=median(select range of cells)` so the first one here was in Row 12 and went `'=median(B2:B21)'`

This was then copied down the column.

Here is a graph of three substances, taken using the cuvette adaptor.

And here is the same data with the smoothing applied



Ideas for Investigation

1) Daylight and artificial lights

If you take pictures of the spectra of daylight or of incandescent light, you will see that they are continuous spectra – though the incandescent light spectrum will have less blue as it has a ‘warmer’ colour.

Comparing this with a spectrum from a fluorescent tube (like the photo on the front page of this booklet, shows that this light is made of a series of discrete bands. Compare different fluorescent sources as well to see how they vary.

2) Filters

If you capture a spectrum from a full-spectrum light source and then repeat it with different filters in between the light source and the spectroscope, you will be able to observe the wavelengths that each filter absorbs.

3) Absorption spectra of chemical compounds

In a similar way to the above, you can pass the light from a full-spectrum source through a solution of a coloured chemical, chlorophyll for example, to see the effect. (You will need to experiment a little with the concentration to get the right magnitude of effect).

4) Emission spectra

You can easily use your spectroscope for examination of the colours from flame tests.

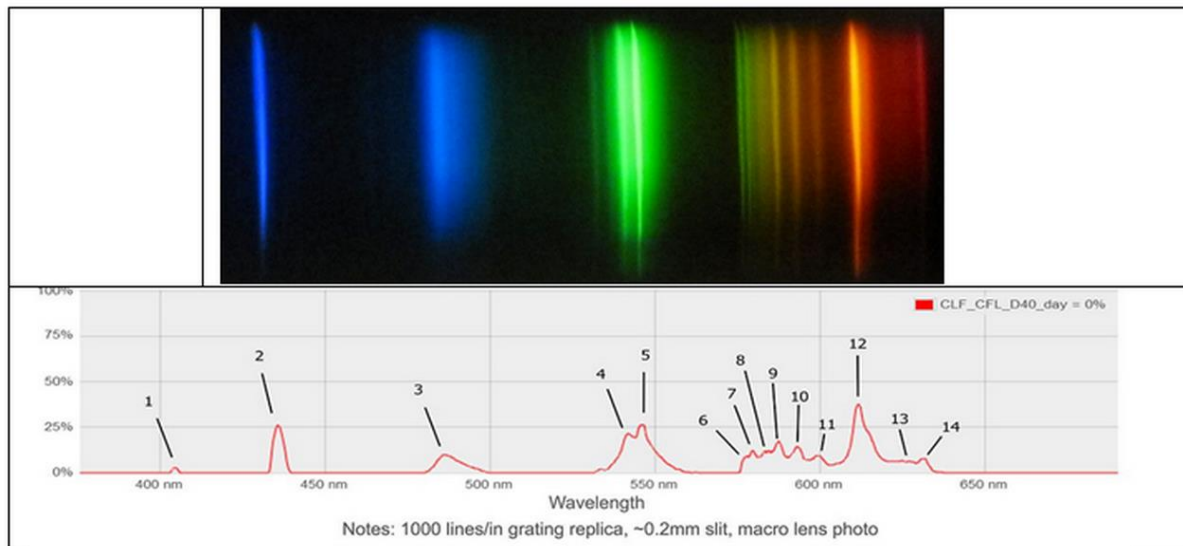
This is best done in a partially darkened room (dim rather than blackout). It can require a bit of coordination to synchronise the creation of the colour and the taking of the photograph but two people working together should be able to manage easily enough. The best method for this seems to be soaking a wooden splint in a solution and holding that in the flame – you get several seconds before the yellow of the burning wood starts.

Alternatively, the demonstration using solid salts and methanol can provide a reasonable, long-lasting colour – be wary of the flammability though.

Compact Fluorescent Data

Here is a more detailed look at the different wavelengths emitted by Compact Fluorescent Sources.

http://users.skynet.be/fc298377/EN_spectro.htm



number	colour	origin of the colour	wavelength
1 (not visible here)	violet but can hardly be seen	mercury	404.66
2	violet	mercury	435.83
3	blue	terbium	~ 485-490
4	green	terbium	~ 543-544
5	green	mercury	546.07
6	green	likely terbium or mercury	~ 578 for Tb or 576.96 for Hg
7	green	mercury or terbium	579.07 for Hg or ~ 580 for Tb
8	yellow	possibly terbium or europium	~ 580
9	yellow	likely europium	~ 587
10	orange	likely europium	~ 593
11	red	likely europium	~ 598
12	red	europium	~ 611
13	red	likely terbium	~ 625
14	red	likely europium	~ 630

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