

Astronomical spectroscopy with the USB 2000 spectrometer

9/29/2012

Your lab reports are due on October 16, 6pm.

Introduction

The USB 2000 spectrometer contains a diffraction grating and a one-dimensional CCD detector array. The CCD array has 2048 pixels in a line, so the spectrum is a list of 2048 data numbers (DN) each number representing the number of photons detected by each pixel. The spectrometer box is shown in Figure 1 and depicted schematically in Figure 2. Light enters via a slit located at the bottom of a threaded connector, which can be used to connect an optical fiber with a SMA plug. This instrument achieves a spectral resolution of about 0.5 nm, and detects wavelengths between 370 - 680 nm.



Figure 1: The Ocean Optics USB 2000 spectrometer. The spectrometer entrance slit is located at the rear of the SMA 905 type threaded connector. Commands to expose the CCD are sent via a USB connection and the data are returned via the same route.

The spectrometer operates from a laptop computer loaded with Ocean Optics' SpectraSuite software, via a USB serial interface. A laptop with SpectraSuite installed is available.

Spectrometer use

We only have one USB 2000 spectrometer. If it gets lost or damaged it cannot be replaced. For that reason the spectrometer must be treated with great care—it is a delicate optical instrument that is sensitive to shock and contamination. The spectrometer will be available for use on the class evenings, as well during some mornings/afternoons in the presence of one of the instructors. We will provide specific days during class.

Inside the “black box”

Figure 2 shows a schematic of the USB 2000 spectrometer from the Ocean Optics web page¹. Light enters the spectrometer through an optical fiber at position (1), passing through a slit (2). An optical filter (3) blocks light that would be diffracted in the second- and third-orders by the grating. A collimating mirror (4) matches to the f-ratio ($F/2.3$) of the optical fiber. Light reflects from this mirror, as a cylindrical, collimated beam, toward the diffraction grating. The grating (5) is installed on a rotating platform that selects wavelength range. After assembly, the grating platform is fixed to eliminate mechanical shifts or drift. A concave mirror (6) focuses the first-order spectrum on the detector plane with pixels having dimensions, $14\ \mu\text{m} \times 200\ \mu\text{m}$. A linear CCD detector (8) with 2048 pixels detects light, a different wavelength at each pixel.

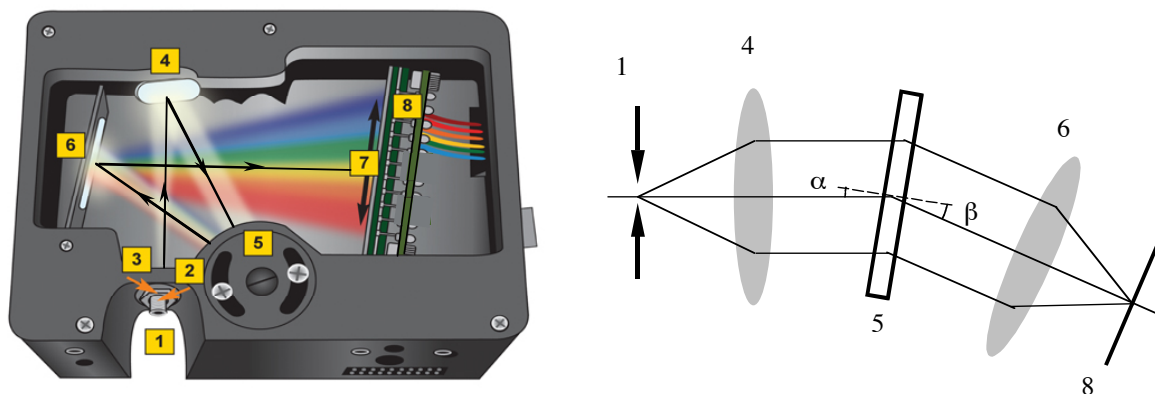


Figure 2: *Left:* The interior of the USB 2000 spectrometer, showing the optical layout. The key optical components are the entrance fiber and slit (1 and 2), the collimating mirror (4) the grating (5), the camera mirror (6) and the detector array (8). *Right:* an equivalent optical diagram using lenses. The angle of incidence and diffraction at the grating (α and β) are shown such that $m\lambda/\sigma = \sin\alpha + \sin\beta$, where m is the order (1, 2, 3...), λ is the wavelength, and σ is the grating groove spacing.

Getting started

First plug in the USB2000 spectrometer into the USB port of the Mac and then fire up the SpectraSuite control software. You should immediately see the control window, which is shown in. If no device shows up in the data sources window (top left) select Spectrometer/Rescan Devices from the menu. If you started the software before plugging in the spectrometer, quit the software and then plug in the spectrometer and try again.

Taking a spectrum

In the default operating mode the spectrometer continuously acquires a new spectrum with a cadence equal to the integration time. Click the blue **S** button to make sure that the plotted spectrum shows raw counts from the CCD. (Pressing the other buttons to the right of **S** activates various processing options such as dark subtraction, which we do not want.)

¹ http://www.oceanoptics.com/products/benchoptions_usb4.asp

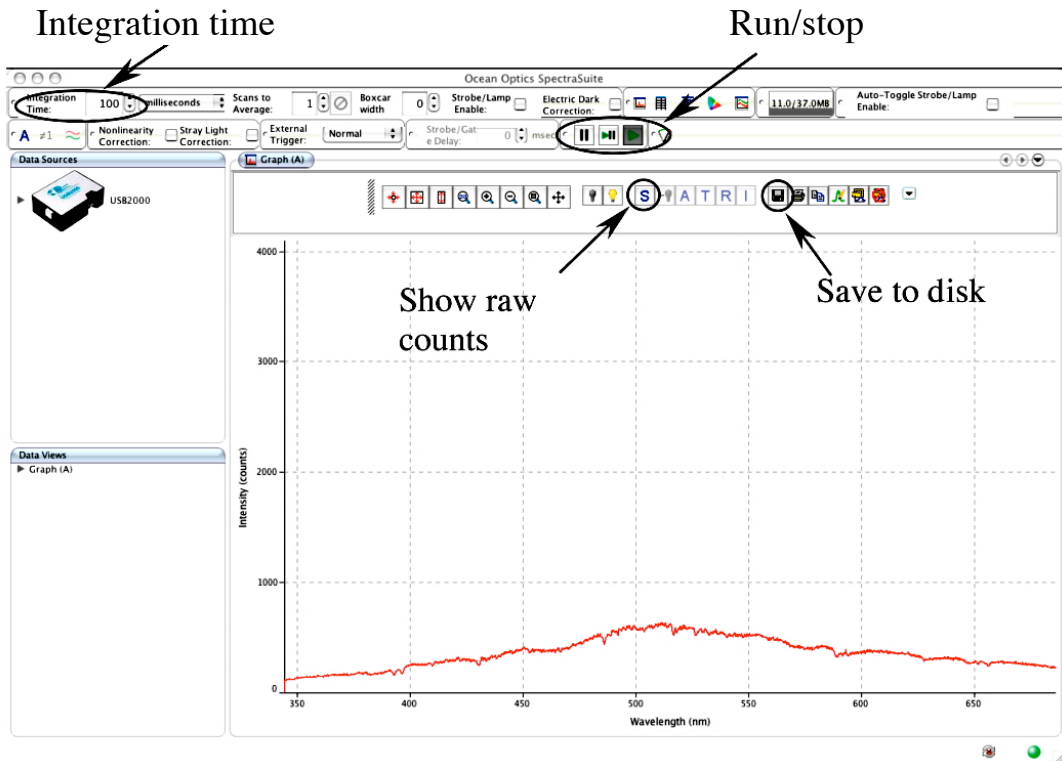


Figure 3: The SpectraSuite control software when it starts up. The red line is a graphical display of the spectrum. The x-axis is displayed in nm or pixels, depending on your setting. Pressing the scope mode button displays unprocessed data.

The spectrum display is “live,” and updates with each new exposure. Wave your hand in front of the entrance aperture and note the change in brightness. The default exposure time is 100 ms, so you should see an immediate response on the plot.

Try changing the integration time in the upper left window from the default 100 ms to a longer time and view the results. Use the set of icons just above the graph to adjust the x- and y-scaling of the graph. If you have a scroll wheel on your mouse, you can use this to zoom in and out.

The easiest way to use the spectrometer is to inspect the live graphical display. This is a very handy option because it lets you see immediately if the light source is bright enough to yield useful data. The plot has some handy tools. For example you can right-click on a feature within the plot window, and a vertical green line will appear. This cursor can be used to read off the wavelength of a feature—when you click this updates the text box at the bottom of the plot with the wavelength in nm and the intensity in counts. By default the plot appears with the x-axis labeled in nm. Choose “Processing” and then “X-axis Units”... to select pixels. No self-respecting astronomer would trust the wavelengths coming from a black box program like SpectraSuite!

What you really want is to save data in each pixel so that you can read them into IDL. When you are happy with the exposure time and other details of the measurement, click the floppy disk icon above the spectrum. Click the “browse” button to select the path and then type a file name in the dialog box. From the “Desired Spectrum” menu, select “Processed Spectrum”—to make sure that what you save is raw counts make sure that you have clicked the blue S button. For a file type to save, choose tab-delimited ASCII text.

Note that the ASCII version comes with “header” that includes the following information:

```

+++++
Date: Sat Aug 16 10:45:11 PDT 2008
User: jrg
Dark Spectrum Present: No
Reference Spectrum Present: No
Number of Sampled Component Spectra: 1
Spectrometers: USB2G5981
Integration Time (usec): 30000000 (USB2G5981)
Spectra Averaged: 1 (USB2G5981)
Boxcar Smoothing: 0 (USB2G5981)
Correct for Electrical Dark: No (USB2G5981)
Strobe/Lamp Enabled: No (USB2G5981)
Correct for Detector Non-linearity: No (USB2G5981)
Correct for Stray Light: No (USB2G5981)
Number of Pixels in Processed Spectrum: 2048
>>>>Begin Processed Spectral Data<<<<<
0.00  0.00
1.00  134.00
2.00  137.00
...    ...

```

This example is from a 30 s, unprocessed spectrum (no dark; no reference; no boxcar smoothing; no electrical dark subtraction; no stray light correction). By inspecting the header you can figure out if you really have raw data. The first number of each pair is the pixel number; the second is the measured signal in data numbers (DN). The default for the first column is the wavelength, but you should always use pixel number to avoid the unreliable manufacturer’s wavelength calibration. The grating may have tilted since construction. In this example the file is truncated after the first three pairs of data.

The method for taking long exposures is accessed from View/Toolbars/Acquisition Controls. The buttons are shown in Figure 4. For a single shot exposure, press the center button.



Figure 4: To change from continuous acquisition mode to single shot mode push the center button. Each time you push the center button a new exposure is recorded in memory. To return to continuous acquisition mode push the right hand button. To pause, push the left button. Save your spectrum by clicking the floppy disk icon on the menu bar above the spectrum.

A convenient option can be found in Tools/Options/SpectralSuite Settings/Current Working Directory, which allows you to set the default directory where data are written. If you don't set this you'll find that a lot of clicking through menus is needed every time you save a file.

Processing Options

The amount of light detected by each pixel is noted by a “data number” (DN), a number that is proportional to the number of photoelectrons detected. (These photoelectrons are generated by the photoelectric effect in each pixel, similar to the PMT light detector of the last lab.) However, the SpectraSuite software also supports some processing options. Even though these should be disabled, it is a good idea to understand these options and make sure that they are turned off before you collect any data for detailed analysis. These options are selected by pushing the button to the right of the blue **S** button.

The most basic corrections are “dark” and “reference”. A “dark” exposure is the DN in each pixel when no light hits the CCD. (This is similar to the “dark” counts from the PMT.) You should take one “dark” exposure, and it should be subtracted from a normal spectrum of any source of light. The final spectrum, $Spec_i$, is the difference:

$$Spec_i = DN_i - Dark_i \quad (1)$$

Thus, if you turn off processing you get raw DN, which is what you want, for both the spectrum and the dark exposures. As you can perform processing operations better in IDL, do not select “dark subtraction” or “reference”.

You can also average multiple scans or boxcar-smooth the spectra; make sure that these are not enabled either. Other, more advanced corrections include non-linearity correction, “electrical dark” subtraction, and stray light correction. The non-linearity correction applies a polynomial correction to the raw data values. The stray light correction is not documented, and should be turned off.

• Taking a Spectrum & Wavelength Calibration

The fluorescent lights in the Undergraduate Lab are gas-discharge lamps. A potential difference of 110 V is sufficient to partially ionize mercury (Hg) vapor that is contained in the tube, and the resultant flow of electric current excites Hg atoms to emit photons at specific wavelengths, called “emission lines”. They have wavelengths predominantly in the UV at 184.9 and 253.6 nm. A phosphorescent material that is painted on the inside of the tube absorbs these UV lines and glows at visible wavelengths producing useful illumination. The chemical composition of phosphors typically includes terbium (Tb), cerium (Ce) and europium (Eu). Not surprisingly the resultant spectrum is quite complex (see Figure 5). In addition to the UV emission lines, Hg emits some visible emission lines that are useful for “wavelength calibration”.

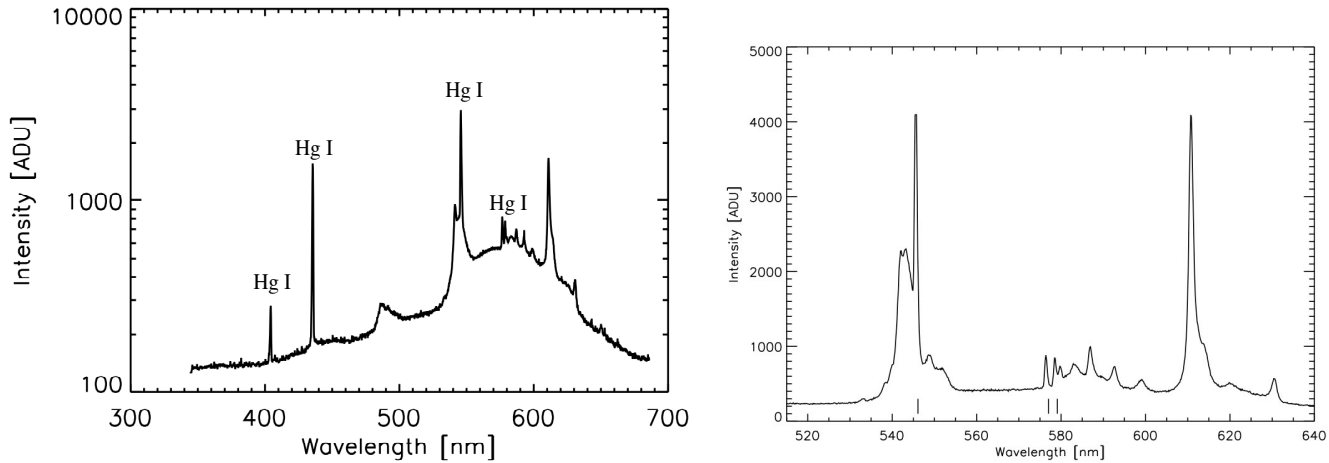


Figure 5: (Left) A 200 ms exposure spectrum of the fluorescent lamps in the Undergraduate Lab obtained with the USB2000 spectrometer. Prominent, narrow lines of atomic mercury (Hg I) are visible together with a broad emission from the phosphor in the lamp. (Not all the narrow lines are from Hg. Some come from Tb, Ce, and Eu.) The wavelength scale here is the nominal factory calibration and is only approximate. The y-axis is plotted on a logarithmic scale. **(Right)** Detail of the spectrum in the 515-640nm range. The vertical tick marks above the bottom axis indicate the expected location of the last three lines in Table 1. Note that the 579.07 nm line is partly blended with another (unidentified) line at a slightly longer wavelength.

Table 1: Bright atomic mercury lines. You must measure their pixel positions.

Relative Intensity	wavelength (nm)	Pixel	Relative Intensity	wavelength (nm)	Pixel
600	365.0153		100	434.7494	
70	365.4836		1000	435.8328	
50	366.3279		500	546.0735	
400	404.6563		50	576.9598	
60	433.9223		60	579.0663	

Every spectrometer must have a “wavelength calibration”, the wavelength of light that hits at each of the 2048 pixels. You will now find an equation that gives the wavelength as a function of pixel number: $\lambda = f(x)$. You will start with a calibration that is a straight line, and then try a parabola.

First take a spectrum of the fluorescent lamp and store it in a file (as per above). Make sure that the strongest lines are not saturated but that the weaker lines can be clearly identified in the spectrum.

In addition to the fluorescent lamp in the Lab, you will also take a spectrum with the Ne lamp, which is characterized by its orange glow. The spectrum of this lamp contains a rich forest of lines beyond 580nm but a remarkable dearth of features at shorter wavelengths, which explains its color (see Figure 6). This is particularly useful to calibrate fully the spectrometer, as the Hg lines you have already identified are at shorter wavelengths. The identification of individual lines in the Ne lamp spectrum can be done using the bottom panel of Figure 6, which provides the wavelengths for all features that can be detected in our lamp spectrum.

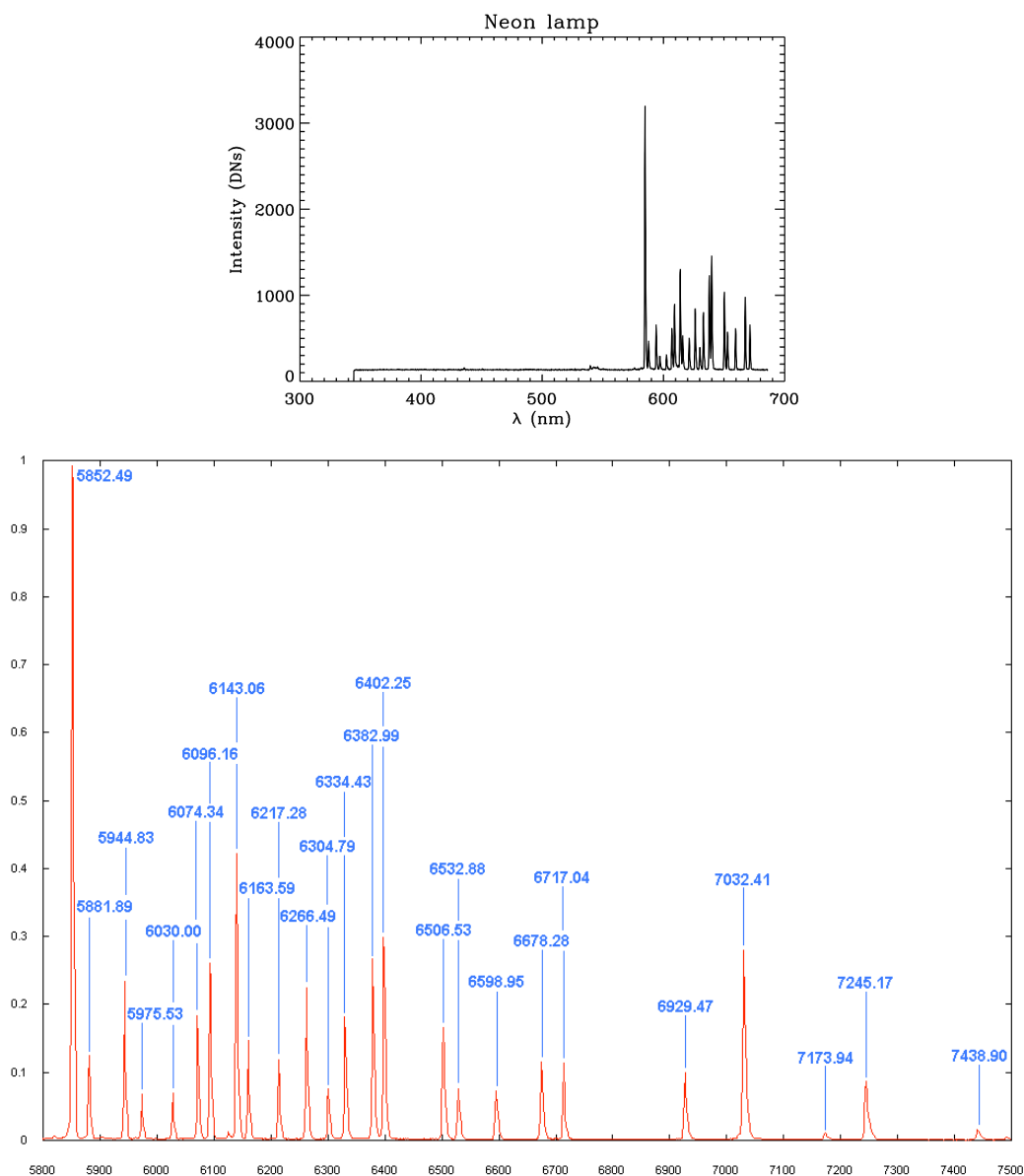


Figure 6: (Top) A 100 ms exposure spectrum of the Ne lamp obtained with the USB2000 spectrometer. All emission lines are from Ne. The wavelength scale here is the nominal factory calibration and is only approximate. **(Bottom)** A Ne lamp reference spectrum with lines identification. The horizontal axis is wavelength (in nm) and the vertical axis is intensity (in arbitrary units). Courtesy of Christian Buil (www.astrosurf.com).

You should also take a spectrum of the green laser pointer, which emits a single emission line at 532nm. You may need to shine the laser at an angle and/or from a distance to prevent saturation.

Transfer all the spectra to the ugaastro computer system disk so that you can use IDL to analyze them. Now give the spectrometer to another group, so they can take a spectrum.

• **Determining the Wavelength Calibration**

To determine the wavelength calibration, you need to find the pixel position of the Hg lamp, Ne lamp and green laser emission lines in the lamp spectra. There are several possible methods to do so. For instance, one can use the “cursor” command in IDL to determine the approximate pixel position of each of the emission lines:

```
IDL> cursor,x,y  
IDL> print,x
```

What do you think is the typical uncertainty on the position of the line using this method? Do you think other methods may help reduce this uncertainty?

Now determine the pixel position of each Hg line and of 3-4 Ne lines (pick wisely among the many available ones and justify your choice) precisely, to the nearest 1/100 of a pixel. To do this, you may write IDL code that determines the “centroid” of the emission line. The centroid is defined as:

$$\langle x \rangle = \frac{\sum x_i DN_i}{\sum DN_i}$$

This is the “weighted” mean position of the emission line, weighted by the DN counts in each pixel. Another possible method consists in fitting a simple functional form to the line. Gaussian and polynomial forms (you may investigate the “gaussfit” and “polyfit” IDL procedures, for instance) are frequently used for this purpose. Other methods might be used. Explain which one you use and why you choose it.

- Construct a table similar to Table 1 that lists the exact pixel position (to within 1/100 pixel) and the wavelength of each of the lines you are using (include the Ne lines). Estimate uncertainties on the pixel position of the lines.
- Make a plot of wavelength vs pixel position for all lines. (Be sure to label axes.)
- Fit a straight line to the datapoints, using the least square method. Give the linear equation in your report.
- Add to the plot, by overplotting that linear fit as a smooth straight line. The line should go through all datapoints. Does it?

- Now use that same straight line equation to predict the wavelengths of each emission line from the pixel position. List the discrepancy (difference) between the predicted and actual wavelength of each line (in nm).
- Plot the discrepancy in wavelength (from above) versus pixel position. What do you notice? Is there a smooth relation? Does this mean a parabola would be better fit to the wavelength calibration than a straight line?
- Now fit wavelength vs. pixel with a parabola: This is a parabolic wavelength calibration:

$$\lambda = c_0 + c_1x + c_2 x^2$$
 Make a new plot that shows the original four points and the overplotted parabola as a smooth curved line. Does the parabola fit the points better than a straight line? How do you know?
- Write the parabolic wavelength calibration in your report, and use this for the remainder of this lab. Compare your results to the wavelength solution provided by the constructor (see Appendix).

Note that IDL's "poly_fit" function is very similar to "polyfit". One difference between the two is that "poly_fit" can perform a fit to data (in this case: the pixel position of each emission line) that are associated to uncertainties. Explain how uncertainties can be propagated in a least square fit. Can you describe in a few sentences how you would use the data at hand to estimate uncertainties on the position of each line?

Sensitivity of the spectrometer

Figure 7 shows the spectrum of a desk lamp (which has an incandescent filament). The spectrum of an incandescent lamp is nearly identical to the Planck function, i.e. a blackbody function. Of course, the Planck function is continuous without any sharp features or wiggles. The wiggles seen in the spectrum represent the spectral response of the spectrograph due to the optical filter transmission, the grating efficiency, and the sensitivity of the CCD to light, all of which vary with wavelength.

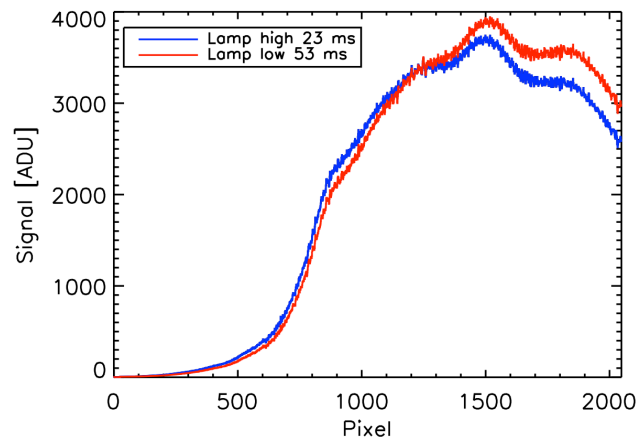


Figure 7: Two spectra of a quartz halogen desk lamp. The lamp has two brightness settings, denoted here high and low. These spectra are the average of 1024 individual spectra. The spectra have been dark subtracted. Note that the spectrum of the lamp in the low setting is

“redder” than in the high setting. The small-scale fluctuations reproduce from spectrum to spectrum suggesting that these represent pixel-to-pixel gain variation across the array (flat field variations).

Take one spectrum of an incandescent lamp. Do you see evidence (wiggles or undulations) in the spectrum that the spectrometer is not equally sensitive to all wavelengths?

Nighttime astronomy

While obtaining spectra of lamps is useful in calibrating the spectrograph, it is only a prelude to observing astronomical objects by using a spectrograph mounted on a telescope. We will gather data with the USB spectrograph mounted on the Leuschner telescope during our field trip there. We will obtain spectra of the blue sky before dawn (which should be similar to that of the Sun) and of the night sky. The latter should be dominated by emission lines from city lights, akin to the lamps in the lab except that city lights are sodium lamps. If feasible, we will obtain data on a few bright stars in the evening sky (Vega, Arcturus, ...). If this fails, we will provide you with spectra of the Moon, Jupiter and Vega obtained with the USB spectrograph mounted on the 14-inch telescope that was located on top of Campbell Hall.

Some example spectra are shown in Figure 8. The top spectrum is from an incandescent lamp, and shows the response of the spectrometer to an approximately 3200 K black body. Note the overall variation of responsivity and fine scale pixel-to-pixel fluctuations. The subsequent astronomical spectra are corrected for the spectrometer response assuming that the lamp radiates like a black body with its temperature:

$$B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}, \quad (1)$$

where $\nu_i = c/\lambda_i$ is the frequency of the i -th pixel. Explain why this is necessary and apply a similar correction to the spectra of astronomical objects.

To do:

- **Plot the spectrum of the night sky and describe it. In particular, are the emission features those expected from sodium lamps?**
- **Plot the spectrum of blue sky and describe it. Do you see absorption features from the solar photosphere? Can you identify the most important ones?**
- **Plot the spectrum of Vega and describe it with respect to that of the Sun. Can you see the Balmer lines in the spectrum? From your wavelength calibration, determine the wavelengths of the Balmer lines. Are they at known, laboratory wavelengths of Balmer lines, consistent with the wavelength calibration that you computed previously, or are the wavelengths different?**
- **Plot the spectra of the Moon and Jupiter. How similar/different are they from that of the Sun? It might be interesting plot the ratio of spectra (e.g., the Moon spectrum divided by the Sun spectrum).**

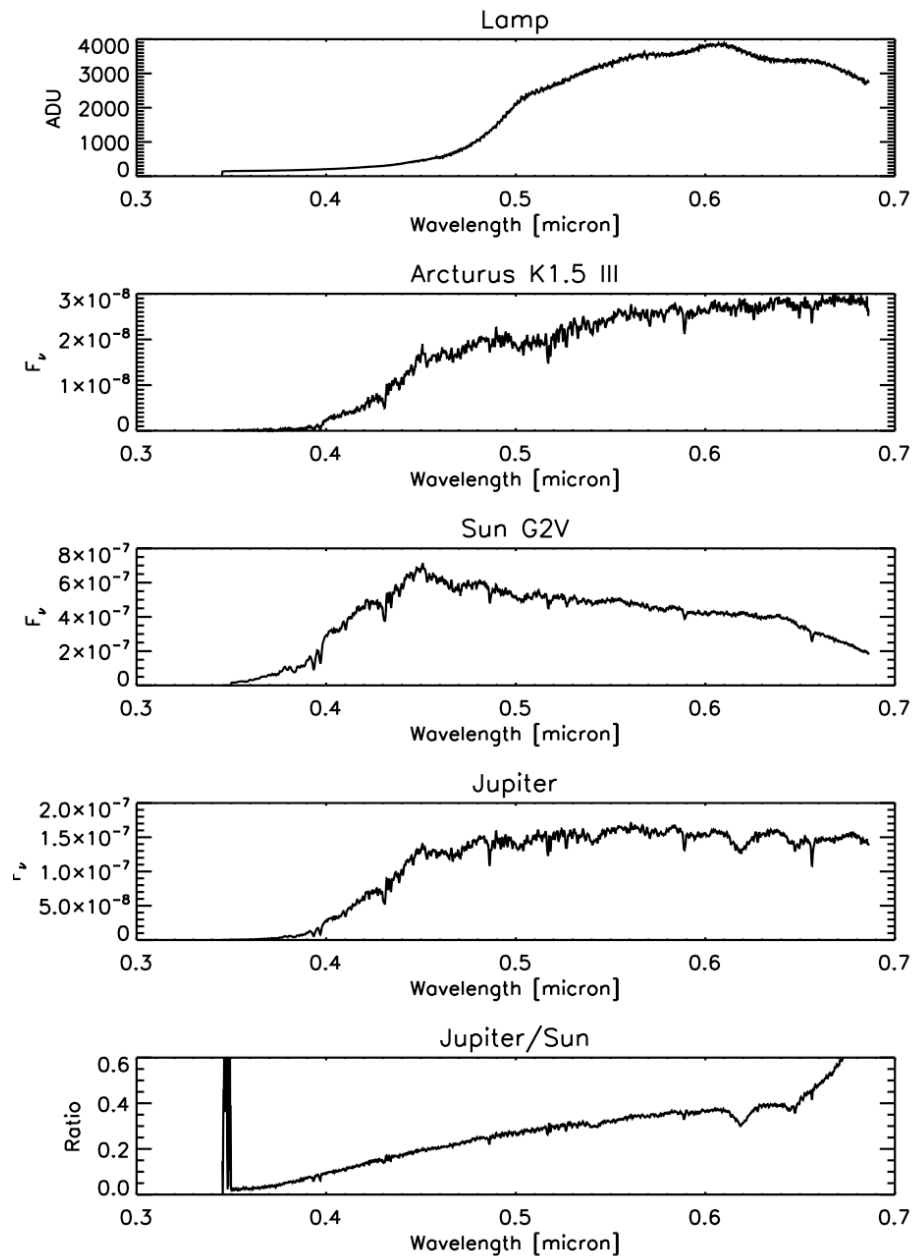


Figure 8: A lamp spectrum and some astronomical spectra. Comparison of Arcturus (4300 K) and the sun (5800 K) shows the effect of Wien's law. The Arcturus spectrum looks noisy—the structure is primarily due to many overlapping absorption lines. In the solar spectrum Ca II H&K 393.37, 396.85 nm, the G band 430.8 nm, H β 486.1 nm, the b and E bands (Mg + Fe) 517, 527 nm, Na D 588.995, 589.592 nm, and H α 656.2 nm are all visible. The spectrum of Jupiter is red, with strong methane absorption at 619 nm. The exposure times are: lamp 23 ms, 1000 frames; Arcturus & Jupiter 500 ms, 100 frames; sun 3 ms, 100 frames. The astronomical spectra are dark subtracted, divided by the lamp spectrum, and multiplied by a 3200 K black body.

Appendix: Manufacturer's Specifications

The data sheet provided by Ocean Optics with the USB 2000 spectrometer lists the nominal properties given in Table 2.

Table 2: Nominal spectrometer properties

Property	Value
Model	USB 2000
Serial No.	USB 2G5981
Grating	1200 line holographic VIS
Bandwidth	350-660 nm
Options	L2 lens, 25 μm slit, WG305 filter
CCD	Sony ILX511 1 \times 2048 pixel
Pixel size	14 μm \times 200 μm
Pixel well depth	62,500 electrons
A/D resolution	12-bit
Dark noise	2.5 counts RMS
Focal length	42 mm input, 68 mm output
Integration time	3 ms—65 s

The image sensor is a 2048-pixel linear CCD manufactured by Sony, part number ILX511. The ILX511 is a rectangular reduction-type CCD designed for bar code hand scanners and optical measuring equipment use. The pixel size is 14 μm \times 200 μm . The chip has a built-in timing generator and clock drivers and packaged in a 22 -pin DIP.

Appendix: wavelength calibration

The spectrometer has a built in processor that uses pre-measured third-order polynomial to convert pixel number to wavelength, so you actually get two columns in the data file, where the first number is an estimate of the wavelength in nm based on a polynomial expression of the form

$$\lambda_i = \sum_{j=0}^3 a_j i^j = a_0 + a_1 i + a_2 i^2 + a_3 i^3 \dots, \quad (2)$$

where i is the pixel value. The manufacturer's values are given in the Table below.

Table 3: Manufacturer's wavelength calibration

Coefficient	Value
a_0	344.311
a_1	0.19743
a_2	-1.4913×10^{-5}
a_3	0.0