4. Discrete Spectra

4.1. Purpose

1. To record several elemental emission spectra using arc lamps filled with each element using the Ocean Optics USB650 spectrometer.
2. To measure the emission lines in the hydrogen, helium and possibly other elemental spectra, and compare these to know values.
3. To measure the emission spectrum of the sun and identify elements of the photosphere by comparison if possible.
4. To identify an unknown element in an arc lamp.

4.2. Ocean Optics Red Tide USB650 Spectrometer Specifications

- Sony ILX511 linear silicon CCD array detector
- Responsive from 350 to 1000 nm
- Sensitivity of up to 75 photons/count at 400 nm
- An optical resolution of ~2.0nm (FWHM)
- Integration times from 3 ms to 65 seconds (15 seconds typical maximum)
- Embedded microcontroller allows programmatic control of all operating parameters EEPROM storage for:
  - Wavelength Calibration Coefficients
  - Linearity Correction Coefficients
  - Other configuration parameters
- Low power consumption of 450 mW
- 12 bit, 1MHz A/D Converter
- 2 programmable strobe signals
- 24-pin connector for interfacing to external products

4.3. Procedure

4.3.1. General

In this lab we will use a Red Tide USB 650 Spectrometer by Ocean Optics in conjunction with a GLX unit. The use of this spectrometer requires a license has been installed on the GLX.

Note that the spectral response of the Ocean Optics spectrometers is not flat for intensity, that is, an intensity of 200 counts at 400nm does not correspond to the same absolute intensity when you see a 200 counts at 600nm. It is quite reliable in terms of wavelength however.

1. Plug in your GLX, and the spectrometer into the USB terminal on the GLX. The spectrometer may have a blue cap covering its detector. Remove the cap.
2. Record the serial number to determine the calibration equation of your spectrometer.
3. Record which "Run #" corresponds with what source. Several runs will be acquired so be sure to know which are the ones to be submitted. The label of the Run can be changed on the GLX if desired.
4. Data will be exported to USB stick and imported into xmgrace for plotting, etc.

4.3.2. Acquiring a spectrum

The data displayed on the GLX will be a graph of Intensity [counts] as a function of wavelength [nm]. There are two main factors that can be controlled that greatly affect the quality of what is recorded. These factors both have influence on the size of the peak. The goal is to avoid too flat a spectrum (no information) and at the other end, avoid saturating the recorded spectrum. The two items are

1. integration time: how long the spectrometer acquires light
2. distance of spectrometer from light source

The goal is to acquire a spectrum that is neither too shallow or so high that it has a flat top. A peak of about 70 to 90 percent of the total available height is very reasonable. By adjusting both the above factors, decent spectra will be acquired.

After you plug in the spectrometer in a few moments you will see the configuration screen come up with the spectrum preview at the top. Among other settings, this screen allows you to adjust the amount of time the spectrometer acquires data. This setting is similar to the exposure length for a camera. Depending on the brightness of the source, you will adjust this value to achieve a good spectrum.

You can always return to this screen by pressing the home key then F1 to open configuration plus the graph screen. From here, F4 will close the configuration dialog and display the full spectrum graph. If the full spectrum graph is on the screen, press F3 to open the tools menu, and the arrow keys to highlight spectrum analysis configuration then press the check mark to select it. Table 4.1 summarizes this behavior.

Table 4.1.: General Configuration keys

Screen showing	Press	To get to screen	use for
Home screen	F1	spectrometer configuration with small graph at top	set integration time
Home screen	F4	Sensor settings for spectrometer	sample rate, type of spectrum
spectrometer analysis/configuration	F4	Data acquisition screen	taking data
Data acquisition screen	F3	spectrometer analysis/configuration	

4.3.3. Required Spectra: Continuous and Discrete

Acquire spectra of several light sources that are available. This includes

- various spectral lamps (discrete): H, He, Na, Hg, Oxygen, Nitrogen, Argon+unknown, possibly others

- room fluorescent lighting
- the sun

Take the following spectra and record the run # and source for reference.

1. Arrange the spectrometer and the integration time so that you can reliably acquire graphs that do not saturate the detector.
2. Collect a spectrum for the various arc lamps.
3. Record a spectrum for the fluorescent ceiling lights.
4. Record a spectrum for sunlight. Take the GLX to either the bright hallway, or outside and change the integration time as needed.

4.4. Importing Data to xmgrace

1. Export your data to a computer for manipulation in xmgrace. The following steps from the Pasco website detail how to do this:
   a) Connect a USB FLASH drive to the USB A port on the GLX. Select Data Files. Select the file you wish to import into xmgrace using the up and down arrow keys. Press F1 to open the data file.
   b) Press the Home button. Press F2 to open the Table. Populate the table with all of the columns of data that you wish to export including the mis-labeled "time" column.
   c) Press the Tables button. Select Export All Data. If you choose to rename the file you are about to export, do not delete the .txt extension.
   d) Change the Export File Format to ASCII. Click OK (F1) to export to the flash drive[1].
   e) Log into a Linux computer and bring up the file manager. Create a folder for your data and then plug in the USB drive to a port on the computer. Copy the files over, taking care that you maintain your original files on the USB stick for a backup.
   f) Open a files to determine which rows have the data you need to plot.
   g) Open xmgrace. Press Data, Import, ASCII. Change the Filter to * so that all files will be listed (it is set to .dat). Find your file in the Files list and click on it.
   h) With more than two columns in the file[2], 'Load as' needs to be set to "Block Data". Other settings are left to their defaults: Data source: Disk, Autoscale on read: XY. Press OK and the block data dialog window will appear
   i) Choose the appropriate columns sor the "X from column" and "Y from column" settings and click on Apply or Accept. Data should now appear in the graph window. If not, press autoscale and/or seek advice from that point.

   You should now see a graph of Intensity in counts as a function of wavelength.[3]
2. Repeat the import and graph creation for each source as per below.

[1]

i. You will see a progress bar when data is being written. These files are reasonably big so it will take a moment to finish.

[2] Row count is present

[3] The GLX displays nanometers on the x-axis but mis-labels it as time. If the x-axis ends up as pixel number (0 to 2047) then either re-import the data and read in the correct column for the x-axis or convert pixel number to wavelength using section 4.4.1.

4.4.1. Converting pixel # into $\lambda[nm]$

The following procedure may not be necessary. The wavelength data is available for export, but is mislabeled in the GLX's software as time. Exporting the "time" column in the GLX is advised.

The CCD of the spectrometer has close to 2048 pixels, each one accumulates a charge proportional to the amount of light that strikes it after reflecting off the diffraction grating. The Ocean Optics company provides a calibration equation to convert pixel number into wavelength. Using p for pixel number, the calibration equation is of the form

$$\lambda = ap + bp^2 + cp^3 + d$$

Consult Table 4.2 below to obtain the constants for your spectrometer. Create a new set by formula in xmgrace will produce the wavelength in nanometers for the horizontal axis.

Serial Number	a nm/pixel	b nm/pixel^2	c nm/pixel^3	d nm
USB2G39925	0.37953	-1.7666E-05	-1.90596E-09	339.148
USB2G40318	0.37585	-1.505E-05	-2.3213E-09	340.669
USB2G40319	0.37955	-1.6416E-05	-2.2904E-09	339.730
USB2G51048	0.38628	-2.6120E-05	3.6696e-10	338.281

Table 4.2.: Calibration constants for Ocean Optics spectrometers

4.5. Data and Analysis

The spectrometers that we are using are well defined in terms of their resolution ($\pm 2nm$), but the intensities at different wavelengths have two problems:

- The intensity values are not absolute. They are merely a count that is proportional to the amount of incident photons at a particular pixel.
- As already mentioned, the spectrometer's sensitivity is not uniform across the wavelength range. So a reading of 400 at pixel 239 and again at pixel 1288 do not mean the light intensity was the same at each location.
- the x-axis in nanometers is well defined and comparisons involving wavelength λ in nanometers can be accurately done.

1. All data must be plotted with wavelength in nanometers on the x-axis. See subsection 4.4.1 for details.
2. Plot the H and He spectra on individual graphs. Pick four or five of the highest intensity emission lines and use the mouse in xmgrace to measure the wavelength of each line. Compare to an on-line resource which has the emission lines measures for each element to gauge the wavelength accuracy of your spectrometer. Create a table these measured and accepted λ values in your report.
3. Plot the sun's spectrum and estimate the temperature of the sun. Examine the solar spectrum and the absorption lines present. Locate any lines in common with the various atomic spectra. You may also see absorption lines or bands due to atmospheric water, oxygen, etc. If so, comment on their presence or lack of their presence.
4. Use your atomic spectra to identify one of the two elements present in the unknown spectral tube. Lines of Argon are in the spectrum, along with one of the other individual knowns collected already.

4.6. Questions

Answer and include with your report.

1. What is the peak wavelength of emission for the human body?
2. Describe a procedure that could be used to calibrate the spectrometer's Intensity readings.