

Hydrogen-Deuterium Mass Ratio

1 Background

1.1 Balmer and Rydberg Formulas

By the middle of the 19th century it was well established that atoms emitted light at discrete wavelengths. This is in contrast to a heated solid which emits light over a continuous range of wavelengths. The difference between continuous and discrete spectra can be readily observed by viewing both incandescent and fluorescent lamps through a diffraction grating; hand held gratings are available for you to do this in the laboratory.

Around 1860 Kirchoff and Bunsen discovered that each element has its own characteristic spectrum. The next several decades saw the accumulation of a wealth of spectroscopic data from many elements. What was lacking though, was a mathematical relation between the various spectral lines from a given element. The visible spectrum of hydrogen, being relatively simple compared to the spectra of other elements, was a particular focus of attempts to find an empirical relation between the wavelengths of its spectral lines. In 1885 Balmer discovered that the wavelengths λ_n of the then nine known lines in the hydrogen spectrum were described to better than one part in a thousand by the formula

$$\lambda_n = 3646 \times n^2 / (n^2 - 4) \text{ \AA} \text{ (angstrom)}, \quad (1)$$

where $n = 3, 4, 5, \dots$ for the various lines in this series, now known as the Balmer series. (1 angstrom = 10^{-10} m.) The more commonly used unit of length on this scale is the nm (10^{-9} m), but since the monochromator readout is in angstroms, we will use the latter unit throughout this write-up.

In 1890 Rydberg recast the Balmer formula in more general form as

$$1/\lambda_n = R(1/2^2 - 1/n^2) \quad (2)$$

where again $n = 3, 4, 5, \dots$ and R is known as the Rydberg constant. For reasons to be explained later, its value depends on the mass of the nucleus of the particular isotope of the atom under consideration. The value for hydrogen from current spectroscopic data is

$$R_H = 109677.5810 \text{ cm}^{-1}[1],$$

and the current value for an infinitely heavy nucleus is

$$R_\infty = 109737.31568525(73) \text{ cm}^{-1}[2].$$

A generalization of the Rydberg formula to

$$1/\lambda = R_H \left[\left(\frac{1}{n_1^2} \right) - \left(\frac{1}{n_2^2} \right) \right] \quad (3)$$

suggested that other series may exist with n_1 taking on the values 1, 3, 4, 5, . . . , subject to the restriction that $n_2 > n_1$. This proved to indeed be the case. In 1906 Lyman measured the ultraviolet spectrum of hydrogen and found the series, now bearing his name, corresponding to $n_1 = 1$. In 1908 Paschen measured the infrared spectrum of hydrogen and discovered the series, now bearing his name, corresponding to $n_1 = 3$. Figure 1 shows some of the lines in these series. The vertical axis in this figure is linear in energy (given in units of electron-volts, or eV, at the right), so you can get some sense of the relative energies of the different series.

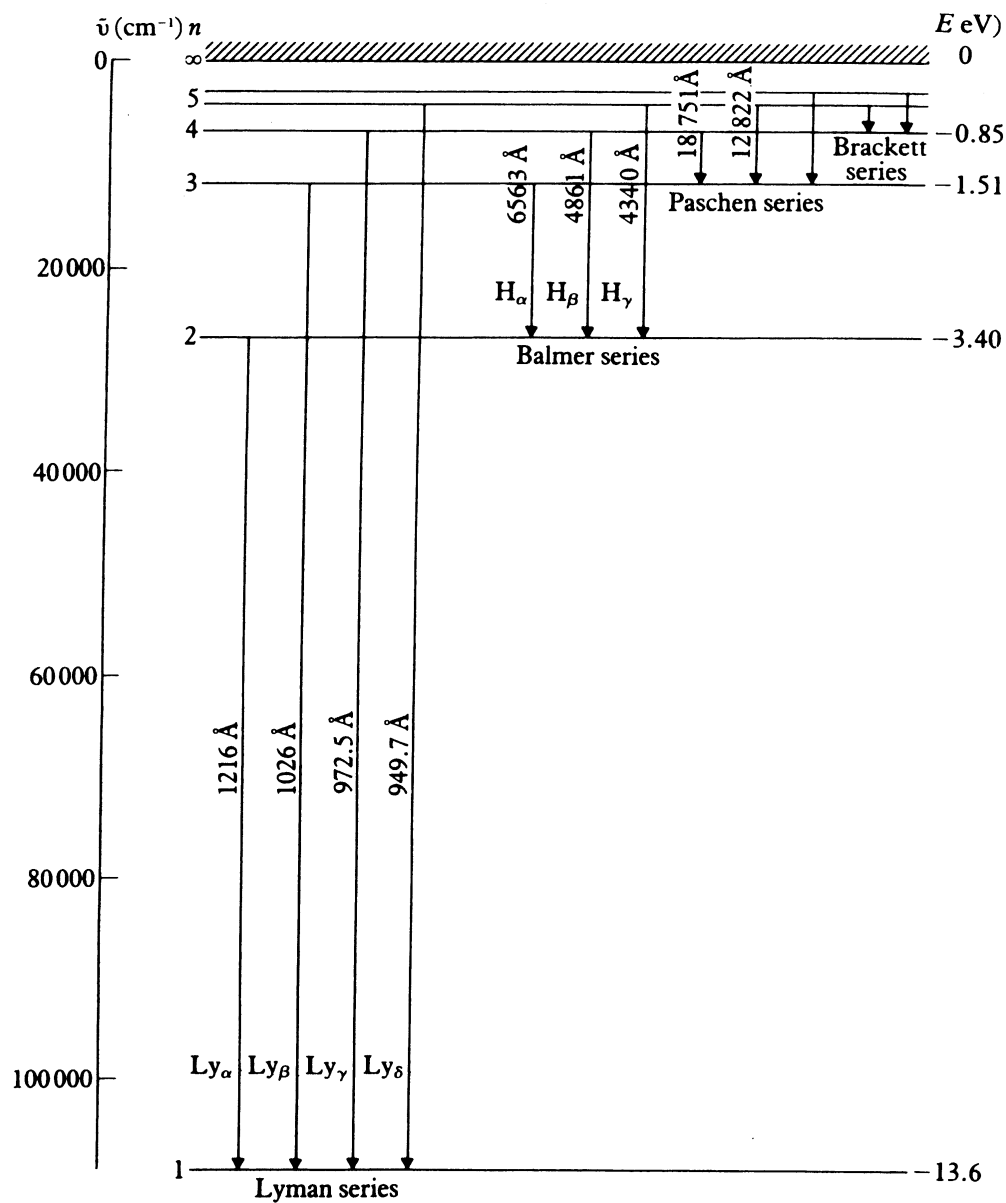
The remarkable success of the Rydberg formula in describing the spectrum of atomic hydrogen was in stark contrast to theoretical understanding of the atom in the early 1900's. Attempts to understand the emission of light at discrete wavelengths, or frequencies, using principles of classical mechanics and electrodynamics proved fruitless, as classical theory does not allow for an electron to circulate about a nucleus in a stable orbit. Rather, classical theory predicted that the negatively charged electron, circulating about the positive nucleus under the influence of a Coulomb potential, would emit radiation due to the centripetal acceleration associated with circular motion (recall that accelerating charges emit radiation). As the electron emitted radiation and lost energy, the orbit would shrink and eventually (in a predicted 10^{-12} seconds!) the electron would spiral into the nucleus, emitting a continuum of radiation in the process. The stability of atoms, and discrete atomic spectra clearly demonstrate that such a theory does not describe atomic behavior.

1.2 The Bohr Postulates

in 1913 the Danish physicist Niels Bohr, working at Ernest Rutherford's laboratory in Manchester, England, proposed a blend of classical and radically new ideas to describe atomic behavior. His three postulates were:

1. The electron moves in a circular orbit about the nucleus under the influence of the Coulomb potential, obeying the laws of classical mechanics;
2. In contrast to the infinite number of orbits allowed classically, the electron can occupy only orbits for which its orbital angular momentum is quantized in units of \hbar , i.e., $L = \text{orbital angular momentum} = n\hbar$ where $n = 1, 2, 3, \dots$. Electrons are stable in such orbits, i.e., they have a well defined energy and do not emit radiation even though they are undergoing centripetal acceleration. Bohr termed these orbits *stationary states*;
3. Radiation is emitted when an electron transitions from one stationary state to another. The energy of the radiation, $E = h\nu$, is equal to the difference in the energies of the initial and final stationary states.

The first postulate is clearly based on classical theory; however the second and third postulates marked a radical departure from classical concepts. Applying these postulates to the hydrogen atom, Bohr's model predicted the total energy of an electron in a stationary state



The spectrum of atomic hydrogen.

Figure 1: Energy level diagram of atomic hydrogen showing the transitions giving rise to the Lyman (UV), Balmer (visible) and Paschen (IR) spectra.

with orbital angular momentum $L = n\hbar$ to be

$$E_n = -\frac{mZ^2e^4}{(4\pi\epsilon_0)^22\hbar^2} \frac{1}{n^2} \quad (4)$$

where m is the mass of electron, Z is the number of protons in the nucleus ($Z = 1$ for hydrogen) and e is the charge of the electron [3]. A transition from a state of higher energy to one of lower energy should result in the emission of radiation with energy

$$E_i - E_f = \frac{hc}{\lambda} = \frac{mZ^2e^4}{(4\pi\epsilon_0)^22\hbar^2} \left[\frac{1}{n_f^2} - \frac{1}{n_i^2} \right] \quad (5)$$

where $n_i\hbar$ and $n_f\hbar$ are the electron orbital angular momenta of the initial and final states, respectively. Comparing this formula with the Rydberg formula we find that R_H should be

$$R_H = \frac{me^4}{8\epsilon_0^2h^3c}.$$

That Bohr's theory resulted in an expression for the Rydberg constant in terms of fundamental constants was a great triumph as it allowed for evaluation of the above expression and comparison to the value derived from spectroscopic data. Then current values for m , e , h and c indicated good agreement between R_H calculated from Bohr's theory and experimentally derived values.

But doubters of Bohr's theory remained, with skepticism on the continent being particularly strong. His brother Harald wrote Bohr in the fall of 1913 from Göttingen, Germany, saying that the physicists there considered Bohr's model to be too "bold" and too "fantastic". Rutherford himself was skeptical, asking Bohr, "How does the electron decide what frequency it is going to vibrate (radiate) at when it passes from one stationary state to another? It seems to me that you would have to assume the electron knows beforehand where it is going to stop."

And skeptics were buttressed by new experimental results. Measurements of the spectral lines of singly ionized helium (one electron orbiting around a nucleus with two protons) showed that the ratio of the wavelengths of corresponding helium and hydrogen lines (same n_i and n_f) was not 1:4 as predicted by Bohr's formula, but rather 1:4.0016. (The ratio 1:4 results from increasing Z from one to two in the above expressions for the electron energy.) Bohr quickly revised his postulates, now requiring that the *total* angular momentum, the combined angular momentum of both the electron *and* the nucleus, be quantized in units of \hbar . The result of this requirement is that in the expression for the electron energy, the electron mass m must be replaced by the reduced mass μ ,

$$\mu = mM/(M + m) \quad (6)$$

where M is the mass of the nucleus. (See the appendix for a derivation of this result.) The expression for the radiation energy of hydrogen-like ions (i.e., one electron orbiting Z protons) is now

$$E_i - E_f = \frac{hc}{\lambda} = \frac{\mu_x Z^2 e^4}{(4\pi\epsilon_0)^22\hbar^2} \left[\frac{1}{n_f^2} - \frac{1}{n_i^2} \right] \quad (7)$$

where μ_X is the reduced mass of atom X . According to Bohr's revised theory, the wavelength ratios between corresponding hydrogen and helium lines should be $4\mu_{\text{He}}/\mu_{\text{H}}$. It turns out that

$$\frac{\mu_{\text{He}}}{\mu_{\text{H}}} = 1.0004 ,$$

(you may wish to verify this) resulting in complete agreement between theory and observation. When Einstein learned of this latest success of the Bohr theory, he responded: "This is an *enormous achievement*. The theory of Bohr must then be right."

The inclusion of the nuclear mass M into the equation for the spectral energies indicates that different isotopes of the same element should show different spectra, since these atoms would have different reduced mass. The existence of the isotope of hydrogen, deuterium, whose nucleus contains one neutron and one proton, was discovered by Harold Urey and his co-workers around 1930 using spectroscopic methods after they successfully produced samples of deuterium-enriched hydrogen by a distillation process [4]. Harold Urey was awarded the Nobel Prize in Chemistry in 1934, "for his discovery of heavy hydrogen."

2 The experiment

Experimental Goal: measure the hydrogen-deuterium nuclear mass ratio.

In this experiment you will measure the wavelengths of both the hydrogen and deuterium spectral lines for four transitions in the Balmer series. From a measurement of the wavelength difference for a given transition, you will derive the ratio of the masses of the hydrogen and deuterium atoms. The four results can then be combined into a final result for the mass ratio.

The spectral lines are produced by a gas discharge lamp. In our setup, the lamp contains hydrogen enriched with deuterium so that both spectra are produced simultaneously. Enrichment of the hydrogen is necessary as the natural abundance of deuterium is about .015%.

From the Rydberg formula corrected for reduced mass, Eq. (7), we see that the wavelength of light emitted from a particular transition is inversely proportional to the reduced mass:

$$1/\lambda_X \propto \mu_X . \tag{8}$$

Because of this proportionality, we see that the nuclear masses of hydrogen and deuterium, M_{H} and M_{D} , are related to the different wavelengths of light produced by each isotope:

$$\frac{\Delta\lambda_{\text{HD}}}{\lambda_{\text{H}}} = \frac{\lambda_{\text{H}} - \lambda_{\text{D}}}{\lambda_{\text{H}}} = \frac{1/\mu_{\text{H}} - 1/\mu_{\text{D}}}{1/\mu_{\text{H}}} = \frac{1 - M_{\text{H}}/M_{\text{D}}}{1 + M_{\text{H}}/m} . \tag{9}$$

The mass M_{H} is, of course, just the mass of the proton M_p , and the ratio of the proton and electron masses is well known, $M_p/m = 1836.15$. Combining this with the results of your measurements, the ratio of the masses of the two nuclei, $M_{\text{H}}/M_{\text{D}}$ can easily be derived and compared to established values:

$$\frac{M_{\text{H}}}{M_{\text{D}}} = \frac{1.007276}{2.013553} = 0.500248 .$$

Extension Ideas

1. Try to measure the H_ϵ peak and compare to your other measurements. Investigate the λ dependence of your measured ratio, if any.
2. Derive the shape of the peak based on the optics of the monochromator.
3. Write a LabVIEW program to digitally record the PMT current while simultaneously recording counts of the number of stepper motor steps. Use this to record the data.
4. Use the setup to measure the emission spectrum of a light source of your choice (some bulb, a mobile phone LED, etc).

3 Apparatus and Procedure

Before describing the apparatus and measurement process, it is instructive to observe the difference between continuous and discrete light sources. Turn off the bright fluorescent tube lights in the experiment area and turn on the smaller overhead lights in the cylindrical shades. Take one of the slide-mounted diffraction gratings and look at the two overhead lights in the cylinders near the experiment and near the desk area. One of the bulbs is incandescent and the other fluorescent. The fluorescent bulb emits light at discrete wavelengths in the mercury spectrum, and the incandescent bulb emits light over a continuum of wavelengths. The colored images overlap, so make sure you identify which image goes with which bulb. Describe the images you see from each bulb, and justify your claim as to which one is the fluorescent bulb.

3.1 Apparatus

A diagram of the apparatus is shown in Fig. 2. Light from a discharge tube containing both hydrogen and deuterium is focused by a lens onto the entrance aperture (slit) of the monochromator. (A monochromator is just a spectrometer that detects one wavelength at a time.) The dispersive element, i.e., the element which separates light according to its component wavelengths, inside the monochromator is a diffraction grating—a fancier version of the hand held grating you used to look at the overhead lights. The angle of the grating and mirrors inside the monochromator can be varied with the wavelength-adjust knob to select the wavelength of the light passing through the exit slit and on to the detector. The detector is a photomultiplier tube (PMT) located inside the housing attached to the exit slit port. The readout dial on the front of the monochromator indicates the wavelength of the detected light to the nearest angstrom.

The output of the PMT is a current, typically a fraction of a microampere at maximum detected light intensity in this experiment. The PDA-700 amplifier converts this current to a voltage which is recorded on an X-Y recorder or digital scope. To record the output light intensity over a wavelength interval, a stepper-motor + reduction-gear drive is attached to the wavelength adjust shaft. Here are some numbers to help you get a sense of the scan rate:

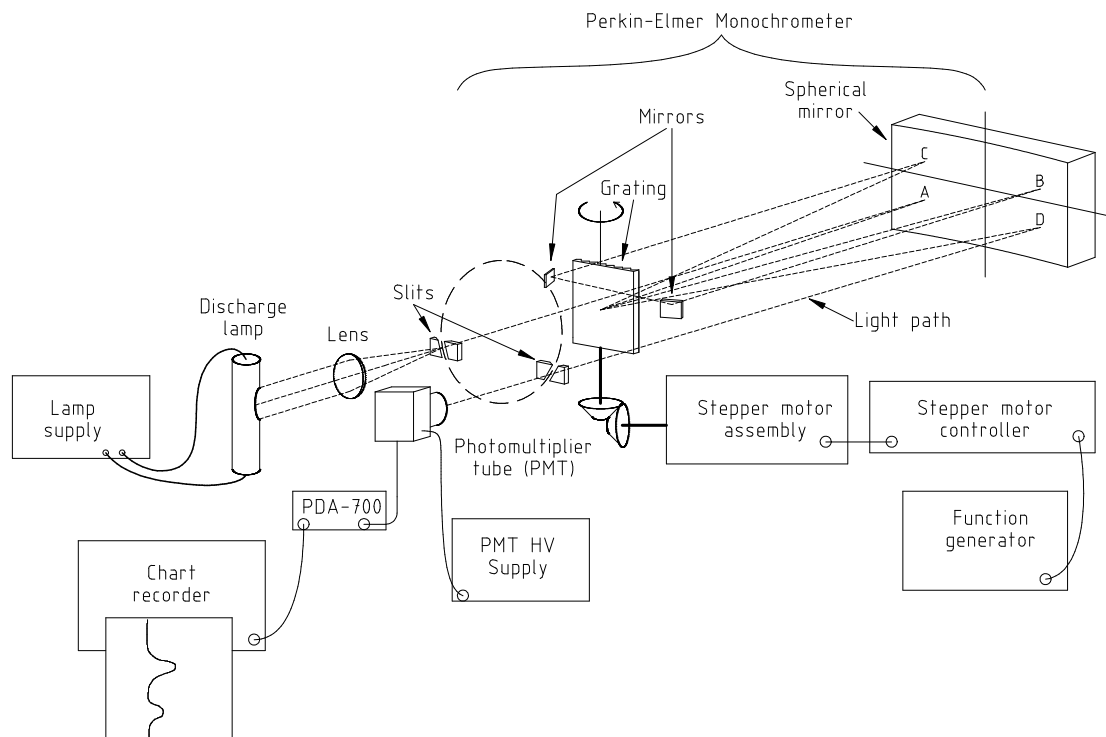


Figure 2: Apparatus used to measure the spectral lines of the hydrogen-deuterium lamp.

Stepper motor: 200 steps per revolution of output shaft
 Reduction gear ratio: 1:36
 wavelength adjust shaft: 20 Å per revolution.

You do want to record data slowly and smoothly, but you don't want it to take all day. You also want to maximize your use of the available plotter or screen space. The following exercise will help you develop a good first set of scanning parameters, you may adjust them from there at your discretion.

Exercise 1 As an initial estimate of the experimental parameters, calculate the difference in wavelengths of the hydrogen and deuterium α lines, assuming that the mass ratio is 1:2. Then also calculate the difference in wavelength of the sodium D lines, listed in section 3.2. What would be the expected ratio of peak separations, $\Delta\lambda_{HD}/\Delta\lambda_{Na}$?

Now assume you have a scope or X-Y recorder that runs at 4 seconds per division and you want to place the D lines 8 divisions apart. What should the stepper-motor control frequency be? How many divisions would this rate give for the α lines?

Feel free to speed up or slow down the stepper motor rate and scan speed from these starting values as you see fit. However, once you are comfortable with your scanning rate, it is recommended to use the same set of values for all of your measurements.

The monochromator does not detect light at just a single wavelength but rather detects light over a small spread of wavelengths centered about the wavelength indicated on the readout

dial. Here we face the common trade-off between signal strength and resolution. The width of the entrance and exit slits is variable, and is set (for both slits simultaneously) by the slit width control. Increasing the slit width allows more light to come through, but degrades the resolution of the monochromator. For the purposes of this experiment, a slit width of about 50 microns allows for a good signal level and more than adequate resolution; the slit readout should show “0 0 50”.

3.2 Calibration standards

As mentioned above, the readout dial indicates the absolute wavelength to the nearest angstrom. We are working with wavelength *differences* on the order of 1 Å, and will want to measure the $\lambda_H - \lambda_D$ interval to fractions of an angstrom, which is not possible using the wavelength readout.

To calibrate the monochromator output, the wavelength difference between the two lines of the yellow sodium doublet, the 3^2S-3^2P transition, is used as a standard. The wavelengths of these two lines are

$$\begin{aligned} D_1: & 5895.92 \text{ \AA} \\ D_2: & 5889.95 \text{ \AA} \end{aligned}$$

The calibration procedure will be described in detail below.

For reference in the next section and for use in data analysis, we also state the wavelengths of the hydrogen lines under investigation:

$$\begin{aligned} H_\alpha: & 6562.852 \text{ \AA} \\ H_\beta: & 4861.33 \text{ \AA} \\ H_\gamma: & 4340.47 \text{ \AA} \\ H_\delta: & 4101.74 \text{ \AA} \end{aligned}$$

It is possible, with some effort, to measure higher energy lines in this series as well.

Exercise 2 *Calculate the wavelengths of the next three higher-energy lines in the Balmer series from Eq. (3).*

3.3 Procedure

Turn on the power supply for the sodium discharge lamp. Press the white button on the power supply if the lamp does not start. It will take a little while for the lamp to reach full intensity, but you can begin aligning the optics and looking for a signal before it is fully warmed up.

The wavelength interval of the sodium lines is used to calibrate the recording apparatus, and the peak separation is much greater for the sodium doublet than for the hydrogen-deuterium

splitting, so it is best to run the sodium scans first to establish the scan settings. (If you are careful, you can get all of your data on one sheet of paper when using the X-Y recorder.)

Turn on the power to the SRS Model PS 325 high voltage power supply and the PDA-700 amplifier. The PDA-700 should be on the “.xxxx” microamp range. This corresponds to a maximum current of $2.000 \mu\text{A}$.

If the stepper motor drive coupling is still attached to the wavelength adjust shaft, remove it. A hex-socket (Allen) wrench is available for attaching and removing the coupling from the wavelength-adjust shaft. Turn the knob smoothly to set the wavelength to approximately 5890 \AA . (Please be gentle: small parts inside the monochromator are easily damaged by rough treatment.)

Remove the plastic dust cover from the lens. Check that the distance from the sodium lamp to the lens is about 240 mm and that the distance from the lens to the entrance slit is also about 240 mm (this corresponds to a carriage position of 725 mm on the optical track). The focal length of the lens is 120 mm, so these distances will result in the formation of an image of the lamp with magnification 1 at the entrance slit. Adjust the lamp position to optimize the focus of the image on the entrance slit.

Exercise 3 *Prove the above claim about the image of the lamp by making a ray diagram.*

Check that the high voltage setting displays “1000” volts. This is the number that should be displayed at the center of the high voltage power supply. Turn on the high voltage with the switch at the lower left of the front panel. The output voltage should read -1000 volts (polarity is negative) within a volt or two. Slowly scan *by hand* through the D_2 line at 5890 \AA while watching the PDA-700 reading; you should see an increase in the PMT output current as you scan through the line. Keep turning the knob and scan through the second D-line, D_1 at about 5896 \AA to verify that you are seeing both peaks. Scan back through the lines and set the wavelength on D_2 to give maximum output current, typically about 0.1 microamp for a slit width of 50 microns. (Note: the exact value is unimportant, and your value may be very different depending on how warmed up your lamp is and how well aligned your setup is.) Then fine-tune the lens position by alternately moving it transversely with the yellow screw and longitudinally along the track so as to maximize the output current, and also fine-tune the focus by moving the lamp carriage along the track, again looking for maximum output. If you are having trouble getting any output, consult with the TA, Professor or Lab Manager.

Once you are getting a signal from the sodium lamp, turn on the power to the chart recorder or oscilloscope and set the sweep speed to about 4–5 seconds per divisions, as you estimated above.

If using the X-Y recorder:

- **do not put a pen in the recorder carriage yet.**
- As a starting point, set the recorder sensitivity to its least sensitive setting, e.g., 50 mV/inch. Check that the RC filter switch is ON (filter is in small metal box),

and observe the displacement of the pen carriage on the recorder as you manually scan through the D lines.

- If you see too much displacement of the pen carriage (or not enough), change the range of the PDA-700 and Y-axis sensitivity on the recorder appropriately. Note that the ranges on the PDA-700 change by factors of ten, but the ranges on the X-Y recorder allow for finer increments.
- You may also vary the signal intensity by changing the slit width, but avoid opening the slit more than 70 microns, or else you will lose resolution. The pen carriage should displace between 2 and 3 inches (2-3 large squares on the graph paper) as you scan through the lines.

If using the scope:

- Turn the horizontal sweep down to 2 to 4 s/Div and select a vertical sensitivity of about 100 mV/Div. Set the trigger to “Automatic/Roll”. (This makes the scope act like a strip-chart recorder.)
- Adjust the trace so it is in the middle of the screen. Observe the trace as you slowly scan (by hand) through the D-line wavelengths. Adjust the vertical sensitivity to display clear peaks, so that they take up most of the vertical space.
- You may want to “invert” the input so the peaks point up. This can be done with the channel controls.

Make sure that the switch box between the function generator and the stepper motor controller is *off*, and turn on the power to the digital function generator. Set the function generator frequency to 20 Hz by using the keypad on the front panel: push **FREQ/PER**, then **2**, **0**, then the units key **Hz Vpp**. Then turn on the switch box briefly to verify that the motor shaft turns. You may safely run the function generator up to 150 Hz for small adjustments, but for data taking, the frequency should be set at a value below 100 Hz, depending on sweep speed.

Set the wavelength 2–3 angstroms less than the D_2 wavelength. Remove the knob from the wavelength adjust shaft and connect the stepper motor drive coupling to the shaft. Select the *increasing* wavelength direction on the stepper motor controller, and turn on the power to the controller.

If using the X-Y recorder, run a “dry” scan (NO PEN) to check that your choice of stepper motor speed and chart scan speed are optimum. Start the stepper motor by flipping the switch on the box between the generator and the stepper-motor controller on, then immediately start the scan by flipping the **Time Base** switch on the X-Y recorder from **RESET** to **SWEEP**. You should see the pen carriage drop and start to move across the cart. Watch to see where the sodium peaks will be recorded. After you have scanned through the lines, **RESET** the time base and turn off the pulse train with the switch box. *Do not turn off the stepper motor controller power.* Your goal should be to have the peaks spaced on either

side of the chart page. A separation of about 10 inches (10 large divisions) is optimum. Adjust either the stepper frequency or the chart speed, and run additional dry scans until it looks good. **Then *and only then* pop a pen in the carriage and record the sodium calibration scan.**

If using the scope, use the START/STOP button to start the scan after you flip the stepper motor switch on, then STOP the scan in time to show both D lines on the screen.

***IMPORTANT:* Once you decide on a stepper-motor frequency and chart speed, you must stick with it for all of the measurements, otherwise your calibration will be ruined. Also, it is a good idea to scan in the same direction of “increasing wavelength” for all runs.**

If using the scope, save the data to a USB stick for later analysis. It is best to save the waveform as “Reduced” resolution and “.CSV” to be able to analyze it with a computer program. See the user manual for details.

While you are taking your good calibration scan, turn on the H-D discharge lamp and the cooling fan (separate power supply). The discharge tube runs very hot, and cooling it with the fan will help extend the lifetime of this expensive (\$500) tube.

After the sodium scan is finished, turn the sodium lamp off, and carefully loosen the carriage screw and lift the carriage and lamp off the track. Place it on the track behind the H-D lamp, and then slide the carriage for the H-D lamp into the same position as the sodium lamp was.

Remove the stepper motor drive. Dial in the approximate wavelength value for the H_{α} line (see table in the calibration standards section). As you did before, scan slowly through the H_{α} and D_{α} lines by hand. Adjust the lens setting and image focus by maximizing the signal on the PDA-700 and chart recorder.

The image of the H-D lamp is much narrower than that of the sodium lamp, so alignment is critical here. Check that the image of the lamp falls on the curved entrance slit to the monochromator (may be necessary to dim lights to see this). To see the slit better, you may want to open it up to 100 microns or more. Note that the lamp needs to be slightly tilted to maximize the coverage of the slit with the image of the lamp, as the slits are off-center of a circle at the focal plane of the monochromator (see Fig. 2) If the image does not fall on the slit, it may be necessary to move the lens back and forth across the light path with the small brass adjust screw marked with yellow tape at the base of the lens holder. If the beam is far out of alignment, it may be necessary to move the entire base on which the lamp and lens are mounted. If this seems to be necessary, please ask for help from the TA, Professor or Lab Manager. After checking the image alignment, reduce the slit width back to approximately 50 microns.

The sodium lamp is considerably more intense than the H-D lamp so it will be necessary to increase the sensitivity of the PDA-700 and/or y-axis sensitivity. *Do not change the x-axis settings on the chart recorder or function generator!* If you do, you will have to repeat the Na calibration.

If using the X-Y recorder, adjust the Y-axis zero offset on the X-Y recorder so that the H-D

scan is vertically separated from the sodium calibration scan. Run a scan (dry first, to set the gain of the PDA-700 and Y-axis input) through both the H_α and D_α lines.

The result of the scan should be a trace showing a pair of peaks of unequal height (fractions of H and D in tube are not equal), with each peak having a symmetric or nearly symmetric shape. If you are not satisfied with the results of the scan, you can repeat it: switch to “decreasing λ ” on the controller, dial the frequency up to 100–140 Hz, run the wavelength back down through the lines, and then repeat the above procedure. *Don't forget to reset the frequency on the generator to the correct value.*

Caution: when you reverse the scan direction, you need to allow the “backlash” in the gears to be taken up before recording your lines. If you fail to do this, you may see significant distortions in your trace: a peak will have a large flat part in the middle of it.

After successfully recording the H_α and D_α lines, remove the stepper motor drive coupling from the shaft. Adjust the wavelength to near the H_β line and repeat the checkout and scan process as above. The signal strength of the H_β and D_β lines is different from that of the α lines. This is due to both a difference in light intensity at these wavelengths, and in sensitivity of the photomultiplier tube. (Study the sensitivity chart for the tube in the book which describes the apparatus; does it make sense?) It may be necessary to switch the PDA-700 to a different range to achieve a suitable displacement on the recorder.

After successfully recording the β lines, proceed to record the γ and δ lines. As the line strength decreases, you may need to adjust the Y-axis input scale or the PDA-700 gain to obtain peaks of reasonable height. You will want to use much of the available vertical space on the page to minimize peak position uncertainty.

After recording the four pairs of lines to your satisfaction, turn off the H-D lamp. You should have at least 5 scans: the sodium lines and the four pairs of H-D lines. (You could also try to get the ϵ lines; these will be noisy.) Make sure that you note which scan is which pair of lines and which direction shows increasing wavelength. It is OK if the scans on a paper chart overlap somewhat. The important thing is to be able to see each peak clearly.

Make a copy of the data for each partner. Each person should carry out the data analysis separately.

After finishing collecting all of your data, please turn off all lamps and electronics, put the plastic cover over the lens, and remove the pen and put the cap back on it.

3.4 Data reduction and analysis

To find the center of a symmetric or nearly symmetric spectral line (peak) on a paper chart:

1. Draw a series of horizontal lines across the width of the spectral line trace. Find the midpoints of each of these lines.
2. Draw the (nearly vertical) line defined by the midpoints.

3. The intersection of this line and the top of the spectral line trace represents the position of the spectral line, and should be very close to the maximum of the line.
4. To get a measure of the uncertainty in locating the position of the spectral line, draw a vertical line that catches most of the midpoints of the horizontal lines you drew *near the top of the spectral line*. The difference between where this line intersects the spectral line and where the line you drew in step 2 intersects the spectral line can be used as the uncertainty in your determination of spectral line position.

The uncertainty in determining the position of the spectral lines is only one possible source of error. Other possible sources are speed variations in the drive trains of the various mechanical systems (stepper-motor + reduction-gear, monochromator, strip-chart recorder). These sources may dominate the uncertainty in the position measurements but are not readily quantified.

To calculate the peak position in a data file:

Load the data file into your favorite computer program (Excel, Python, Matlab, etc.). Then you have a few options:

1. Carry out an analysis similar to the above: make a plot and use the plotting viewer options to determine the peak position or trace out bisecting lines as described.
2. Make a curve fit to each peak, and use the fit parameter for center of the peak. This works best with symmetric peaks, because most peak functions are symmetric about their center, such as a Gaussian or Lorentzian.
3. Calculate a “centroid” which is a weighted average of the counts per channel. The centroid would be given by the formula

$$X_{\text{centroid}} = \frac{\sum x_i n_i}{\sum n_i}, \quad (10)$$

where the index i runs over the channels included in the peak. Note: a “channel” is a time value in scope file.

After you have found the peak positions, and determined the statistical uncertainty in each, use your Na D lines to make a calibration conversion: change the horizontal separation from inches or time into ångstroms of wavelength difference.

Then make a plot. Equation (9) suggests a relationship that should be constant. How can you plot your data in a way that gives that constant from a line fit?

Some things to think about and discuss:

- How consistently do the data follow the predicted relationship? Are there obvious outliers?
- How should you deal with the fact that your calibration (the Na Lines) is also a measurement with uncertainty?
- What would happen if the calibration lines had a mistake (say, by being too far apart)?

Appendix – Reduced mass

Consider a classical system of two particles of mass M and m interacting via central forces (i.e., Coulomb or gravity). Let the position vector between the two particles be \vec{r} . When no external forces act on the system, the center of mass \vec{R} will be at rest with respect to some inertial reference frame S . The center of mass is defined as

$$\vec{R} = \frac{M\vec{X} + m\vec{x}}{M + m}, \quad (11)$$

where \vec{X} and \vec{x} locate the particles of mass M and m with respect to the origin of S , and $\vec{x} = \vec{X} + \vec{r}$. Since the center of mass is at rest with respect to S , a physically equivalent reference frame S' has its origin at the center of mass itself; in S' , the center of mass of the system

$$\vec{R}' = \frac{M\vec{X}' + m\vec{x}'}{M + m} = 0. \quad (12)$$

Hence $M\vec{X}' = -m\vec{x}'$. It is still true that $\vec{r} = \vec{x}' - \vec{X}'$, since \vec{x} and \vec{X} are related to \vec{x}' and \vec{X}' by a simple translation. These two equations can be solved to yield

$$\vec{X}' = -\frac{m}{m + M}\vec{r}, \quad (13)$$

$$\vec{x}' = \frac{M}{m + M}\vec{r}. \quad (14)$$

In S' the energy of the two particle system is given by

$$E = \frac{1}{2}m\dot{x}'^2 + \frac{1}{2}M\dot{X}'^2 + V(r), \quad (15)$$

where the “dot” notation indicates a derivative with respect to time and $V(r)$ is the potential energy between the two particles. Upon taking derivatives of Eqs. (13) and (14) and substituting the result into the energy equation one obtains

$$E = \frac{1}{2} \left(\frac{mM}{m + M} \right) \dot{r}^2 + V(r). \quad (16)$$

Clearly, the expression in parenthesis in the above equation is the reduced mass μ . An advantage of expressing the energy in terms of μ is that one transforms the problem of two particles of masses m and M into a problem of one particle of mass μ . A similar calculation shows that one can write the angular momentum about the center of mass in a similar way:

$$\vec{L}' = \left(\vec{x}' \times m\dot{\vec{x}}' \right) + \left(\vec{X}' \times M\dot{\vec{X}}' \right) = \vec{r} \times \mu\dot{\vec{r}}. \quad (17)$$

In the Bohr model and in the subsequent Schrödinger theory, these classical results translate directly into their quantum equivalents.

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Prepared by J. Stoltenberg, D. Pengra, and J. A. Detwiler
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