CONCAVE DIFFRACTION GRATING SPECTROGRAPH

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Diffraction gratings are widely used for high resolution spectral studies. The grating available in the lab is a holographically-produced, concave grating of 600 lines/mm and radius R = 1075 mm. It is placed in a *Rowland* mounting. In such a mount, the grating is constrained to be on a circle of diameter equal to the radius of curvature of the grating (the Rowland circle) on which the entrance slit (the slit through which light is incident on the grating) is also located. If the entrance slit and the grating are on the circle, the slit image will be in focus on the same circle. Concave gratings are often used in the ultraviolet portion of the spectrum where their focusing properties eliminate the need for UV-transmitting lenses. In this experiment, strong lines from the visible part of the spectrum of the elements mercury and cadmium are used to calibrate the spectrograph. The spectrograph is then used to measure the wavelengths of the lines in the visible spectrum of hydrogen (Balmer series) from which a value of the Rydberg constant for hydrogen can be obtained. The lamp used also contains the isotope of hydogen, deuterium, so the spectrum of deuterium can be obtained as well; for this part, we use a CCD array detector which allows a more accurate measurement to be made of the separation betwen similar lines of the two isotopes, and also allows the experimenter to make a quantitative measurement of the resolving power of the spectrograph.

REFERENCES

- 1. Hecht, Optics (4th ed.), pp. 476–481 (general properties).
- 2. Thorne, Anne P., *Spectrophysics*, 2nd ed., Chap. 6, pp. 144–170 (types of diffraction gratings and mounts, focusing property of concave gratings).
- 3. Davis, Sumner P., *Diffraction Grating Spectrographs* (practical information on the alignment and auxiliary optics for diffraction gratings).
- 4. Tipler, Modern Physics, pp. 144-151 (reduced mass correction).

APPARATUS

The apparatus is pictured in the Fig. 1 with the Rowland Circle shown as a dashed line. The radius S of the grating is 1075 mm (\pm 2 mm), the width of the grating is 25 mm, and the grating constant is 600 lines/mm (error unknown). The grating is blazed to give maximum intensity in the first order. The grating mounting has been carefully adjusted and should not be disturbed. A movable carriage holds a viewing microscope (and CCD array), which can be focused on the slit image. A set of cross-hairs in the microscope allows for precise location of the spectral line under observation.

The distance x from the slit to the slit image can be measured on a wooden meter stick + associated vernier to a precision of about 0.1 mm. For a Rowland mounting with the angle of reflection (i.e., the angle between the grating normal and the axis of the detector) $\theta_r = 0^\circ$, the grating formula becomes $d\sin\theta = d\frac{x}{S} = m\lambda$, where d is the line-to-line separation on the grating, θ is the angle of incidence of the light on the grating, x is the slit to image distance, S is the grating-to-image distance, m is the order of the spectrum (m = 1, 2, etc.), and λ is the wavelength of the spectral line.

CALIBRATION OF THE SPECTROGRAPH

The wavelength of a spectral line can be determined from a measurement of x and use of the grating equation, but this method has significant limitations. The grating equation is only as precise as the values of d and S, and it depends on positioning the entrance slit exactly above the zero of the meter stick scale, a result difficult to achieve in practice.



Figure 1: The concave grating spectrograph. The carriages with the grating and detector (microscope or CCD array) move perpendicular to each other along tracks, so that the distance between them S stays constant, even though the angle θ changes. The image of the slit is focused by the grating, which is slightly concave, on the detector. Because S stays constant, the spectrograph stays in focus over the range of angles θ . The grating, detector and entrance slit lie on an imaginary circle of fixed diameter called the "Rowland circle".

To avoid these limitations, the spectrograph is calibrated by measuring x for a number of spectral lines the wavelengths of which are known precisely. An empirical relation is then established from which the wavelength of an unknown line as a function of x can be obtained more precisely than it can from the grating equation. The wavelengths for the spectral lines of mercury and cadmium that may be used to calibrate the spectrograph are listed below:

$oldsymbol{\lambda} \ (nm)$	Element	Color
643.85	Cd	deep red
579.07, 576.96	Hg	saffron yellow doublet
546.08	Hg	bright green-yellow
508.58	Cd	medium green
479.99	Cd	light blue
467.81	Cd	dark blue
435.83	Hg	bright violet-blue
404.66	Hg	dark violet

You do not need to measure *all* of these lines, but pick at least 5 widely-spaced lines to give a good lever-arm to your calibration graph. The calibration obtained from the measurements of these lines is to be used for all subsequent wavelength determinations.

PROCEDURE

Position the large carriage supporting the mercury/cadmium lamp assembly so that the small piece of white tape on the left edge of the carriage is above the 570 mm mark on the metal rail, and clamp the carriage securely to the rail with the silver clamping knob. If the hydrogen lamp is in the way, slide it back and clamp it to the rail before positioning the mercury/cadmium lamp. The hydrogen lamp assembly is delicate – please handle it carefully.

Position the smaller carriage directly beneath the mercury/cadmium lamp housing so that the small piece of yellow tape on the near edge of the carriage is above the 179 mm mark on the small metal rail, and clamp this carriage in position. Turn on the power supply for the mercury/cadmium lamp.

Check that the lens is positioned so that the small piece of white tape on the left edge of its carriage is above the 835 mm mark on the metal rail. With the lamp and lens in these positions, the lamp image is focused on the slit with 1:1 magnification (to see the image hold a white card next to the slit).

Adjust the slit width (using the small lever marked with red tape) to approximately 0.2 mm. The width scale is marked on the slit housing. For $x \approx 35$ cm, the green line should be clearly visible.

Before looking through the microscope, make sure that its base is firmly seated on the platform. The spring-loaded screws on the adjacent rails insure that the microscope does not shift on the platform.

If the observed line is not in focus, adjust the focus with the large focusing knob on the right side of the microscope assembly. Maximize the brightness of the line by adjusting the transverse position of the lens using the knob marked with yellow tape. Also move the small carriage beneath the mercury/cadmium lamp housing back and forth to maximize the brightness of the line and again clamp the carriage in position. The slit width can now be decreased to allow for more precise location of the center of the line.

1. Make five or more independent measurements of the position of the green line. Move the carriage with the microscope well away from the line, then reset it so the cross-hairs are centered on the line. From these measurements determine the precision with which you can locate a line. Each student in the group should make this set of measurements.

- 2. Compute the positions of the calibration lines in the first order (i.e., m = 1) from the grating equation. These computed positions need not be especially precise, but they will help in identifying the correct calibration lines.
- 3. Carefully record the positions of the calibration lines in first order. Plot each point carefully on the graph paper provided after you measure a line. Plot x (in cm) on the vertical and λ (in nm) on the horizontal. Choose the scales for x and λ so that the data nearly fill the page. Visually verify that a spectral line of the right color exists at that value of x. Use a straight edge to draw a line through the data points. If you have correctly identified each line and measured its position carefully, the plotted points will lie on a straight line as closely as you can plot them. If not, remeasure the lines that are off.

When you have finished recording the calibration lines, look at several of them (green & yellow) in the second order. Notice how much dimmer these lines are than their first order counterparts. This is the result of the grating being blazed so that maximum intensity is reflected in the first order. After looking at the second order lines, turn off the mercury/cadmium lamp.

Later, when you write your report, also do the following:

- 4. Use EXCEL (or another curve fitting program such as KaleidaGraph or Mathematica) to fit a leastsquares straight line to the calibration data. Obtain the slope s, the standard deviation in the slope σ_s , the intercept x_0 , the standard deviation in the intercept σ_{x_0} , and the standard deviation in an individual measurement of x, σ_x . Comment on the value of the intercept you obtained. Is it reasonable? Why might the intercept be nonzero?
- 5. From the slope and the radius R calculate the lines per mm in the grating and the standard deviation in this number. Compare this to the nominal value of 600 mm⁻¹, and comment on how any difference might arise.

BALMER SERIES AND THE RYDBERG CONSTANTS

The visible spectrum of hydrogen consists of a series of lines that result from transitions terminating on the energy level with principal quantum number n = 2 and originating from higher-lying energy states for which n = 3, 4, 5, etc. The series of lines is named after Johann Balmer who, in 1855, published a numerical relation accurately describing their wavelengths. Starting with the longest (red) wavelength, the lines are labeled H_{α} , H_{β} , H_{γ} , etc. The Balmer series wavelengths for hydrogen are described by the Balmer formula

$$\frac{1}{\lambda} = R_H \left(\frac{1}{2^2} - \frac{1}{n^2} \right), \quad n = 3, 4, 5, \dots$$
(1)

The constant is called the Rydberg constant for hydrogen. A similar expression applies for deuterium, but the Rydberg constant for deuterium, R_D , is slightly larger than that for hydrogen. The difference arises from the effect of the greater mass of the deuterium nucleus. A larger nuclear mass results in a larger value for μ_e , the electron reduced mass. The reduced mass of the electron arises from the fact that the two-body problem of an electron and a nucleus can be recast into an effective one-body problem involving the reduced mass of an electron only. The formula for the reduced mass is

$$\mu_e = \frac{m_e}{1 + m_e/M} , \qquad (2)$$

where m_e is the mass of an electron and M is the mass of the nucleus. See the reference by Tipler and the material on the class website for the derivation of this formula. The Bohr (and Schrödinger) theories of the hydrogen spectra give a formula for the Rydberg constant:

$$R = \frac{\mu_e e^4}{8\varepsilon_0^2 h^3 c} , \qquad (3)$$

where e is the charge of an electron, ε_0 is the permittivity of free space, h is Planck's constant, and c is the speed of light. The Rydberg constant for an infinitely heavy nucleus R_{∞} , which is the same as Eq. (3) with $\mu_e = m_e$, is one of the best known constants in physics, $R_{\infty} = 10\ 973\ 731.568\ 549(83)\ m^{-1}$ [CODATA recommended values of the fundamental constants 1998]. Note that this is larger (by a small amount) than the value of the Rydberg constant for hydrogen.

In the next exercise, you will take data in order to determine R_H .

Move the large carriage supporting the mercury/cadmium lamp toward the lens carriage and clamp it a cm or so from the lens carriage. Move the small carriage and mercury/cadmium lamp housing toward the wall, out of the light path, and clamp it in position. Move the carriage supporting the hydrogen/deuterium lamp assembly forward until the small piece of white tape on the left edge of the carriage is above the 515 mm mark on the metal rail, and clamp the carriage with the silver clamping knob. With the lamp and lens in these positions, the lamp image is focused on the slit with 1:1 magnification (to see the image hold a white card next to the slit).

You may need to make some adjustments of the lens in order to optimize the position and the focus of the image of the hydrogen/deuterium lamp.

The hydrogen/deuterium lamp gets very hot after being on for a period of time, and as its temperature increases, the intensity of the emitted light decreases. To help keep the lamp cooler and the intensity higher, a small fan is positioned at the base of the black tubing, which protects the lamp. **Turn on the power supply for the fan**, and then turn on the power supply for the lamp.

For $x \approx 42$ cm, the red (Balmer α) line should be visible. If the line is not uniformly bright, it may be necessary to adjust the transverse position of the lens and/or the longitudinal position of the hydro-gen/deuterium lamp.

The hydrogen/deuterium lamp draws 20 milliamperes (mA) of current at 5000 volts potential difference across the tube. 20 mA can be a lethal current so it is important to handle the hydrogen/deuterium lamp assembly carefully and touch it only at grounded surfaces.

To change the position of the lamp, slightly loosen the knob marked with blue tape, and rotate the lamp holder by grasping the short horizontal rod marked with orange tape. **Do not touch the black tubing protecting the lamp or the white caps holding the tube in place.** When you have achieved maximum brightness by adjusting the lens and lamp positions, clamp the lamp in position by tightening the knob marked with blue tape.

Once you have found the Balmer α line, reduce the slit width in order to see the separation between the hydrogen and deuterium lines. Which line corresponds with which element? Hint: study Eqs. (1) through (2). When you have figured out which lines are the hydrogen lines, focus the cross-hairs of the microscope on those lines.

Measure the position of the three visible Balmer lines, $(\alpha, \beta \text{ and } \gamma)$ for hydrogen in first order. (The other lines in the Balmer series fall outside the visible range.) Note: there are a number of lines in the spectrum of the lamp that come from impurities rather than from hydrogen or deuterium. These tend to be notably dimmer than the hydrogen lines, but you can use your calibration from the mercury/cadmium lamp to make sure you are observing the correct lines.

6. Determine the value of R_H from measurements of the Balmer lines of hydrogen. Extract the Rydberg constant for hydrogen R_H from the parameters of a straight-line fit (done with EXCEL or other program) to an appropriately chosen plot of your data. Hint: The Balmer formula can be reduced to a linear equation by substituting the proper functions of λ and n. See Eq. (1). Calculate an uncertainty in your value of R_H , and compare your result with the accepted value of R_{∞} adjusted for the reduced mass of hydrogen.

THE ISOTOPE EFFECT & THE RESOLVING POWER OF THE SPECTROGRAPH

The ability of the spectrograph system to resolve small differences in the spectral lines of a source depends on many factors: the quality of the optical components and their alignment, the width of the entrance slit, the quality and properties of the grating, the resolution of the detector system (whether it is someone's eye or an electric photodetector), and the inherent properties of the light source.

The resolving power \mathcal{R} of a diffraction spectrograph is described by the formula

$$\mathcal{R} = \frac{\lambda}{\Delta \lambda_{\min}} , \qquad (4)$$

where $\Delta \lambda_{\min}$ is the wavelength difference between two spectral lines that are *just resolved* (i.e., seen as separate lines). The contribution of the grating itself to the resolving power is given by theory (for a perfectly made grating) to be

$$\mathcal{R}_{\text{grating}} = mN \,, \tag{5}$$

where m is the order number and N is the total number of lines in the grating that are illuminated by the light source. In practice, the resolving power will always be less than this theoretical value.

In this next exercise, you will use a CCD ("Charge-Coupled Device") array to measure the separation between the Balmer lines of hydrogen and deuterium. The fact that there is a separation is called the "isotope effect." You will also estimate the resolving power of the spectrograph from the width (specifically, the full-width at half-maximum) of these spectral lines.

The CCD array has 1024 equally spaced sensing elements (pixels) in the space of 7.99 mm, so it is capable of resolving very closely spaced lines. The array electronics "reads out" the array periodically according to an internal clock circuit. The output of the array circuit is fed to a homemade amplifier that allows a DC offset to be applied to the signal. The amplifier output is sent to a digital oscilloscope. A second output from the array circuit is used to trigger the oscilloscope to produce a stable trace. We will use the features of the oscilloscope to reduce noise in the CCD signal.

Before switching to the array, you should make sure you can see the two lines with your eye. Position the microscope carriage to observe H_{α} line. Adjust the slit width until you see two very closely spaced red lines; these are the H_{α} and D_{α} lines. The CCD array will allow you to make a quantitative measurement of their separation.

Carefully lift the microscope assembly and set it aside, taking care not to move the microscope/detector carriage. Loosen the silver clamping knob on the black post holder and swing the CCD array board into position so that the plane of the board is perpendicular to the light path. Clamp the array in position. The sensing elements of the array are beneath a glass cover on a small "chip" near the lower center of the circuit card.

Turn on the power to the oscilloscope and the power supply connected to the CCD card and amplifier box. Grab a flashlight and turn off the room lights; the CCD is very sensitive, and you'll need to work in the dark for this part. Set the scope sweep speed to (about) 10 milliseconds (ms) per division, and the vertical gain to (about) 0.5 volt per division. Check that the "trigger" menu shows the scope on external (EXT) trigger with a trigger level between 200 and 250 mV, and that the "Acquire" menu is set to "Sample".

If you do not see a "bump" in the trace that moves as you slide the carriage a small amount, open the slit up completely, and hold a white card in front of the CCD card and look for the hydrogen lines. If the room is dark, you should be able to see the red α and turquoise β lines. Use the card to help you see where to move the carriage so that the red line crosses the detector window. You should now be able to see a large bump in the signal trace on the scope, similar to the signal shown in Fig. 2a. If you can't find the signal, ask for help.



Figure 2: Scope traces showing the CCD array output. (a) The Balmer α lines with the entrance slit too wide to resolve the difference between H_{α} and D_{α} . Note the ≈ 2.5 V readout cycle start spike directly below the trigger marker ("T"). (b) The α lines resolved into the H_{α} and D_{α} components. Note that the carriage has been moved so that the lines are near the start cycle spike, and the horizontal and vertical scales have been greatly increased so that the steps corresponding to individual pixels are visible.

Once you can see the signal of the α lines, reduce the slit width enough to split the large bump into two smaller bumps. Then loosen the silver knob on the side of the post holder that supports the CCD card assembly and, while watching the scope, slowly rotate the card assembly back and forth to find the position which makes the peaks the highest and narrowest possible. This optimizes the position of the CCD detector so that it is at the focus point of the grating.

Next, slide the carriage slowly along the track to position the peaks near the beginning of the CCD readout cycle, which is marked by the short "spike" or "blip" of about 2 volts amplitude (See Fig. 2a). The vertical position of the trace on the scope is determined by two knobs: the vertical "Position" knob on the scope panel sets the position of zero volts, as denoted by the channel marker on the left side of the display, and the "Offset" knob on the amplifier box, which applies a DC offset to the CCD signal. It is helpful to position the channel marker about two large divisions below the centerline of the display, and then adjust the "Offset" knob to park the trace at this spot. This is shown in Fig. 2a; note the marker for channel 1 at the left.

Increase the sweep speed to about 400 μ S/div in order to zoom in on the peaks. Then, make successive *small* adjustments of the CCD card position, carriage position, slit width, and oscilloscope controls in order to make the peaks on the scope as narrow and as distinct as possible. You should be able to obtain an image similar to that shown in Fig. 2b. Note the significant change in both the vertical sensitivity ("CH 1") and horizontal sweep speed ("M") between Figs. 2a and 2b. When you have zoomed in on the peaks, the trace will be quite jumpy because of electrical noise. You can quiet this noise by using the averaging feature of the scope. Press the MENU button in the ACQUIRE column, then press the Average button to the right of the scope screen next to the Average selection. An average of 32 sweeps will make for a steady display. To change the number of sweeps in the average, rotate the knob with the \oplus on it at the upper right of the screen. Trace averaging was done in Fig. 2b.

At this point, the H_{α} and D_{α} lines should be clearly resolved. The readout from individual pixels should now be visible on the scope: each pixel shows up as a flat section with a faint spike at the edge.

A very nice hard copy of the CCD readout can be obtained with the Tektronix TDS 3012 digital scope. If there are waveforms displayed other than Channel 1 (yellow), you can remove them from the display by pushing the appropriately colored button (white for REF, red for MATH), and then pushing the OFF button. To print the scope display, press the button at the lower left of the screen with the printer icon on it; retrieve your print from the printer below the scope.

By counting pixels (the "stair-steps" in Fig. 2b), you can measure the separation between the two peaks and estimate the full-width at half maximum (FWHM) of the peaks. But to relate the pixel counts to the change in wavelength, you need a conversion factor, which you can determine by using the CCD array and the *alpha* lines as follows.

Set the sweep speed back to 10 ms/div, so that you can see an entire readout cycle of the CCD array. Move the carriage to the left so that the very top of the largest peak is just at the left edge of the CCD readout. Note the x reading (call it " x_1 ") on the meter stick. Now move the carriage to the right so that the very top of the same peak is just at the right edge of the CCD readout, and again note the x reading (x_2) on the meter stick. Hint: if you understand how this system works, you can get a more accurate result by moving the horizontal position marker, or "trigger point" to the middle of the screen, and then increasing the sweep speed sufficient to see individual pixels. Then at one extreme, the peak will be on the right side of the cycle-start spike, and at the other extreme, the peak will be on the left side of the cycle-start spike.

From your original calibration you can derive the wavelength associated with x_1 and x_2 , and thereby the wavelength difference $\Delta \lambda = \lambda(x_2) - \lambda(x_1)$ across the 1024 pixels. The change in wavelength per pixel will be $\Delta \lambda/1024 = \Delta \lambda_{\text{pixel}}$.

After you have obtained your pixel calibration data and printout for the α lines, repeat the procedure to measure the H_{β} and D_{β} lines. You will need to increase the vertical sensitivity on the scope, since these lines are less intense, and the CCD is less sensitive to this wavelength. Make sure to turn off the Averaging feature when first locating the β lines. After locating the lines, and parking them close to the cycle-start point, increase the sweep speed and vertical sensitivity to see the lines in more detail. Turn on the Averaging feature to get rid of the bounce in the display.

Since the β lines produce a much smaller signal than the α lines, the background pixel-to-pixel variation of the CCD readout will visibly affect the line shapes. To eliminate this background variation, the REFERENCE and MATH features of the scope can be utilized. After finding the β lines and getting them displayed on the digital scope, proceed as follows.

- 1. Cover the slit assembly with the black paper (or slide the carriage a wee bit to one side so that the lines move off screen).
- Press the REF button, turn Ref 1 on (press the button below the Ref 1 selection on the screen), and store Channel 1 to Reference 1 by pressing the "Save/Recall" button to the right of the knob marked ⊕, and chosing the appropriate softkeys on the screen.
- 3. Remove the black paper covering the slit, (or move the carriage back to its original position).
- 4. Now press the MATH button, and select the subtraction operation (-), with the first source set to Channel 1, and the second source set to Reference 1.

The MATH trace (red one) will now display the difference between the signal and background, with the pixel-to-pixel variation largely eliminated and the line shapes displayed much more cleanly. This effect is shown in Fig. 3.

Make a print out of the β lines for later analysis. If you have time, you may wish to explore whether you need to calibrate the pixel width versus wavelength for the β line measurements. Can you think of a reason why it might differ from that of the α lines?

Copies of the scope display for both the H_{α}/D_{α} and H_{β}/D_{β} lines are available in the lab, so you can see what sort of data you should be able to obtain.



Figure 3: Scope traces in the acquisition of the β lines. This picture shows the effect of subtracting the random pixel offsets from the signal. The lowest trace, near the marker "R1", shows the CCD output without the lines. The middle trace, near the marker "1" shows the CCD output with the lines in view. The topmost trace, near the marker "M" shows the difference between the two lower traces, as calculated using the "Math" feature. On the right of the figure is the Math menu, with Ch 1 subtracting Ref 1.

SHUTDOWN

When you are finished please move the CCD array out of the way, put the viewing microscope back in place, and put the covers back over the optics.

Shut off all lamp power supplies and electronics.

POST DATA-COLLECTION ANALYSIS

With your printouts and calibration data in hand, carry out the following analyses for your report:

7. Obtain estimates for the resolving power of the spectrograph by studying the widths of the hydrogen/deuterium lines.

Estimate the width (FWHM) of each peak to one-half of a pixel. (You should have four peaks to look at.) Multiply this number by $\Delta \lambda_{\text{pixel}}$ to obtain a minimum resolvable $\Delta \lambda$, and a value for \mathcal{R} . Make sure to calculate an estimate on the random error of this value of \mathcal{R} .

Calculate the theoretical value of $\mathcal{R}_{\text{grating}}$ for this grating, using Eq. (5). Then use this value of $\mathcal{R}_{\text{grating}}$ to estimate how many pixels this resolving power would correspond to. Compare this theoretical limit to the values you measure, and discuss: Why is this experimental value for \mathcal{R} likely to be less than $\mathcal{R}_{\text{grating}}$? What other factor do you think affects the resolving power the *most*? Justify your choice based on your observations.

With this instrument, how close in wavelength could two lines be and still be resolved? Explain the criteria you apply to make this estimate. Hint: you may want to read Hecht, pp. 471–481 to help you think about this problem.

8. Determine the mass ratio of deuterium to hydrogen from the difference in wavelength of the α and β lines.

Use your printouts and calibration data to determine the difference in wavelength $\Delta \lambda_{HD} \equiv \lambda_H - \lambda_D$ between the H_{α} and D_{α} lines and the difference in wavelength between the H_{β} and D_{β} lines. Then calculate $\Delta \lambda_{HD} / \lambda_H$ for each pair of lines, along with an uncertainty in this ratio.

Use Eqs. (1), (2) and (3) to prove the following relationship:

$$\frac{\Delta\lambda_{_{HD}}}{\lambda_H} = \frac{1 - M_H/M_D}{1 + M_H/m_e} \,, \tag{6}$$

where M_H and M_D are the masses of the hydrogen and deuterium nuclei.

Finally, use the result of Eq. (6) along with your measurements to calculate the ratio of the of the masses of the hydrogen and deuterium nuclei, M_H/M_D , along with its uncertainty. You will need to use the proton/electron mass ratio $m_p/m_e = 1836.15/1$. If the nuclear mass ratio you calculate is not close to 1/2, try again.