Spectroscopy - Identifying Unknown Elements

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The identification of two unknown elements was accomplished in this experiment through the use of spectroscopy. By passing the light emitted from two known elements (helium and neon) through a diffraction grating and determining the angle and order of diffraction, the diffraction grating spacing d was determined, where $d = 1826 \pm 0.5440$ lines per mm. This value allowed for calculation of the wavelengths λ of each spectral line for each of the unknown elements. These values for λ were then compared with the spectra of various elements on a spectral chart, and the unknown elements were identified as mercury and helium[1]. The standard deviation σ_{Hg} in the values of λ for mercury was $\sigma_{Hg} = 61.1$ nm, and the standard deviation σ_H for hydrogen was $\sigma_H = 115$ nm. Each value of λ for the wavelength of each spectral line for the two unknown elements was within one σ of the accepted values.

I. INTRODUCTION

The objective of this experiment was to use spectroscopy to identify two unknown elements in the form of rarefied gas in spectral tubes. This was accomplished by examining the emission spectra of two known gases, helium and neon, and determining the diffraction grating spacing based on the diffraction angles at which constructive interference occurred and the order of diffraction, in conjunction with the known wavelengths of each spectral line. Once the diffraction grating spacing was determined, the wavelengths of the two unknown elements' spectra were calculated and compared with various elements' spectra on a spectral chart. In this fashion, the identities of the two unknown elements were determined[2][3].

A. Theory

Passing a high-voltage discharge through a rarefied gas contained in a tube causes electrons to collide with atoms throughout the tube. During these collisions, the electrons produced in the discharge cause atomic electrons to gain energy and jump to higher energy levels through a process called excitation. The electrons that were bumped into a higher energy level remain there for a short time before reverting to the original energy state. When these electrons return to their original energy levels, they release photons in the process at particular wavelengths[2][3][4][5].

The various wavelengths of light emitted from the discharge tube can then be identified using a spectrometer. The emitted light passes through a small slit and diffraction grating, which contains many slits and results in numerous wavefronts. If the distance between the two slits in the diffraction grating happens to be an integer multiple of the wavelength of the emitted light, then constructive interference will occur, in which the waves passing through the diffraction grating will be in phase and appear to be enhanced at certain angles relative to the diffraction grating. The following equation describes this relationship[3]:

$$dsin\theta = n\lambda \tag{1}$$

where d is the diffraction grating spacing, θ is the angle between the diffraction grating and the point at which constructive interference occurs, n is any positive integer, and λ is the wavelength of the emitted light.

Measuring the angle of diffraction θ, the order of diffraction n, and the wavelengths λ of the spectrum of a known element enabled the determination of the diffraction grating spacing d. Once d was known, the wavelengths of the spectrum of an unknown element could be determined and compared with known values from spectral charts[3][6].

II. PROCEDURE AND EQUIPMENT

The description of the experiment apparatus and the procedure may be found in "Diffraction and Spectral Analysis" [3].

A. Equipment

The equipment for this experiment consisted of a spectrometer, gas discharge tubes, a 5000-V discharge tube stand, a diffraction grating, and a dark cloth with which to cover the apparatus. The spectrometer consisted of a collimator with adjustable slit, a spectrometer table on which the diffraction grating was placed, a telescope with adjustable eyepiece, and a vernier table with degree markings for measuring diffraction angles. The experimental apparatus may be seen in Figure 1 below.

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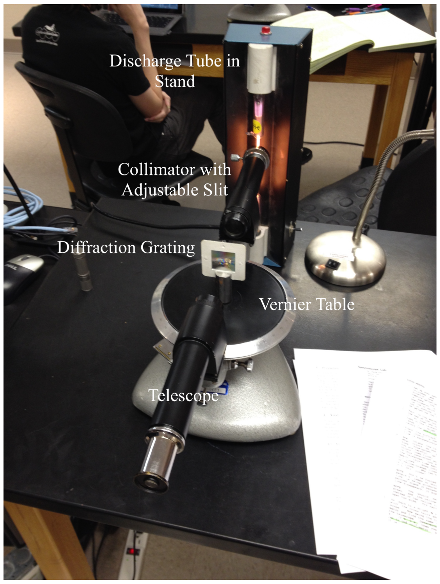

FIG. 1. The experimental apparatus consisted of a discharge tube with 5000V discharge tube stand, a collimator, vernier table, diffraction grating, and telescope. Light emitted from the discharge tube passed through the adjustable slit attached to the collimator, through the diffraction grating, and through the telescope. The telescope was able to move to either side of the normal to the diffraction grating via the vernier table. Emission spectra could only be seen at certain diffraction angles, which were marked on the vernier table.

B. Procedure

Each portion of the procedure was carried out in accordance with the instructions contained in "Diffraction and Spectral Analysis" [3].

The spectrometer was configured to ensure that the discharge tube, collimator, and telescope were all collinear, and the focus of the telescope was adjusted until the discharge tube was in focus. One of the known gases, helium, was then placed in the discharge tube stand, which was then given power. The slit in the collimator was then adjusted until a bright but narrow image appeared in the telescope. The telescope was also adjusted so that the image was aligned with the crosshairs in the telescope's eyepiece. The angle at which this occurred was recorded as the zero point θ_z, which was equal to $0.0 \pm 0.05°$.

The diffraction grating was then placed in the center of the vernier table and perpendicular to the collimator. The apparatus was then covered with a dark cloth to enable easier viewing of the spectral lines and to minimize any interference from outside light sources, such as computer screens or ceiling lights.

The telescope was rotated to the right (counterclockwise) until spectral lines appeared, beginning with purple, then blue, green, and yellow-orange lines. The telescope was then rotated to the opposite side of the diffraction grating (clockwise) until the same lines were visible.

The green spectral line was most clearly visible and was chosen to calibrate the apparatus. This process consisted of recording the diffraction angles on each side of the diffraction grating in which the green line was visible, and determining whether these angles were equal. The values of each angle were $\theta_1 = 15.8 \pm 0.05°$ for the right-hand side, and $\theta_2 = 15.8 \pm 0.05°$ for the left hand side. Since $\theta_1 = \theta_2$ relative to θ_z, the diffraction grating was perpendicular to the collimator, and the apparatus was deemed properly calibrated[3].

The angles for each first-order spectral line ($n = 1$) were then recorded on each side of the diffraction grating. The averages of these angles were then taken and recorded according to the following equation:

$$\theta_{av} = \frac{\theta_1 + \theta_2}{2} \tag{2}$$

The wavelength λ was then determined for each spectral line based on color and by referring to the known values for helium[1].

The same process was repeated for neon gas, and the diffraction grating d was then determined by plotting the wavelength λ versus the sine of the average diffraction angle $sin\theta_{av}$ for helium and neon. The slope of the straight line fit through the data points was equivalent to the diffraction grating spacing, and this value was used to determine the wavelengths of each spectral line emitted by the two unknown gases. The data collection process for the two unknown gases was identical to the data collection process for the two known gases, except that the values of λ were obtained using Equation 1[3].

It should be noted that only the first-order spectral lines ($n = 1$) could be seen for each gas, since higher-order lines were either barely visible or not visible at all.

III. DATA

For each known gas, the color of the spectral line, the two diffraction angles θ_1 and θ_2, the average diffraction angle θ_{av}, and the wavelength λ were recorded. For the unknown gases, the wavelengths λ were not recorded, since the diffraction grating spacing d was unknown at the time.

The data for the spectra of helium and neon may be seen in Tables I and II below, where all angle measurements were recorded in degrees:

TABLE I. Spectrum of Helium

Line Color	θ_1	θ_2	θ_{av}	λ(nm)
Purple	14.0 ± 0.05	14.1 ± 0.05	14.05 ± 0.04	447.1
Blue	14.8 ± 0.05	14.9 ± 0.05	14.85 ± 0.04	471.3
Blue − Green	15.5 ± 0.05	15.6 ± 0.05	15.55 ± 0.04	492.2
Green	15.8 ± 0.05	15.9 ± 0.05	15.85 ± 0.04	501.6
*Yellow*1	18.7 ± 0.05	18.7 ± 0.05	18.70 ± 0.04	587.6
*Yellow*2	18.7 ± 0.05	18.8 ± 0.05	18.75 ± 0.04	587.6

TABLE II. Spectrum of Neon

Line Color	θ_1	θ_2	θ_{av}	λ(nm)
Blue	14.7 ± 0.05	15.0 ± 0.05	14.85 ± 0.04	471.0
Blue − Green	15.8 ± 0.05	16.1 ± 0.05	15.95 ± 0.04	500.5
Green	16.9 ± 0.05	17.2 ± 0.05	17.05 ± 0.04	540.1
*Yellow*1	18.3 ± 0.05	18.7 ± 0.05	18.50 ± 0.04	588.2
Red	20.2 ± 0.05	20.7 ± 0.05	20.45 ± 0.04	640.2

It should be noted that the spectral line colors listed for each gas above were the most clearly visible of those present, and therefore were most easily measured.

The data for the two unknown gases may be seen in Tables III and IV below, where all angle measurements were recorded in degrees:

TABLE III. Spectrum of Unknown Gas I

Line Color	θ_1	θ_2	θ_{av}
Purple	13.5 ± 0.05	14.0 ± 0.05	13.75 ± 0.04
Blue − Green	15.3 ± 0.05	15.7 ± 0.05	15.50 ± 0.04
Green	17.1 ± 0.05	17.5 ± 0.05	17.30 ± 0.04
*Yellow*1	18.1 ± 0.05	18.5 ± 0.05	18.30 ± 0.04
*Yellow*2	18.2 ± 0.05	18.6 ± 0.05	18.40 ± 0.04

TABLE IV. Spectrum of Unknown Gas II

Line Color	θ_1	θ_2	θ_{av}
Purple	13.5 ± 0.05	13.9 ± 0.05	13.70 ± 0.04
Blue − Green	15.2 ± 0.05	15.5 ± 0.05	15.35 ± 0.04
Red	20.7 ± 0.05	21.2 ± 0.05	20.95 ± 0.04

IV. RESULTS AND ANALYSIS

The diffraction grating spacing d was calculated by plotting the wavelength λ versus the sine of the diffraction angle θ for each known gas, and fitting a straight line through the data points. The slopes of these lines corresponded to the diffraction grating spacing based on Equation (1), and the average of these two values was used as the final value for d, which was equal to 1826 ± 0.5487 lines per mm.

For helium, the slope of the best-fit line was $m = 1795 \pm 0.5392$, while the slope of the best-fit line for neon was $m = 1856 \pm 0.5487$.

Using the above value for d in Equation (1), the wavelengths of each spectral line for each unknown gas were calculated, and may be seen in Table V below:

TABLE V. Wavelengths for Unknown Gases I and II

Line Color	λ for UI (nm)	λ for UII (nm)
Purple	434.0 ± 70.9	432.5 ± 71.0
Blue − Green	488.0 ± 70.4	483.4 ± 70.4
Green	543.0 ± 69.7	
*Yellow*1	573.4 ± 69.3	
*Yellow*2	576.4 ± 69.3	
Red		652.9 ± 68.2

Based on these values, Unknown Gas I was determined to be mercury, and Unknown Gas II was determined to be hydrogen. The known values for the wavelengths of each spectral line for both gases may be seen below in Table VI[1]:

TABLE VI. Known Wavelengths for Mercury and Hydrogen

Line Color	λ for Hg (nm)	λ for H (nm)
Purple	435.8	434.0
Blue − Green	491.6	486.1
Green	546.1	
*Yellow*1	577.0	
*Yellow*2	579.0	
Red		656.3

The standard deviations σ in the calculated wavelengths for mercury and hydrogen were $\sigma_{Hg} = 61.1$ and $\sigma_H = 115$, respectively. Each calculated value for wavelength λ for each unknown gas was well within the accepted value of λ, which indicated that each unknown gas was correctly identified.

A. Error Analysis

The main sources of error in this experiment were due to the placement of the diffraction grating and the measurement process of each diffraction angle. The diffraction grating was placed as perpendicularly as possible relative to the collimator and discharge tube, to ensure that each diffraction angle measurement was as accurate as possible. However, each diffraction angle measured on either side of the diffraction grating was often not exactly equal to the other, and thus the average of the two angles was used for calculations of wavelength in order to minimize any effects this discrepancy may have had on the final values of λ. The resulting differences between the calculated values and accepted values for λ were all less than 5 nm, which indicates that taking average angle measurements effectively minimized any error due to the placement of the diffraction grating.

In addition, the measurement process of each diffraction angle was also subject to other factors, such as ambient lighting and experimenter visual acuity in near darkness. This may have increased the difficulty in seeing fainter spectral lines, resulting in increased uncertainty in the angle measurements. This was minimized by placing a dark cloth over the apparatus and turning off as many lights in the laboratory as possible, in order to decrease the effects of outside lighting. This also allowed low-light vision to become more effective, resulting in more accurate measurements.

Finally, the selection of the brightest spectral lines for measurement purposes minimized the uncertainty in line color identification, especially when multiple spectral lines of nearly the same color appeared relatively close together when viewed through the telescope. During the calculation process, each resulting value of λ was compared with known values for that particular element, along with a visual representation of the element's spectrum, to ensure that line color identification was correct. Based on the relatively small disparities between calculated and accepted values of wavelength, this strategy worked effectively.

V. CONCLUSION

The objective of this experiment was to identify two unknown elements through the use of spectral analysis. This was accomplished by analyzing the spectra of helium and neon gas and determining the diffraction grating spacing d by plotting wavelength λ as a function of the sine of the diffraction angle θ for each gas. The slope of the best-fit line for each gas corresponded to the diffraction grating spacing d. Using the resulting value of $d = 1826 \pm 0.5487$ lines per mm, the wavelengths of each spectral line for the two unknown gases were calculated according to Equation (1). The unknown gases were subsequently identified as mercury and hydrogen, based on a comparison of the calculated wavelengths with the known wavelengths of emission spectra for each element.

The calculated and known wavelengths of the emission spectra for mercury and hydrogen may be seen below in Tables VII and VIII[1]:

TABLE VII. Mercury

Line Color	Calculated λ(nm)	Accepted λ (nm)
$Purple$	434.0 ± 70.9	435.8
$Blue - Green$	488.0 ± 70.4	491.6
$Green$	543.0 ± 69.7	546.1
$Yellow1$	573.4 ± 69.3	577.0
$Yellow2$	576.4 ± 69.3	579.0

TABLE VIII. Hydrogen

Line Color	Calculated λ(nm)	Accepted λ (nm)
$Purple$	432.5 ± 71.0	434.0
$Blue - Green$	483.4 ± 70.4	486.1
Red	652.9 ± 68.2	656.3

Since the differences between the calculated and accepted values for λ were less than 5 nm for each spectral line, the elements were positively identified. The standard deviations in the calculated wavelengths for mercury and hydrogen were $\sigma_{Hg} = 61.1$ and $\sigma_H = 115$, respectively.

More sensitive equipment, such as an electronic light detector instead of a telescope, may improve future experiments by enabling measurement of second- and third-order diffraction angles, thereby increasing the accuracy to which the diffraction grating spacing could be measured, and increasing the accuracy of wavelength calculation for unknown elements. In addition, any spectral lines outside of the visual range could also be detected through the use of an electronic detector rather than a telescope, resulting in a more complete picture of the full emission spectrum of an element.

[1] C. Nave, "Atomic spectra," (2014).
[2] D. Smith, "Spectroscopy lab - identifying unknown elements," (2014).
[3] D. Smith, "Diffraction and spectral analysis," (2015).

[4] K. Krane, *Modern Physics* (John Wiley and Sons, Inc., 2012).
[5] H. D. Young and R. A. Freedman, *University Physics* (Pearson Education, Inc., 2012).
[6] A. C. Melissinos and J. Napolitano, *Experiments in Modern Physics* (Academic Press, 2003).