Experiment 1.
Atomic and Molecular Structure

Experimental Procedure

- Objectives
- Introduction
- Experimental Procedure
- Report Sheet

OBJECTIVES

- To view and calibrate visible line spectra
- To identify an element from via visible line spectra
- To identify a compound from its infrared spectrum
- To predict the three-dimensional structure of molecules and molecular ions

Introduction

According to quantum mechanics, energies of electrons in an atom are quantized, which means all the electrons can possess only the particularly allowed energies.

When an atom of an element absorbs a certain amount of energy, (which has the exactly same amount with the difference between energies of two different states) the electrons within it absorb the energy and reach excited states.
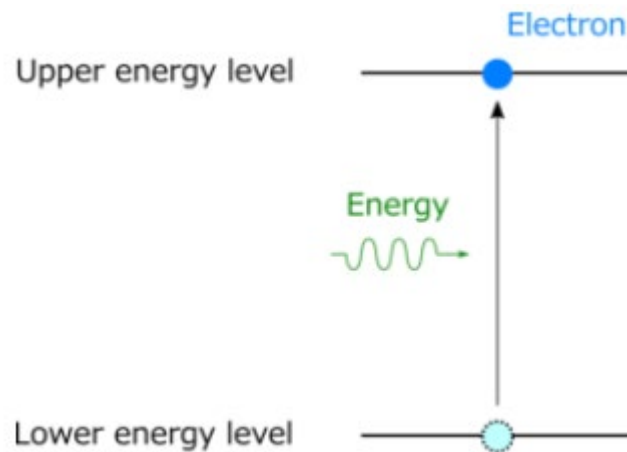

Electrons can acquire a certain amount of energy because the energies of allowed states are quantized.

After an electron reach an excited state, the electron returns to the ground sate by various pathways. One of the most frequent ways is fluorescence, a radiative procedure where a photon possessing a certain amount of energy comes out.
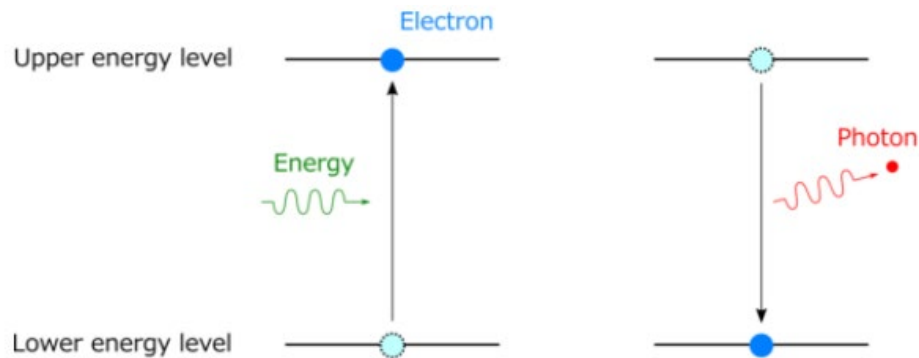
These photons can have only the allowed energies (due to the energy quantization). The energies are different according to the elements, which makes emission spectrums of various elements much different.
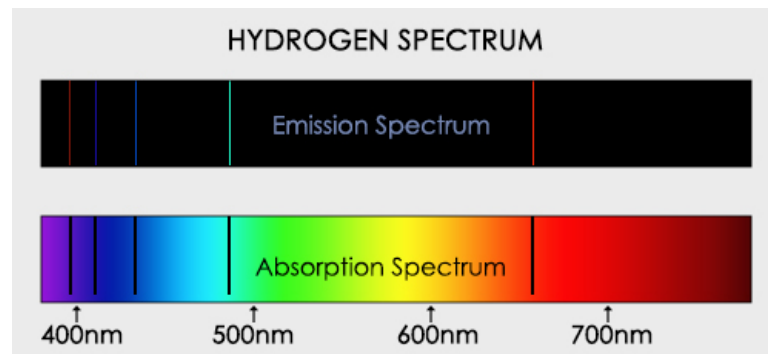
IR spectroscopy is a tool to identify what bonds a target molecule possesses. This analysis method utilizes a concept of molecular vibration. (You will learn this concept in GenChem 2)

The only thing you have to remember is that each bond
has its own characteristic vibrational frequency. You may refer
to Table D3.2 in the experiment manual.

Bond	Stretching Frequency (cm^{-1})	Intensity
O—H	3200–3650	Weak to strong (strongest when H-bonded)
N—H	3100–3550	Medium
C—H	2700–3300	Weak to medium
C=C	1600–1680	Weak to medium
C=O	1630–1820	Strong
C—O	1000–1250	Strong
C—C	1670 – 1640	Not interested

Lewis structure is a powerful tool to represent molecules into 2-D diagrams. It explains basic information about molecules such as bond order, lone pairs, hybrid orbitals, and so on.

However, one of its weakness is that it lacks information about 3-D geometry, which defines many features of chemicals. Chemists needed to identify the 3-D structure, so they invented a new model called Valence Shell Electron Pair Repulsion, or VSEPR theory.

VSEPR Theory (Molecular Shapes)

A = the central atom, X = an atom bonded to A, E = a lone pair on A

Note: There are lone pairs on X or other atoms, but we don't care. We are interested in only the electron densities or domains around atom A.

Total Domains	Generic Formula	Picture	Bonded Atoms	Lone Pairs	Molecular Shape	Electron Geometry	Example	Hybridi-zation	Bond Angles
1	AX	A — X	1	0	Linear	Linear	H_2	s	180
2	AX_2	X — A — X	2	0	Linear	Linear	CO_2	sp	180
	AXE	A — X	1	1	Linear	Linear	CN^-		
3	AX_3		3	0	Trigonal planar	Trigonal planar	$AlBr_3$	sp^2	120
	AX_2E		2	1	Bent	Trigonal planar	$SnCl_2$		
	AXE_2	X — A	1	2	Linear	Trigonal planar	O_2		
4	AX_4		4	0	Tetrahedral	Tetrahedral	$SiCl_4$	sp^3	109.5
	AX_3E		3	1	Trigonal pyramid	Tetrahedral	PH_3		
	AX_2E_2		2	2	Bent	Tetrahedral	$SeBr_2$		
	AXE_3		1	3	Linear	Tetrahedral	Cl_2		

Total domains (or Steric number): Groups of atoms / Lone pairs

EXPERIMENTAL PROCEDURE & RESULT VIDEOS

A. The mercury spectrum

1. The color plate

Notice the various experimental emission line spectra on the color plate (It is on the back cover of the book).

A continuous spectrum appears at the top, the line spectra for various elements appear in the middle (unknown elements, 1~10), and the Hg spectrum appears at the bottom.
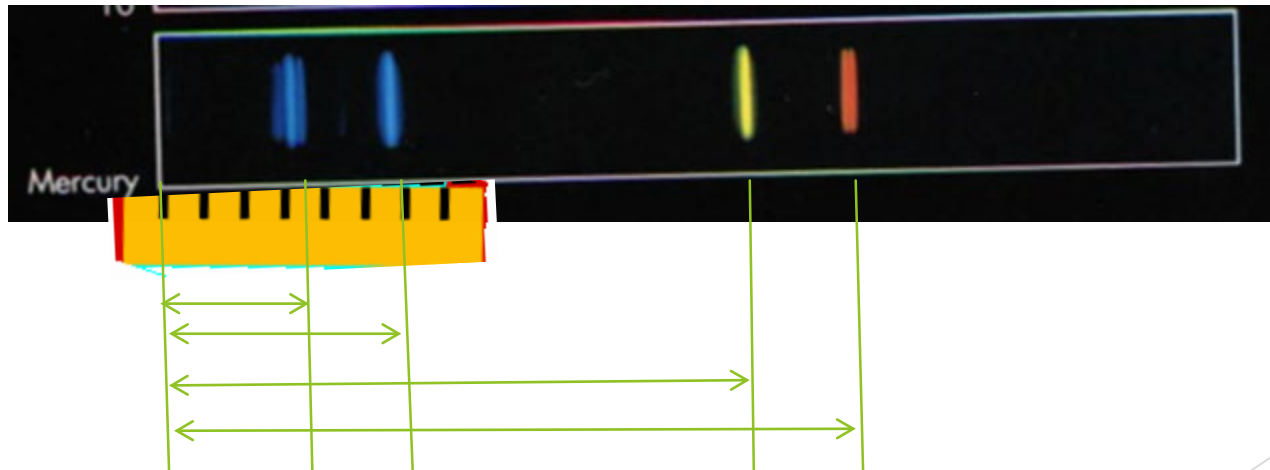
Continuous spectrum
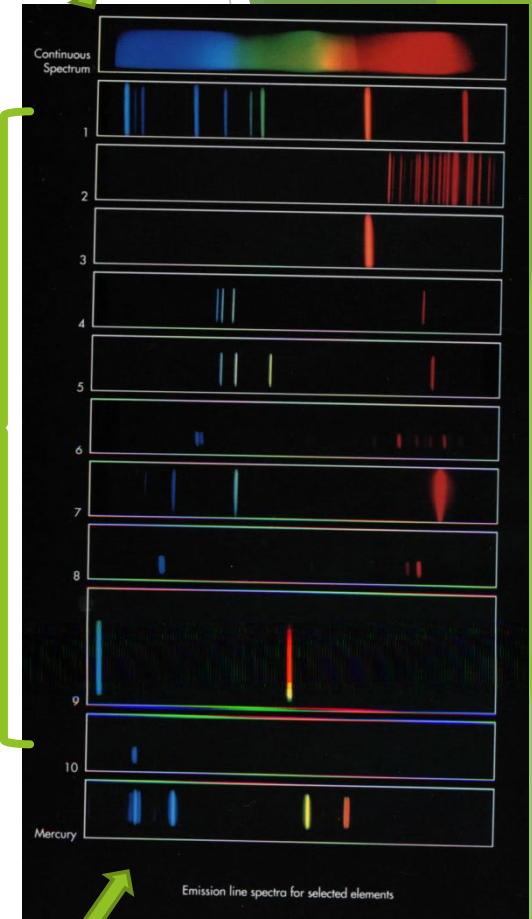
Unknown elements (1~10)

Hg spectrum

Emission line spectra for selected elements

2. Calibrate the spectra of the color plate

Match the lines of Hg spectrum on the color plate with the wavelengths in Table D3.4.

Use a ruler to measure where the lines of Hg spectrum are located.

The distances between two lines of spectrum is proportional to the differences between the wavelengths of themselves.

So using the lengths we measured and the wavelengths in **Table D 3.4**, we can know wavelengths of any lines on the color plate by measuring their locations.


Emission line spectra for selected elements
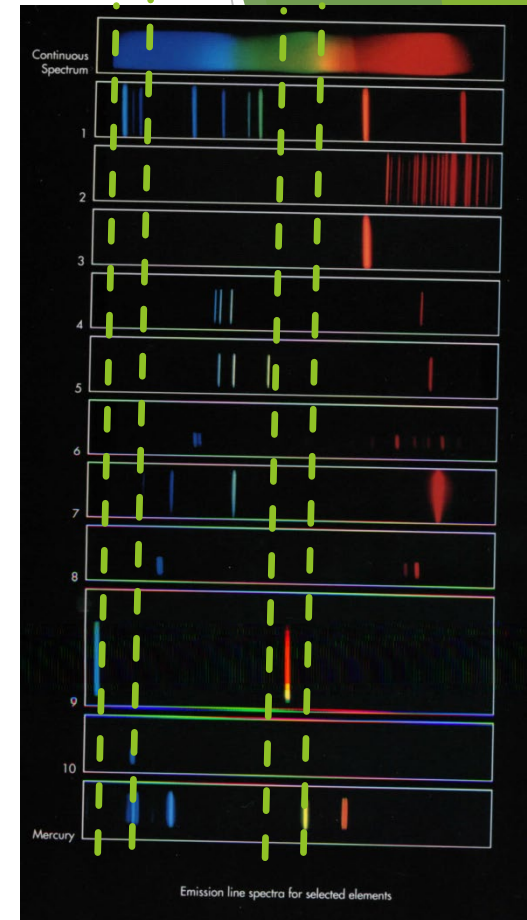
| Table D3.4 Wavelengths of the Visible Lines in the Mercury Spectrum	
Violet	404.7 nm
violet	407.8 nm
Blue	435.8 nm
Yellow	546.1 nm
Orange	577.0 nm
Orange	579.1 nm

B. The spectra of elements

1. Hydrogen spectrum

Use **Figure D3.3**, page 158, to identify which of the emission spectra on the back cover is that of hydrogen. Justify your selection.

Figure D3.3 Formation of the line spectrum for hydrogen
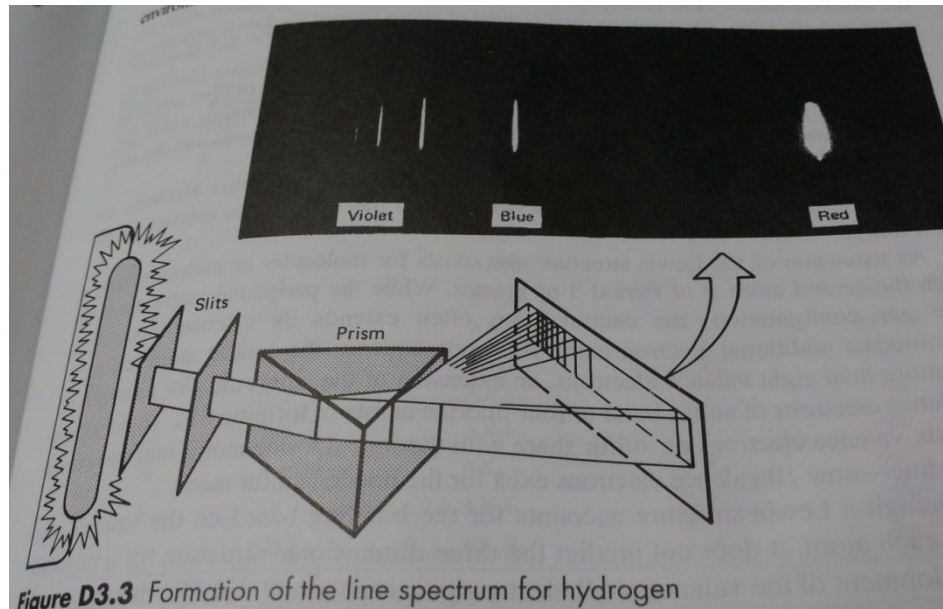
2. Unknown spectra

Your TA will assign to you one or two emission spectra from the color plate (1~10).

Use a ruler to measure where the lines of spectra are located.
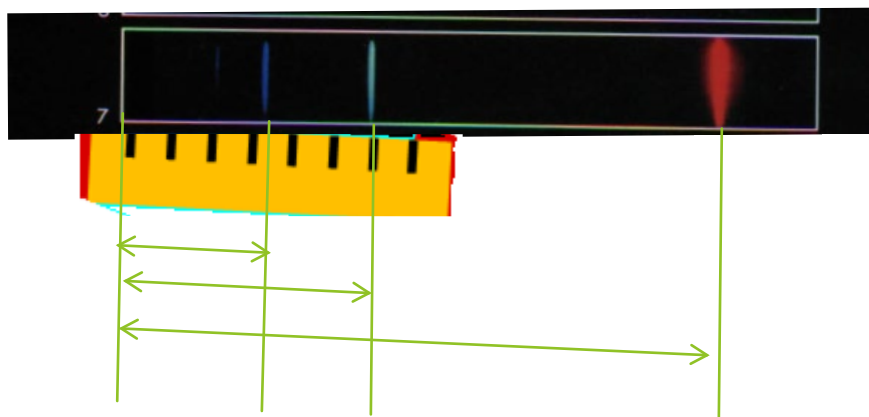
Calculate the wavelengths of them by using the data from Hg spectrum and **Table D 3.4**.

Compare the wavelengths of the most intense lines with the data in **Table D.3.5**. Identify the elements having the assigned spectra.

Additional Experiment : Observing Real Spectra

Spectrum Tubes contain one or more elements as gaseous atoms or molecules. Energy is supplied through an electric field applied between electrodes at the ends of the tubes. Ions and electrons formed by the field are accelerated; collisions convert the increased Kinetic energy to other types, one being electronic. Electrons in energetic or excited atoms occupy one of many well-defined states. An electron with high energy E_3 will return to a lower energy state E_2 simultaneously emitting a photon of energy E_3-E_2 =ΔE= hc/λ; where h = 6.63X10^{-30}J-s is Planck's constant, c = 3X10^8 m/s is the speed of light and λ is the wavelength of light (in meters) in the emitted photon.

Each excited atom type emits characteristic wavelength determined by energy level differences ΔE present in that species. One may observe a particular color with the eyes; analysis with a spectrometer will reveal a series of sharp (monochromatic) emission lines.
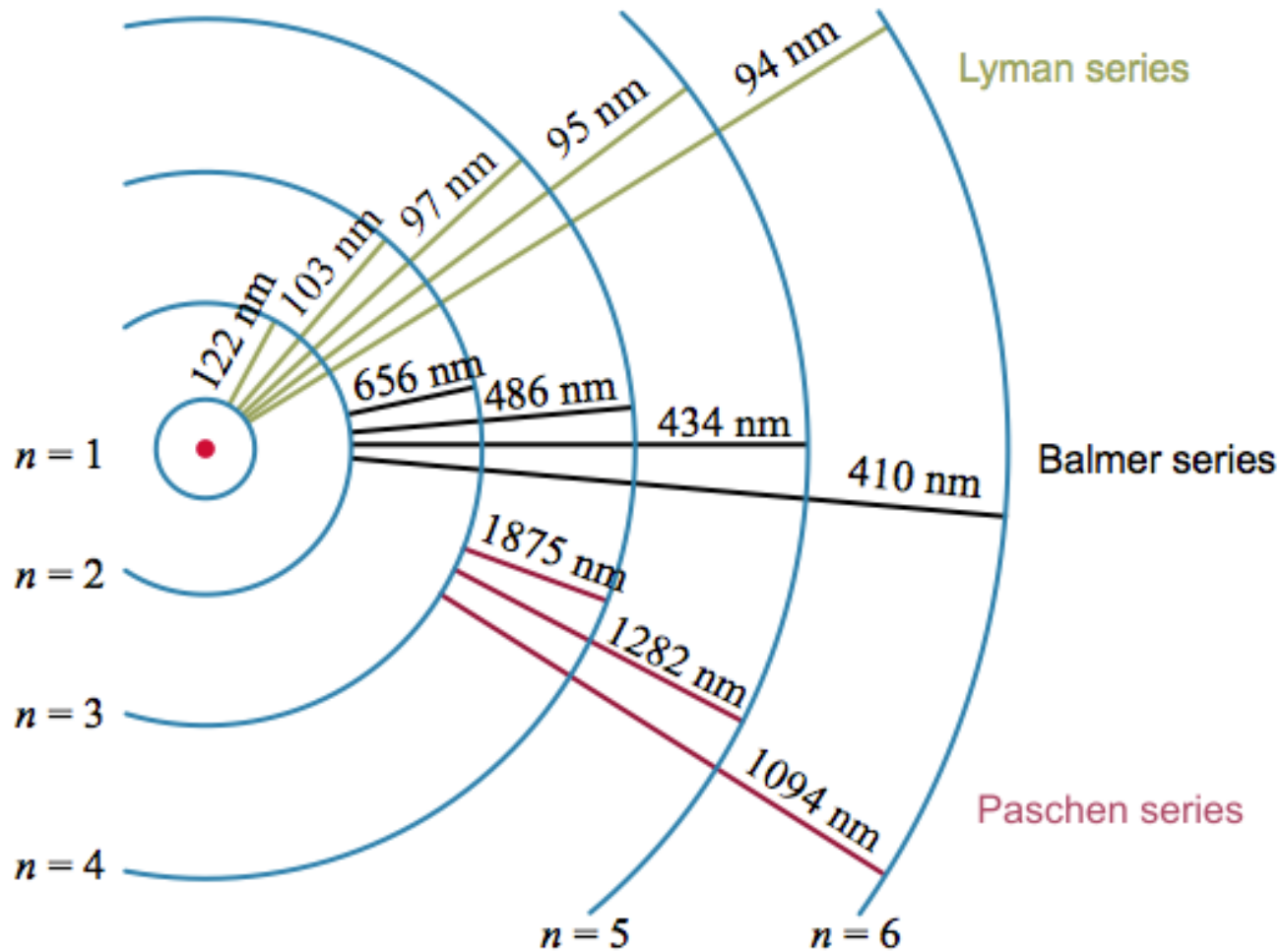
In this part of the lab, you will look at the emission spectra produced by samples of hot gas. The samples are installed in the Vernier spectrum tube carousel power supply, which is shown in the picture to the right. Spectra can be measured using the Logger Pro software. The fiber optic cable of the spectrometer can be mounted in the plastic holder attached to the carousel.

There should be seven gas samples in the carousel: hydrogen, helium, nitrogen, neon, argon, carbon dioxide, and air. To move from one sample to the next, carefully rotate the middle part of the carousel until the next sample clicks into position.
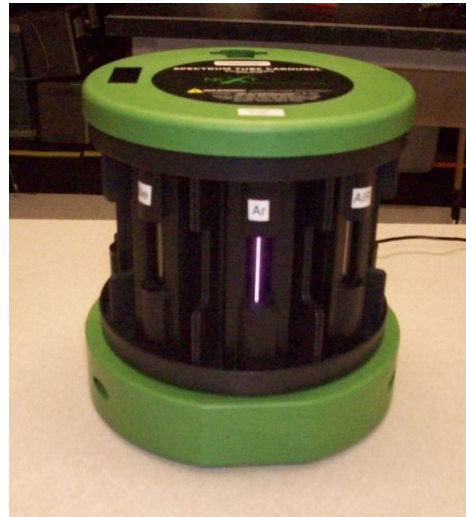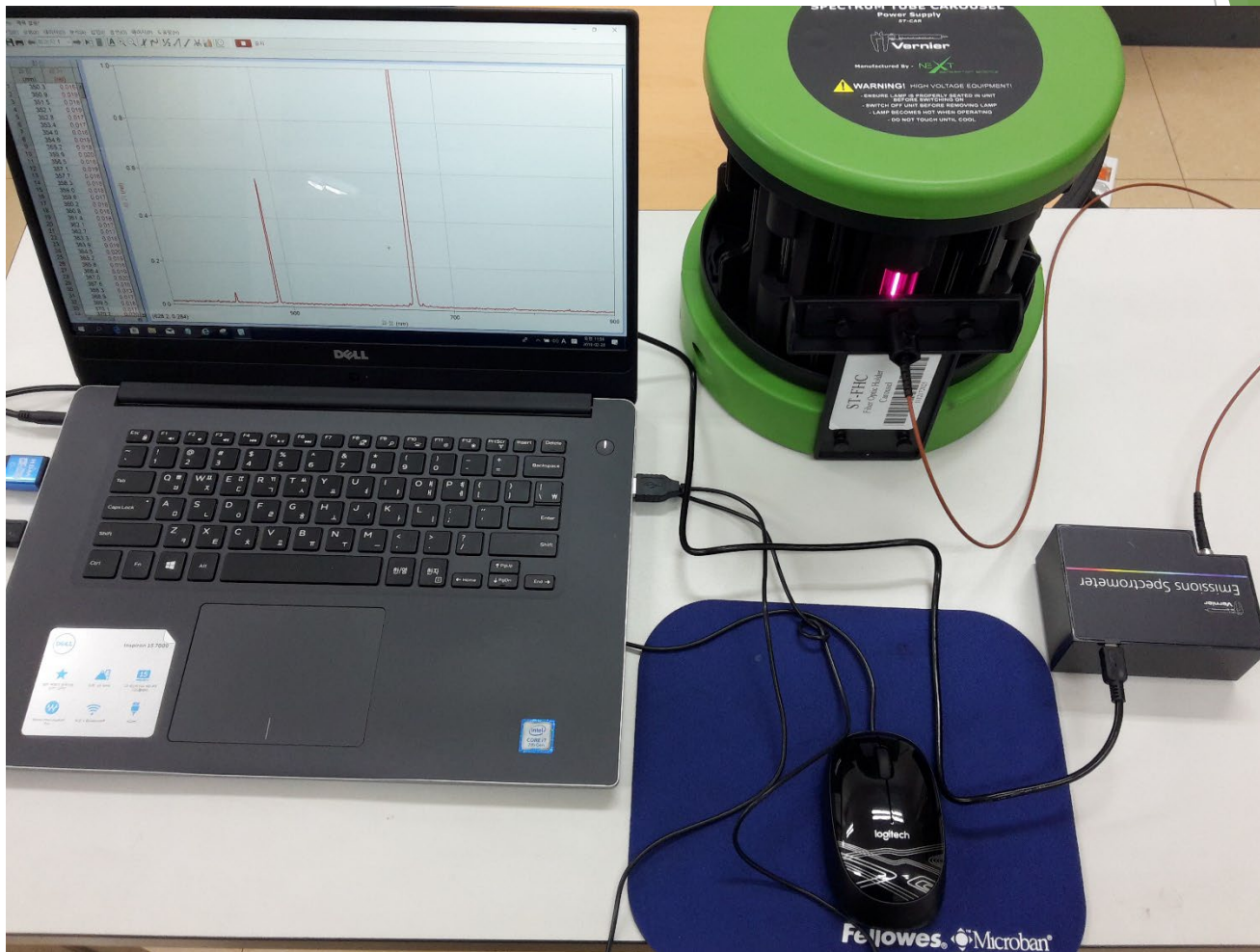
Emissions spectrometer

Emissions fiber

**Spectrum Tube Carousel Power Supply**

NOTE: Turn off the spectrum carousel when you are not actively viewing a gas sample. The gas samples will burn out after extended use, particularly the hydrogen sample, which has a useful lifetime of approximately 40 hours.

1. Begin by observing the spectra of hydrogen and helium. Note the wavelength and intensity of the emission lines in each spectrum in your worksheet. You will need to devise a way of describing the intensity, or strength, of the individual lines.

2. Measure the spectra of neon and argon and observe the colors they make when discharging. Can you explain why these two gases glow with the colors they do?

Sample Data
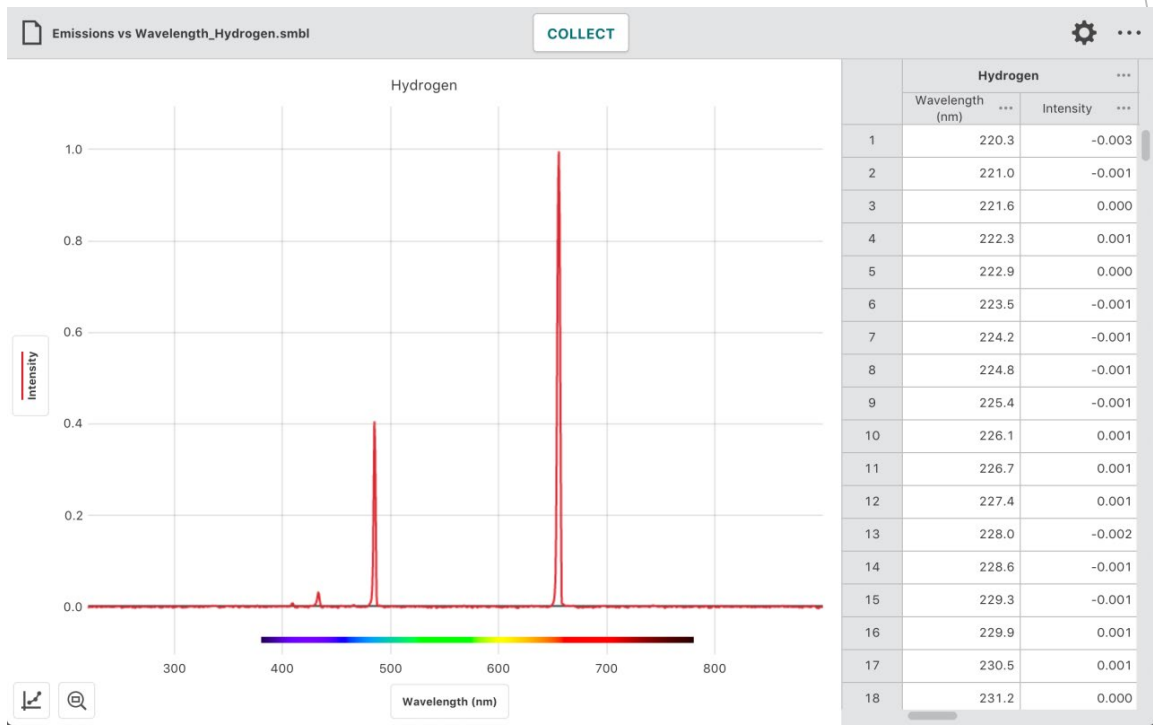
Video: Vernier Emissions Spectrometer - Tech Tips

Also let's observe it through a Direct-Reading Spectroscope that is a replica diffraction grating instrument with an internal scale that shows students the wavelength in nanometers.

It is used for the detection and identification of elements by their characteristic spectral emission lines. The light source may be from salts in a flame or from electrically excited tubes filled with elemental gases, such as helium or nitrogen. The grating has 600 lines per mm. The scale reads from 380 to 720nm and has an actual length of approximately 35mm. The entire spectrum can be seen at once. The slit is adjustable and a reflector is provided to back-light the scale. The housing is a one-piece aluminum casting, finished with light gray polyurethane paint, mounted on a stainless steel post and supported on a cast iron tripod base.
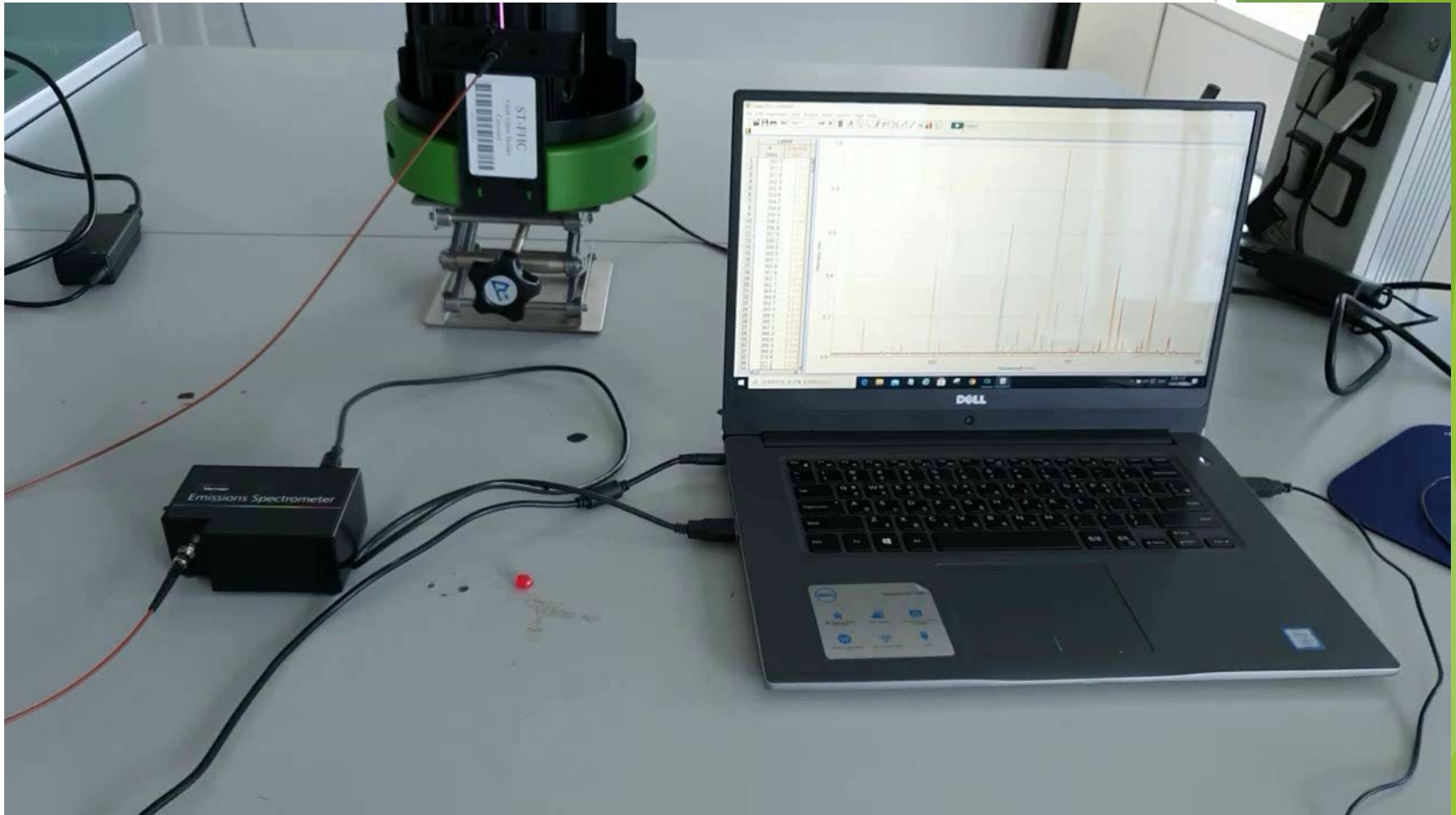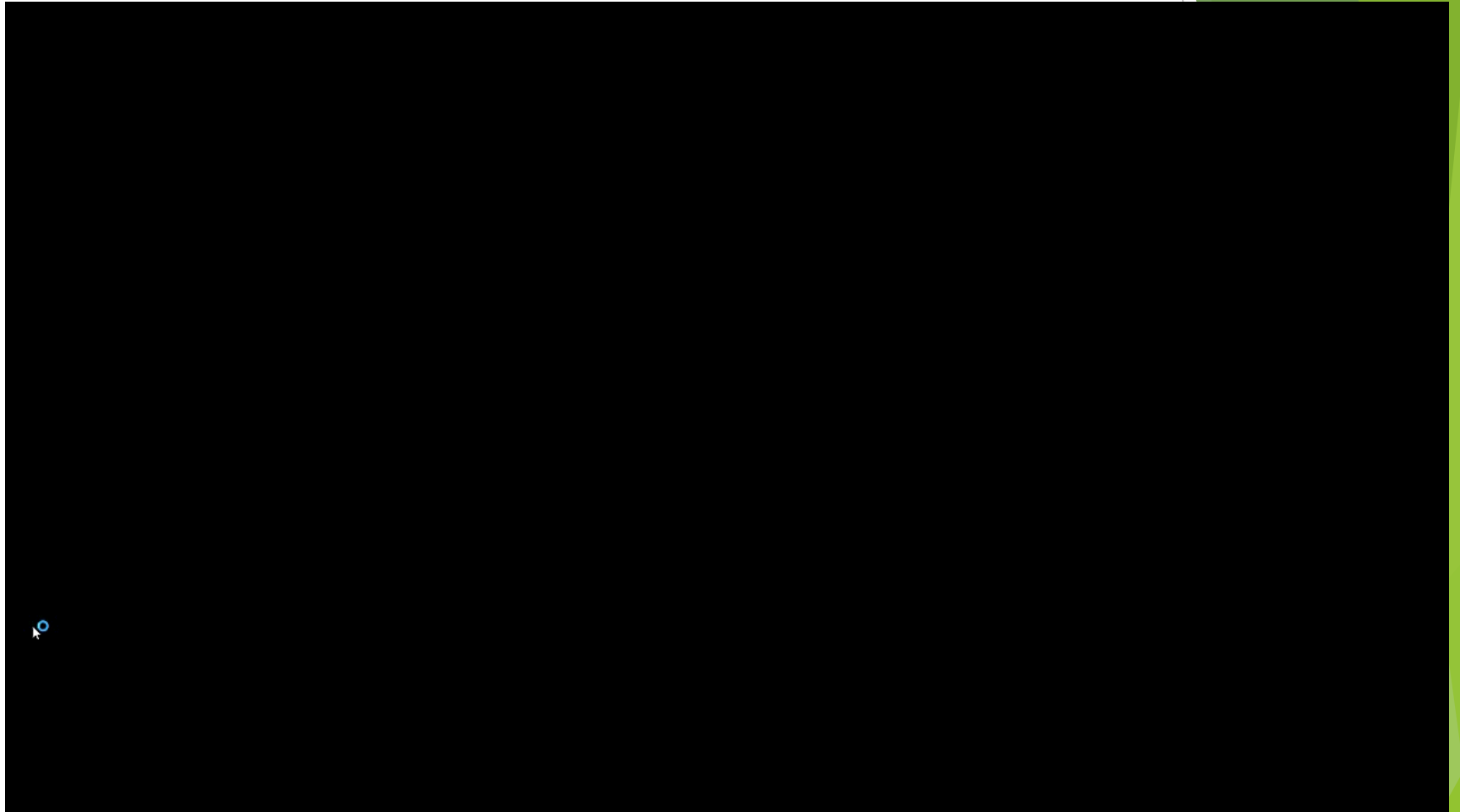
.

Experimental Results

You indirectly can obtain some results and data sets from the experimental video clips and pictures conducted by TA. Both qualitative and quantitative data must be included in your lab report.
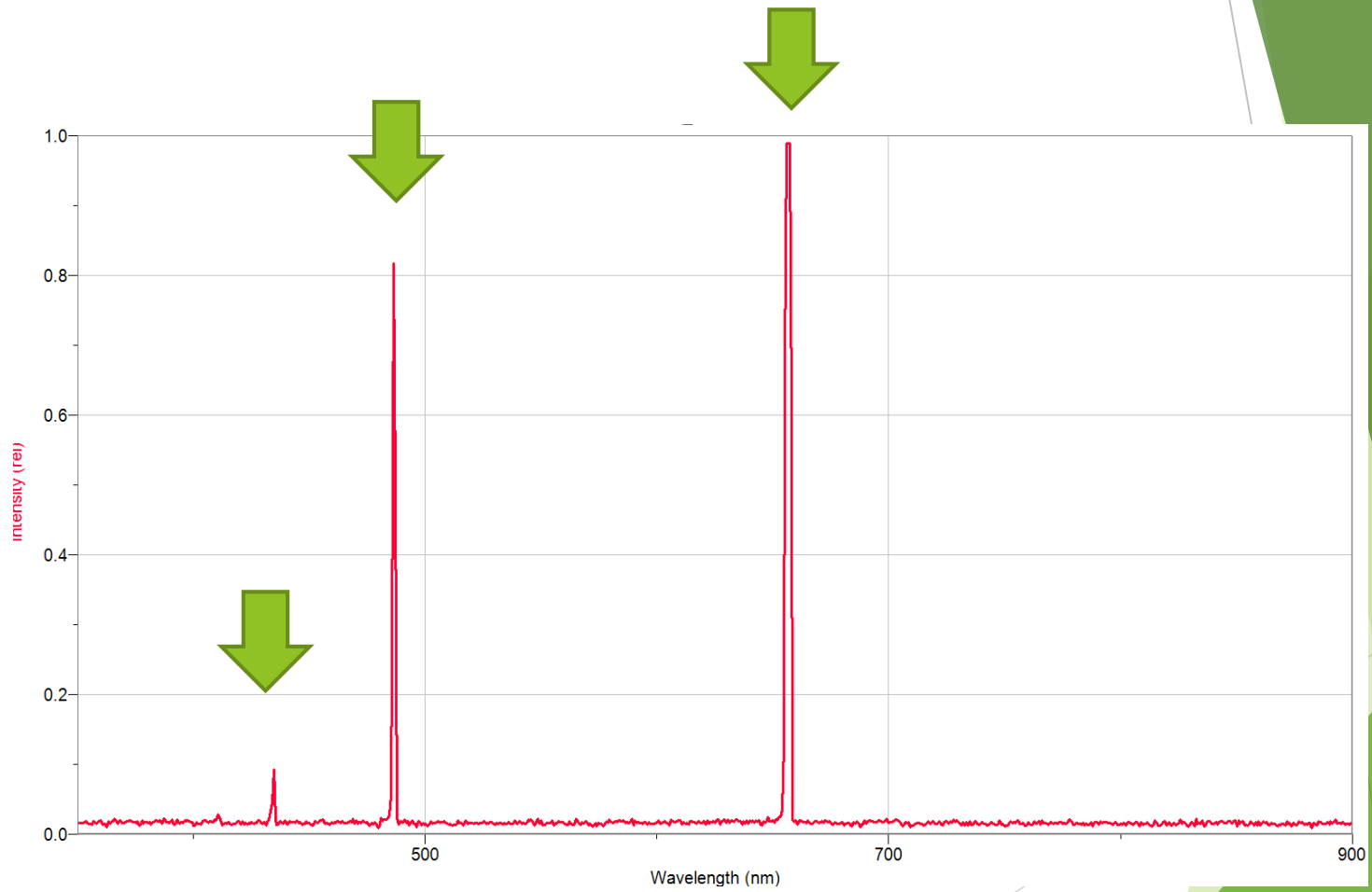
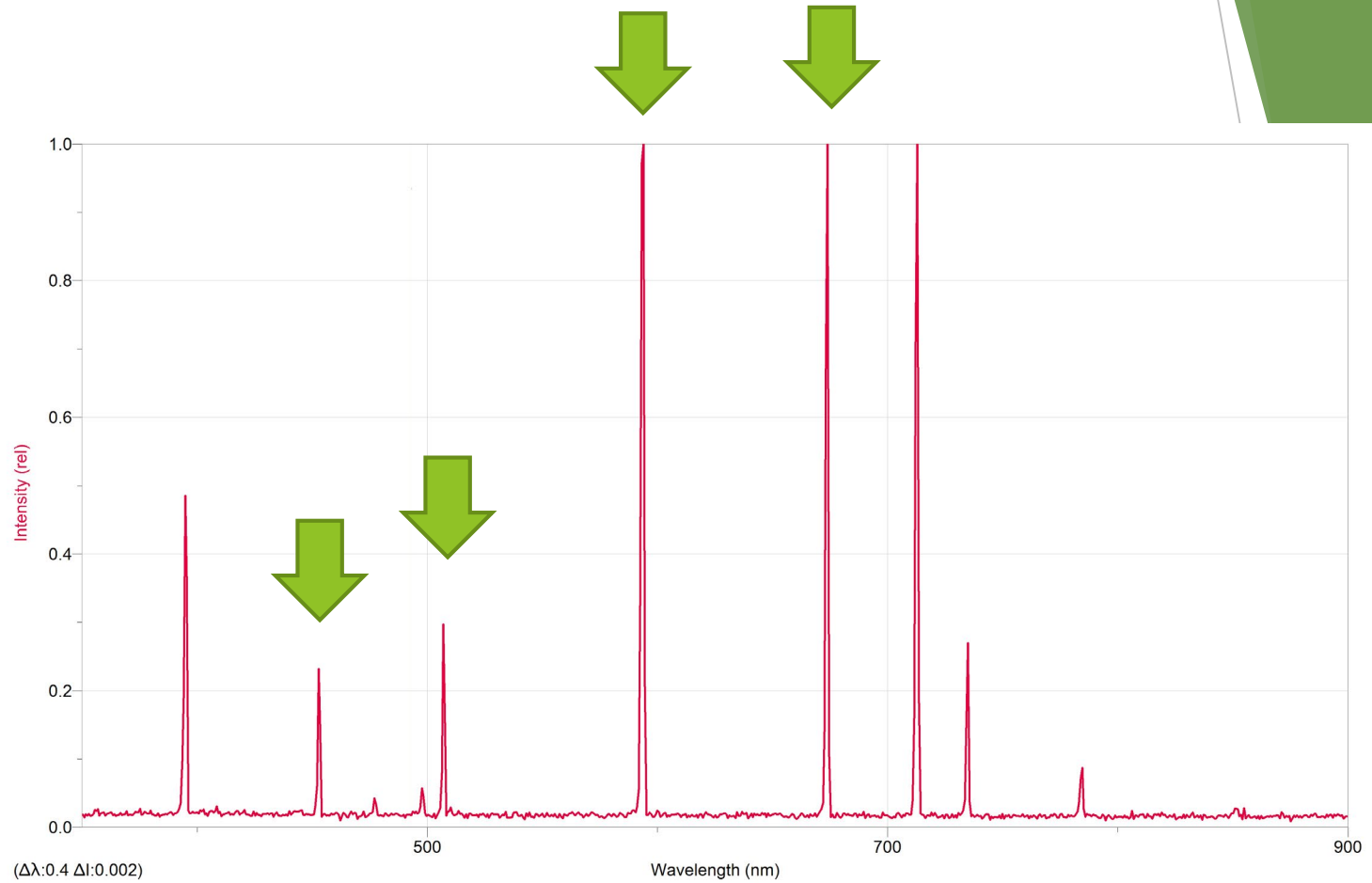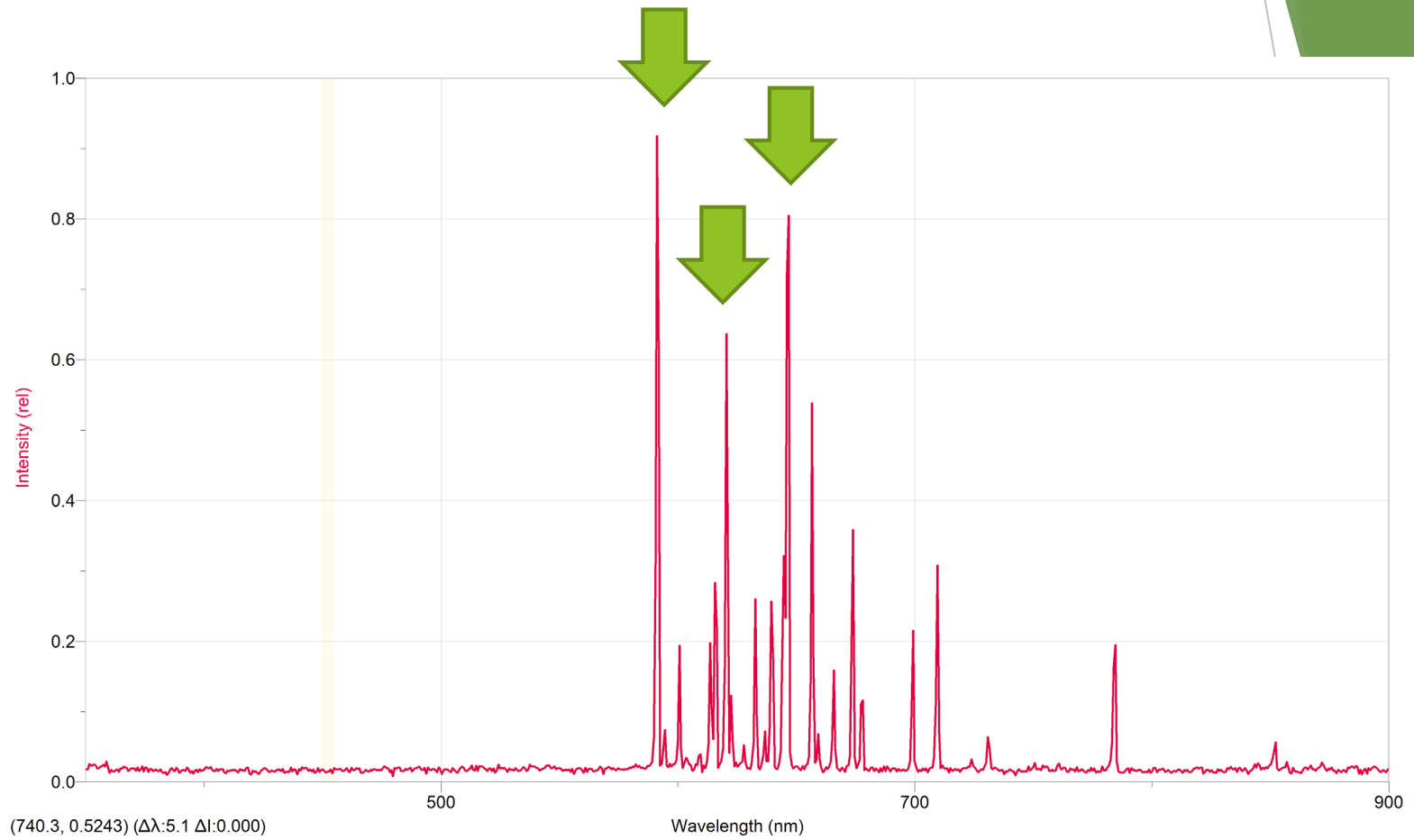**1. Observing real spectra via the fiber optic cable of the spectrometer with *Logger Pro* program**
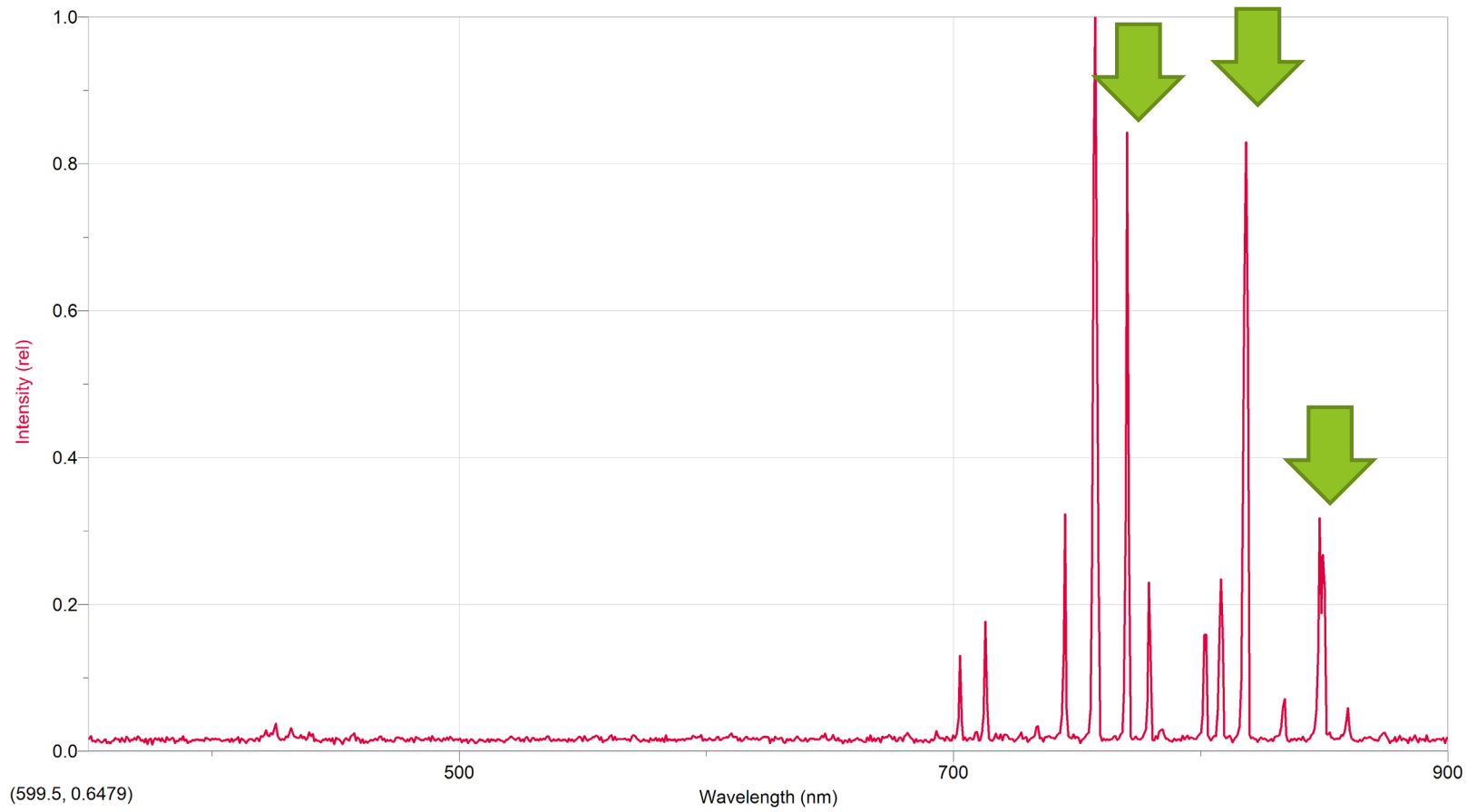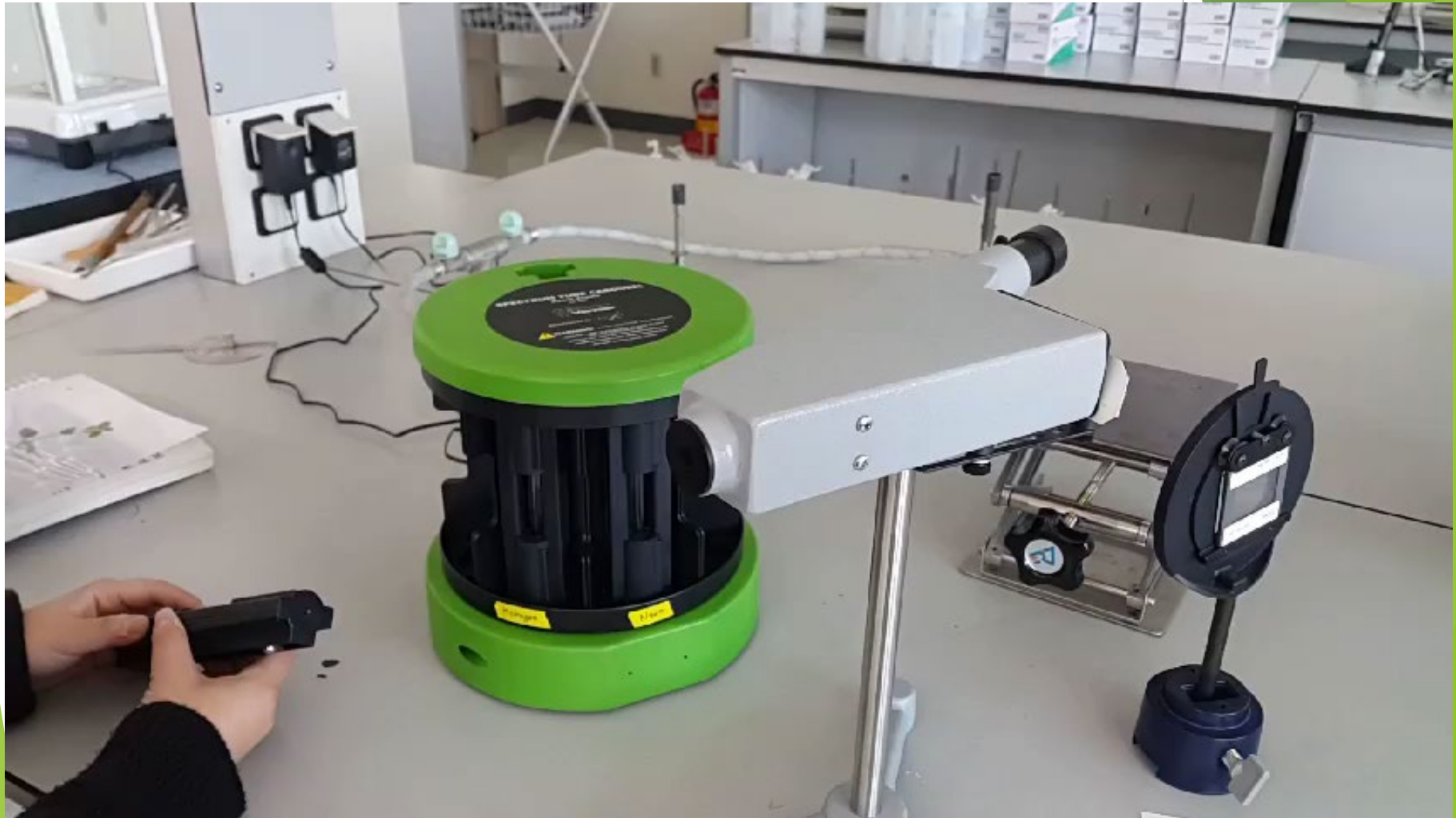
# In-screen Recording

1) Hydrogen

2) Helium

3) Neon

4) Argon

2. Observing real spectra through the spectroscope

Spectrum Carousel

C. Infrared Spectra of Compounds (Homework)

Match of molecules with infrared spectrum (Figure D3.5A~5D). The absorption bands characteristic of atoms in bonds are listed in **Table D3.2**, page 158, to assist in the match.

H_3C-CH_3 H_3C-OH

Molecules

$H_3C-O-CH_3$ $H_3C-\overset{\overset{O}{\|}}{C}-CH_3$
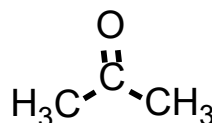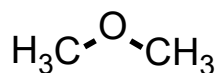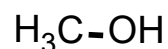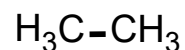
Table D3.2 Infrared Absorption Bands for specific Atoms in Bond Arrangements in Molecules

Atoms in Bonds	Wavenumbers (cm^{-1})	Wavelengths (µm)
O-H	3,700 to 3,500	2.7 to 2.9
C-H	3,000 to 2,800	3.3 to 3.6
C=O	1,800 to 1,600	5.6 to 6.2
C-O	1,200 to 1,050	8.3 to 9.5
C-C	1,670 to 1,640	6.0 to 6.1

■ Video clip

About molecular structures

- **VSEPR Theory**
- **Polarity**
- **Hybrid orbitals**
- **Molecular orbitals**

(From Standard Deviants, DVD, Learn CHEMISTRY 3)

D. Structure of Molecules and Molecular Ions

1. Five basic structures

By using molecular model set provided by TA, construct the five basic three-dimensional structures shown in **Table D3.3**, page 159.
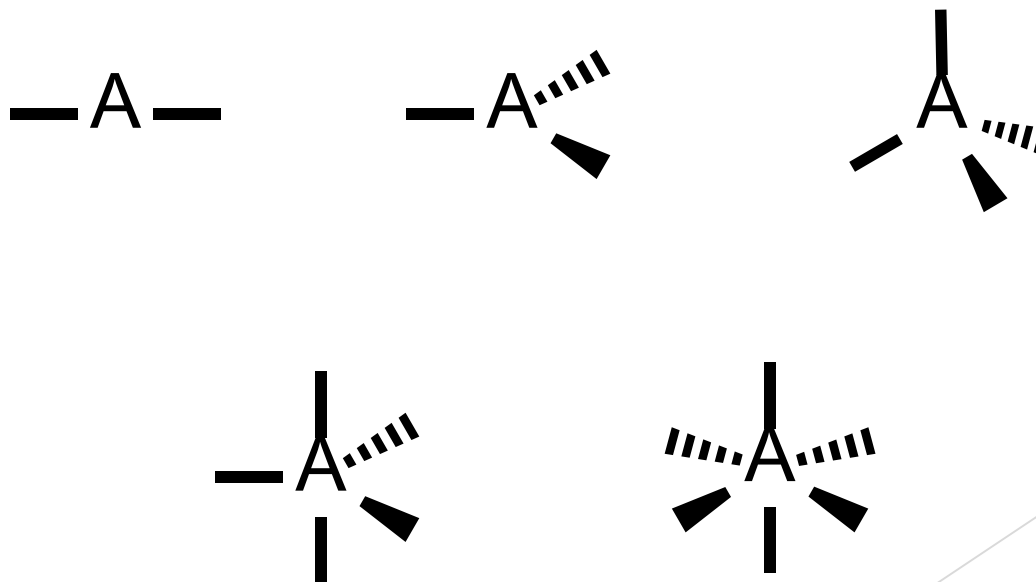
Five Basic three-dimensional structures from Table D3.3

2. Determine three dimensional structures

On a separate sheet of paper, set up the following table (with eight columns) for each of the molecules/molecular ions in 'D. Structure of Molecules and Molecular ions' on the **Report Sheet** (164p.) that are assigned to your group.   Determine their geometric shapes and approximate angles by using the molecular model set and a protractor.

molecule or molecular Ion	Lewis Structure	Valence Shell Electron Pairs	Bonding Electron Pairs	Nonbonding Electron Pairs	VSEPR Formula	Approx. Bond Angle	Geometric Shape
CH_4	H:C:H with H above and H below	4	4	0	AX_4	109.5 °	tetrahedral
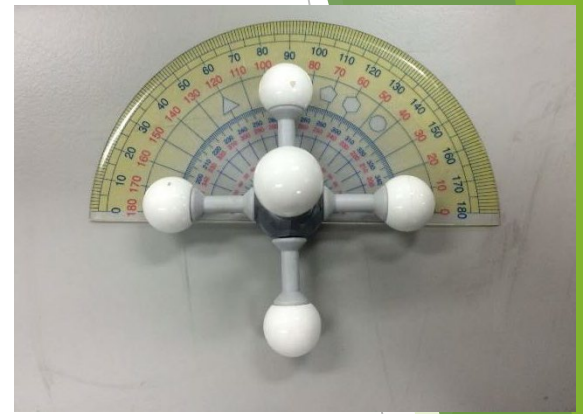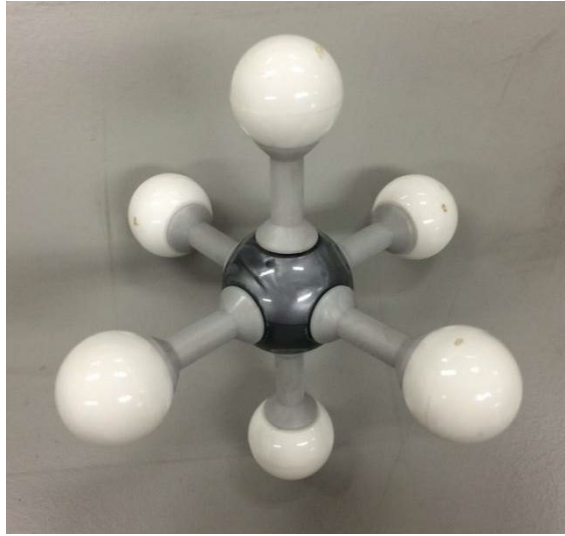
Experimental Results

You indirectly can obtain some results and data sets from the experimental video clips and pictures conducted by TA. Both qualitative and quantitative data must be included in your lab report.

1. Molecular structure and bond angle
- How to make molecular structure model

1) CO_2

2) COCl$_2$

3) CH$_4$

4) PCl$_5$

5) SF$_6$
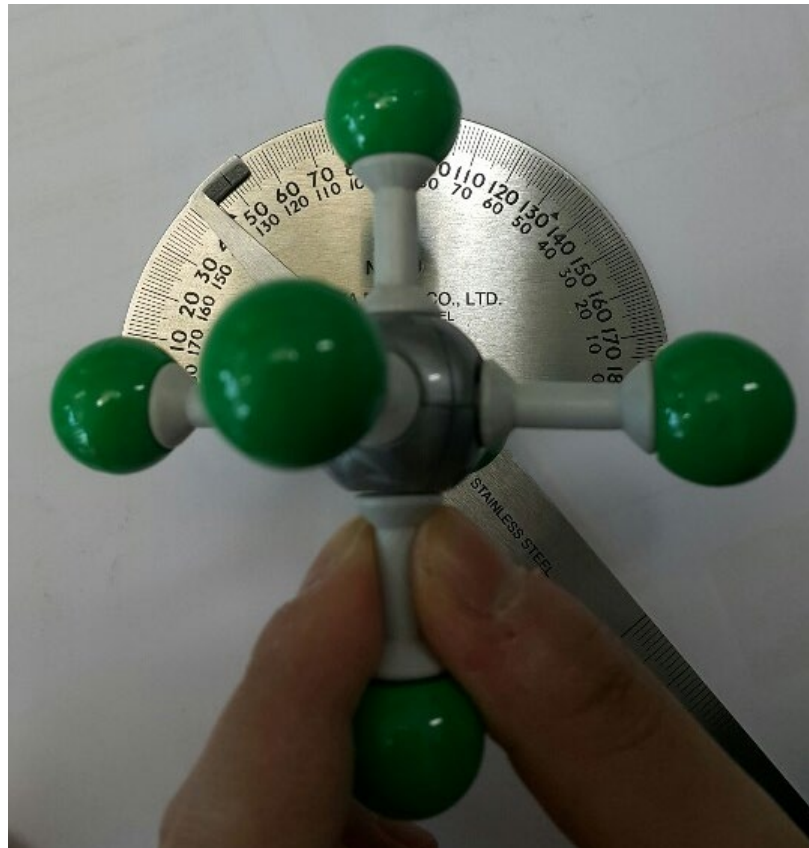
REPORT SHEET

A. The Mercury Spectrum

TA's approval of the wavelength grid of the spectra on the color plate (back cover)

B. *The Spectra of Elements*

1. Spectrum number (   ) is the emission line spectrum for hydrogen on the color plate.
   What are the wavelengths and colors of the emission lines of the visible spectrum of hydrogen?

2. *Identification of Spectra*

a. Spectrum number (   )
Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

b. Spectrum number (   )
Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

C. Match of Molecule with Infrared Spectrum

Complete the following table.

Molecule Assigned	Atom-in-Bond Arrangements	Absorption Bands (cm^{-1})	Infrared spectrum Figure No.

Observing Real Spectra through the spectroscope

Spectrum of Hydrogen
   Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

Spectrum of Helium
   Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

Spectrum of Neon
   Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

Spectrum of Argon
   Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

Observing real spectra *via* the fiber optic cable of the spectrometer with *Logger Pro* program

Spectrum of Hydrogen
    Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

Spectrum of Helium
    Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

Spectrum of Neon
    Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

Spectrum of Argon
    Intense lines in the spectrum: (   )nm; (   )nm; (   )nm; (   )nm; (   )nm; (   )nm;

D. Structure of Molecules and Molecular Ions

On a separate sheet of paper, set up the following table (with eight columns) for the molecules/molecular ions that are assigned to you/your group. The central atom of the molecule/molecular ion is italicized.

Molecular or Molecular Ions	Lewis Structure	Valence Shell Electron Pairs	Bonding Electron Pairs	Nonbonding Electron Pairs	VSEPR Formula	Approx. Bond Angle	Geometric Shape
1. CH_4							

D-1. *Complete the table (as outlined above) for the following molecular/molecular ions, all of which obey the Lewis octet rule. Complete 4 ones that are assigned by your TA.*

D-2. *Complete the table (as outlined above) for the following molecular/molecular ions, none of which obey the Lewis octet rule. Complete* 5 molecular/molecular ions *that are assigned by your TA.*

D-3. *Complete the table (as outlined above) for the following molecular/molecular ions. No adherence to the Lewis octet rule is indicated. Complete* 5 molecular/molecular ions *that are assigned by your TA.*

D-4. *Complete the table (as outlined above) for the following molecular/molecular ions. For molecules of molecular ions with two or more atoms considered as central atoms, consider each atom separately in the analysis according to Table D3.3. Complete* 5 molecular/molecular ions *that are assigned by your TA.*