LAB 3: RAMAN SPECTROSCOPY

LAB GOALS

Raman spectroscopy is a powerful tool for identifiying the vibrational and rotational energies within a material. In this lab, you will learn to work with a laser, optics, and a spectrometer. You will measure the Raman spectra of various materials in order to identify them and learn about their molecular structure.

In Week 1 of this experiment you will make some absorption measurements that characterize the two optical filters. You will then set up your optical train, calibrate your spectrograph and take the Raman spectrum of three known plastics and an unknown.

This is a 2 week lab. You will work with partners for this lab. There is a 30 minute prelab lecture on BrightSpace. There will be a 10 minute quiz at the beginning of lab of the first lab.

You will use Jupyter as your lab notebook again. Use Jupyter on the lab computers because you will be importing pictures from the computer software. Save the Jupyter notebook to the desktop to make your life easier.

Upload your Jupyter notebook to BrightSpace as by PDF by the end of each lab day. You and your partner can submit the same lab notebook. Write the name of your lab partner at the top somewhere.

1. Transmission Properties of Bandpass & Notch Filters

- **Never touch the surface of any lens, mirror or filter. Be extremely careful, the cost of a filter is over $200, and they are difficult to clean.**

You are going to use two optical filters in this lab, a bandpass and a notch filter. In this part of the lab, you are going to use an absorption spectrometer to measure the transmission properties of both filters in order to figure out which one is which.

1) Select filters F1 and F2 from the set of optical components and take them to the absorption UV-VIS spectrometers that you used in the previous lab. Set the spectrometer with the following parameters (NOTE: *some set-ups may have different parameters*):

START	END	INCREM.	INTEGR.	CYCLES	DWELL	DELAY	MONO2
600	700	1.0	500	1	1290	0	0

2) In the LabView folder, open the file "RamanFilters.vi". We will run trials for the light source (blank), the bandpass filter and the notch filter. The percent transmission of these filters will be calculated by:

% Transmittance of filter = 100% • (filter / blank)

3) Start a new code cell and import <u>either</u> the data (ideal if data is in csv format) and plot a figure or import an image of a plot of your data directly.

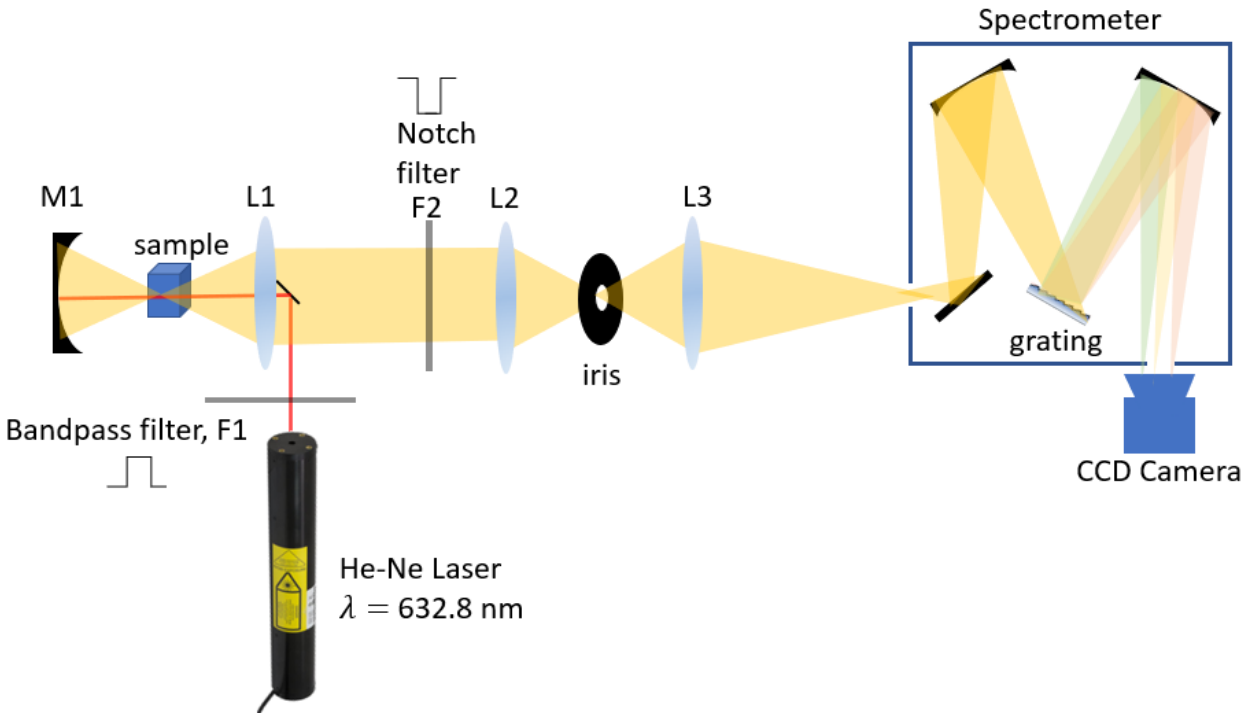
> Hint: You can import images directly by copying and pasting them in a Markdown cell. This works especially well with Window's Snip tool. Just take a snip, copy, open your markdown cell, and paste.

4) From these plots, decide which filter is the bandpass filter and which filter is the notch filter. The bandpass filter allows only a narrow region or "band" of wavelengths to pass. The notch filter acts in a manner opposite to the bandpass filter in which it allows all wavelengths to pass except a narrow region or "notch". Start a new text cell and label it "# Problem 1.3". Record the approximate wavelengths of the pass and notch bands. Use the wavelength value at which 50% of the light is allowed to pass through the filter to define where the regions start or stop. Return these filters to the optical rack.

In your experiment, you will be using the passband in front of the laser to block any wavelengths from the laser outside the passband, since those would appear in our Raman spectrum. You will send the scattered light through the notch filter to get rid of the laser light and Rayleigh scattering, which also is at the laser wavelength.

2. Alignment of the Optics and Spectrometer

In this section, you will align the optics so that the Raman scattered light is focused into the slit of the spectrometer. This is challenging so take your time! Here is a schematic of the experiment you will build and description of each part.



- He-Ne laser: The He-Ne laser emits light with a wavelength of 632.8 nm, or a wavenumber of 1580 cm^{-1}.
- F1: The bandpass filter only allows 632 nm through.
- Prism and sample: The prism glued to lens L1 reflects the laser light towards the sample, which will be placed on the wood block.
- L1 and M1: The scattered light in yellow from the sample is collected by both lens L1 and mirror M1. After the lens L1, the scattered light is collimated, meaning that the light is neither converging nor diverging.
- F2: The notch filter filters out any of the laser light or Rayleigh scattering, so that only Raman scattered light remains, which has a different wavelength than the laser light.
- Spatial filter: The lens L2 focuses the Raman scattered light to a small spot, which is sent through an iris to filter out light coming from any other sources besides our sample.

- L3: The lens L3 focuses the light down to a spot at the entrance slit of the spectrometer, which is 1 cm inside the spectrometer.
- The spectrometer uses a grating to separate different wavelengths and focus them down into an image onto a low noise CCD camera. The reflection angle from a diffraction grating is approximately $\theta \approx \lambda/d$, where d is the spacing of the grooves on the grating.

Lens Table	M1	L1	L2	L3
Focal Length	50 mm	50 mm	50 mm	35 mm

- **Never touch the surface of any lens, mirror or filter.**
- **Do not adjust the sliders that move the optical elements perpendicular to the optical rail.**
- **Double check to see that the laser shutter is closed before inserting optics into the system.**

1) Place the filter that you have determined is the Band Pass Filter (BPF) into the post holder in front of the laser with the mirrored side towards the laser.

2) Open the shutter on the top-front side of the Helium-Neon laser. Adjust the BPF so that the laser passes through the center of the filter and securely tighten down the locking screw on the post holder of F1.

3) Place L1 into post holder on the optical rail. Face the turning prism toward the spectrograph.

4) Adjust the position and height of L1 until the laser beam spot is centered on the prism. You can accomplish this by placing the white card behind the prism and observing the shadow cast by the prism while checking to see that the laser spot is centered on the front of the prism. Tighten down the locking screw on the horizontal slider.

5) Slide the wooden block with the two white focusing cards back and forth along the optical axis on the left side of L1 (i.e. side away from spectrograph) until the reflected red focused spot appears on the spectrograph and is as small as possible.

6) Adjust L1 until the laser spot on the spectrograph is centered both vertically and horizontally on the entrance slit on the monochromator. This is the most critical step.

7) Securely tighten down the locking screw on the post holder of L1.

8) Using a ruler, roughly adjust the center of the post holder for L3 so it is around 10 cm from the monochromator by sliding it along the optical rail. Note that the spectrograph slit is inset by 1 cm from the spectrograph faceplate. Tighten down the locking screw on the horizontal slider just enough to keep the post holder in place.

9) Roughly adjust the center-to-center distance of the post holder for the pinhole (PH) so it is around 15 cm from the monochromator. Tighten down the locking screw on the horizontal slider to keep the post holder in place.

10) Again, roughly adjust the center-to-center distance of the post holder for L2 to a distance equal to the focal length of L2 (50 mm) from the post holder for the pinhole. Tighten down the locking screw on the horizontal slider just enough to keep the post holder in place.

11) Place the pinhole (PH) into the correct post holder. Slowly close the pinhole down by rotating the outer ring. NOTE: The pinhole will not close completely. Do not force it or it will break.

12) Slide the wooden block with the two white focusing cards back and forth to the left of L1 until a focused laser spot appears on the pinhole. Adjust the height of the pinhole so that the focused laser spot is centered on the pinhole. Make sure that the pinhole is perpendicular to the optical rail. NOTE: Do not adjust L1; only adjust the height of the pinhole. Securely tighten down the locking screw of the post holder for the pinhole.

13) Slide the wood block (sample holder) with the white cards all the way to the right, up against the left side of the post holder for L1. This is required for focusing onto the spectrograph.

14) The white focusing card on the sample block represents the focal distance for L1. It is important to keep the focusing card as perpendicular as possible to the sample block. Place L2 into its post holder with the flat side of the lens towards the pinhole. Adjust the height of L2 until the laser spot is roughly centered on the pinhole. Now loosen the slider screw for L2 and gently slide it along the optical rail until a sharp focus is achieved on the pinhole. Tighten down the slider screw and readjust the height and angle of L2 until the laser spot is centered on the pinhole. Securely tighten down the locking screw of the post holder for L2. Now, carefully increase the size of the pinhole so that it is the same size as the laser beam.

15) In a manner similar to Step 14, align and adjust the focus of L3 (again with the flat side of the lens towards the pinhole) to the entrance slit of the spectrograph. Be sure to keep the white focusing card at the marked focal distance of L1 on the sample block. Securely tighten down the locking screw of the post holder for L3.

16) Roughly adjust the center of the post holder for the parabolic mirror (M1) to a distance equal to the focal length of M1 from the line on the sample block (again check to make sure the sample block is placed up against the post holder for L1). Place M1 into its designated post holder, and remove the white cards from the wooden block. Adjust the height of M1 until the laser spot is centered on the pinhole. Securely tighten down the locking screw of the post holder for M1 and tighten down the locking screw on the horizontal. NOTE: The alignment of M1 is not critical; a rough alignment to the pinhole center is all that is needed.

17) Center the post holder for the notch filter about two inches to the right of L1. Place the notch filter into the post holder making sure that the open side is towards the spectrograph and the filter is perpendicular to the optical rail. Place the white focusing card at the focal line and center the notch filter on the scattered laser light that may fall onto the edge of the filter. Securely tighten down the locking screw of the post holder for the notch filter.

18) Carefully place the plastic light shield so that the partially closed end is between F2 and L2. Gently slide the light shield back against the spectrograph. Make sure not to disturb any of the aligned optics.

19) Close the laser shutter.

3. Calibration of the Spectrometer

The spectrometer will focus different wavelengths to different pixels on the CCD camera. We will need to use a calibration source in order to figure out which pixel corresponds to which wavelength or wavenumber. We will use a neon lamp as the calibration source because it emits visible photons at discrete wavelengths when excited in the region of wavelengths that we will be measuring. By using a neon calibration graph, you will match the wavelengths for specific neon peaks with their corresponding pixels from the CCD camera.

Before we are able to calibrate our window, we must first acquire a neon spectrum. DO NOT adjust the micrometer setting on the spectrograph at any time or you will have to recalibrate the spectrograph and retake all of your data!

1) In the "CCDOps" program, check to see that the camera temperature is -4.0 degrees Celsius by looking in the Status window. Click on the "Grab" icon, and set the exposure time to 0.30 seconds. DO NOT hit return yet or you will acquire a spectrum. Turn the neon lamp ON and place it between the notch filter and the plastic lens cover. Try to center the neon lamp on the optical axis while holding it stable. Click the "OK" button to acquire a spectrum. Once the spectrum is taken, save the file with FILE → Save As… as an ASCII file called "neon.txt" into the folder where your Jupyter notebook is saved.

2) Open the Jupyter notebook called "raman.ipnyb" on your desktop or download it from Brightspace. Copy the first cell into your notebook and run it. This cell imports libraries that you have used before (numpy, matplotlib, pands, and scipy), and defines functions for importing and calibrating data in this lab. Do not change these functions.

3) Start a new cell. We are now going to use a function defined in the cell you copied called import_image("filename.txt"), which imports the image, and sums of the rows to make a 1D list of counts. It outputs three variables x_pixels, y_img1d, img. Look at the red text where the function is defined to see a description of these variables.

```
# Import the data and plot vs pixels
x_pixels, y_img1d, img = import_image("neon.TXT")

# Plot original image
plt.imshow(img)
plt.show()

# Plot image summed over rows
plt.plot(x_pixels, y_img1d) # sum over rows
plt.title('Neon Calibration Spectrum')
plt.xlabel('pixels')
plt.ylabel('counts')
plt.grid()
plt.show()
```

4) Start a new cell. You should several peaks in the 1D plot of the image. We are now going to use a function called 'peak_finder(y_img1d, threshold)' to output the pixel locations of those peaks. You must enter a threshold value to find peaks that go above that threshold. The function outputs a spectrum plot with a horizontal line drawn at the threshold value. **Note that you should change the value of 'threshold' to obtain about 6 peaks (you will need at least 4, but the more the better). The value below of 1e6 will probably not work for you.** The function will print the list of found peaks and mark them in a plot.

```
# Find the peaks
peaks = peak_finder(y_img1d, threshold=1e6)
```

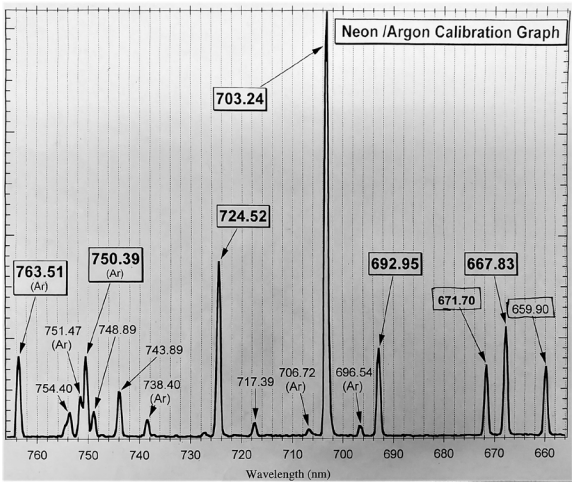
5) Start a new cell. Now you have a list of pixels corresonding to the peaks in the neon spectrum. Look at the neon spectrums below to identify the wavelength in nm of each peak. Make a numpy list of those peaks in nm, which will look something like

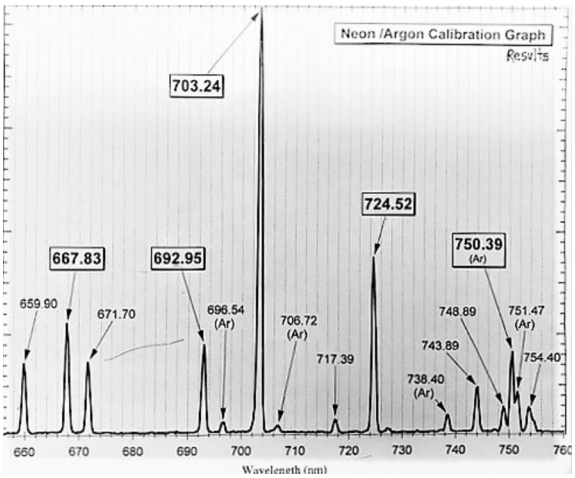
```
wavelengths = np.array([763.51, 750.39, 724.52, 703.24, 692.95, 671.70, 667.83])
```

Note that the length of 'wavelengths' should be the same length as 'peaks', because every wavelength should correspond to a peak pixel location.

Make a quick plot of 'peaks' vs 'wavelengths' to make sure it is linear. We know it should be linear because the reflection angle from a grating is approximately $\Delta\theta \approx \lambda/d$, where d is the spacing of the grooves on the grating.

Neon spectrum (the wavelength axis of the left and right panel are just flipped):





6) Now you have a list of pixel location of the peaks and a list of the corresponding wavelengths, which is approximately linear. We are now going to use a function called 'calibrate_pixel_to_wavelength()' that fits a polynomial model to this data, and then uses that model to convert all the pixels in 'x_pixels' to wavelenghts. See the red text in the function definition for more information.

```
x_wavelengths = calibrate_pixel_to_wavelength(x_pixels, peaks, wavelengths)
plt.plot(x_wavelengths, y_img1d) # sum over rows
plt.xlabel('Wavelength (nm)')
plt.ylabel('Counts')
plt.title("Neon spectrum with pixels calibrated to wavelength")
plt.grid()
plt.show()
```

7) Convert variable 'x_wavelengths' to wavenumbers, and call it 'x_wavenumbers'. A wavenumber has units cm^-1, and is defined as $\frac{1}{\lambda(cm)}$, where the wavelength λ is in units cm. Right now 'x_wavelengths' is in units nm. Note that I have already defined nm=1e-9 and cm=1e-2 for you in the imported cell. Now plot the neon callibration data 'y_img1d' vs 'x_wavenumbers' and label your axes and give it a title.

8) Create a new variable 'x_shifted' which subtracts the laser frequency to get difference frequency from the laser frequency. As long as you don't change the alignment of the spectrometer, you can now use this variable 'x_shifted' for all of your data.

```
x_shifted = 15803 - x_wavenumbers
```

4. Raman Measurement of Plastics

The identification of plastics is important in recycling programs because different plastics cannot be mixed together for processing. Raman spectroscopy is ideally suited for the task of identifying plastics because each plastic presents a unique vibrational fingerprint that allows it to be easily characterized. You will acquire the spectrum of three known plastics, polymethylmethacrylate (PMMA), polycarbonate (PC), and Polyethylene Terephthalate (PETE). Then you will acquire the spectrum of an unknown plastic, and by comparing the unknown spectrum to the spectra of the known plastics, you will determine the type of plastic that the unknown is made of.

Now that we have calibrated the pixels to wavelengths, we can begin collection of Raman spectra from our plastics. Initially we will have to acquire a background blank so that fixed pattern noise or any light leaks into our system can be removed from our Raman spectrum. Once this background blank has been collected and loaded, we will then subtract the background blank off all the Raman spectra that we acquire.

Acquisition of Background Blank

1) Begin by making sure the shutter on the laser is <u>open</u>, and the black cardboard box is over the sample holder. Click on the CCDOps program, click the "Grab" icon and set the exposure time to 60 seconds; click the "OK" button to acquire a background blank. Save this background spectrum with FILE → Save As… as an ASCII file called "background.txt" in the same folder as your Jupyter notebook.
2) Start a new cell. Import the background image and name the 1D image array 'y_background.' You will later subtract this from your Raman spectrum. In the same cell, plot the background spectrum and label the axis and title.

```
_, y_background, _  = import_image("background.txt")  # import_image outputs 3 variables, and we use _ to ignore 2 of them
plt.plot(x_shifted, y_background)
plt.show()
```

ACQUISITION OF PLASTIC SPECTRA

1) Open the shutter on the laser and place the PMMA sample at the focal line on the sample block. If the sample will not stand on its own, use a brace to support it. Use the dock to bring the CCDOps program to the front. Click on the "Grab" icon and set the exposure time to 60 seconds; click "OK" to acquire the plastic's Raman spectrum. Save this PMMA spectrum with FILE → Save As… as an ASCII (.txt) file "PMMA.txt" in the folder with your Jupyter notebook.

   HINT: You should see faint verticle lines, however it is likely that you will not see anything on your first try. Raman scattered light is millions of times less bright than the laser. Make sure the wood is up against L1. Take the notch filter and try to get as much of the red light into the spectrometer slit as possible.

2) Repeat the procedure for the remaining plastics and the unknown in the following order, naming them PC, PETE, and Unknown.

3) Start a new cell and import the four spectra, calling the 1d image array 'y_PMMA', 'y_PC', 'y_PETE', and 'y_Unknown.' Subtract the background from each of these variables, and plot all the background subtracted spectra on the same plot. In the example below, only the PMMA and PC data are plotted, but you will need to include all 4 sets of data.

```
_, y_PMMA, _ = import_image("PMMA.txt")
y_PMMA = y_PMMA - y_background # subtrack the background
plt.plot(x_shifted, y_PMMA)
plt.grid()
plt.xlabel("Wavenumber (cm^-1)")
plt.ylabel("Counts")
plt.title("PMMA")
plt.show()
```

4) You should be able to visually compare the spectra for the three known plastics to that of the unknown and assign the unknown plastic to one of the known types. Start a text cell and discuss which plastic you think the unknown is.

THIS IS THE END OF WEEK 1. UPLOAD YOUR NOTEBOOK TO BRIGHTSPACE AS A PDF. SAVE A COPY OF YOUR FILES AND IMAGES SO THAT YOU CAN USE THEM NEXT WEEK.

WEEK 2

In Week 2, you will measure the Raman spectra of pure acetone, an acetone/water mixture, and an acetone/THF mixture to study the structural changes to the acetone molecule that occur when it is solvated. You will also collect the Raman spectra of *cis*- and *trans*-1,2-Dichloroethylene; in which the *trans* isomer possess a center-of-inversion. This center-of-inversion provides a unique opportunity to study the complimentary behavior between IR and Raman spectroscopies as will be explained later.

Start a new Jupyter notebook. You can copy code that you need from your Jupyter notebook from last week, including the cell with the defintitions and libraries.

1. CALIBRATION OF THE SPECTROMETER

Following the procedure from the first week, use the neon lamp to calibrate the spectrometer. The spectrometer settings might have changed, so you will need to again 1) import the neon image 2) find the peaks with 'peak_finder()', create a calibrated x-axis with 'calibrate_pixel_to_wavelength()', and then convert wavelength to wavenumber in a variable 'x_wavenumbers'. You will use that for all your plots today.

2. RAMAN INVESTIGATION OF ACETONE MIXTURES

- **DO NOT, under any circumstance, open any of the solution vials.**

Raman spectroscopy provides a way to examine the vibrational structure of molecules in situ, in different environments, and examine directly the effect of the environment on chemical bonds. As a case in point, we shall investigate acetone, and see what happens to it on the molecular level when we place it in the hydrogen-bonding environment of an aqueous solution and the polar aprotic solvent tetrahydrofuran (THF).

The Raman spectrum of pure acetone features the following strong bands:

the **C-C-C** symmetric stretch	787 cm^{-1}
the **CH**, bending mode	1430 cm^{-1}
the carbonyl **C=O** stretch	1710 cm^{-1}

In aqueous solution, water protons form hydrogen bonds with the acetone carbonyl oxygen. This can be expected to pull electron density from the C=O double bond, and alter the hybridization of the central carbon. In contrast to water, the aliphatic hydrogens on THF will tend to cluster around the methyl groups of acetone. How might these solvents affect the vibrational spectrum of the acetone? Do you think that we will be able to detect the effects of water-acetone hydrogen bonding and THF-acetone interactions in the Raman spectrum of solvated acetone?

Solution Key for Vials:

Pure Acetone = 1	*cis*-1,2-dichloroethylene = 4
Acetone/H_2O = 2	*trans*-1,2-dichloroethylene = 5
Acetone/THF = 3	

1) **Acquisition of Background Blank**

In order to remove any Raman scattered photons that may result from the glass vials, we must acquire the spectrum of an empty vial. Place the empty vial onto the sample block inside the marked circle. This should leave about 1/3rd of the vial face extending over the focal line. Open the shutter on the laser and slide the vial perpendicular to the optical axis until the series of laser spots on the front of the vial overlap, this ensures that the laser is positioned on the center of the vial. In the CCDOPS program, click on the "Grab" icon and set the exposure time to 90 seconds; click "OK" to acquire the background vial Raman spectrum. Save this Background Vial spectrum with FILE → Save As… as an ASCII (.txt) file called 'BackgroundVial.txt' in the same folder as your Jupyter notebook. Load the background in your Jupyter notebook, like you did last week. Plot the 1D spectrum and label the plot and your axes. The x-axis should be wavenumbers. You will subtract this background plot from the acetone solution spectra.

2) **Acquisition of Acetone Solution Spectra**

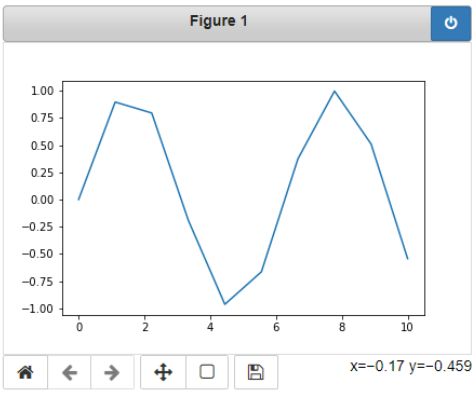
Place pure acetone (solution 1) onto the sample block inside the marked circle leaving about 1/3rd of the vial extending over the focal line, align the vial using the same procedure for the blank vial. In the CCDOPS program, click on the "Grab" icon and set the exposure time to 90 seconds; click "OK" to acquire a Raman spectrum. Save this spectrum with FILE →Save As… as an ASCII (.txt) file as "AcePure" into the folder with your Jupyter notebook. Repeat this procedure for the other acetone solutions (see Solution Key above for identification), naming them AceH2O, and AceTHF. Load the Raman spectra into your Jupyter notebook. Subtract the background spectrum of the empty vial, and plot all three spectra.

Start a text cell and answer these questions. Label each problem.

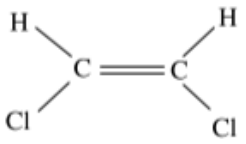
1) How do the peak frequencies shift (relative to pure acetone) for the acetone/water mixture and for the acetone/THF mixture?
2) What physically is occurring to the solvated acetone molecules to cause the frequencies to shift?
3) Why do different solvents cause different shifts in the peak frequencies?

Hint: You will have to estimate the location of different peaks. By running '%matplotlib notebook', the figure will have options at the bottom for zooming. You will need to run '%matplotlib inline' when you are finished to return the Jupyter notebook to the default setting. You also plot grid lines with 'plt.grid()'.

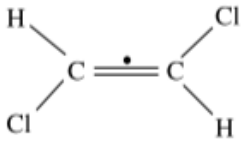
```
%matplotlib notebook
x = np.linspace(0,10,10)
y = np.sin(x)
plt.plot(x,y)
plt.show()
```



3. Raman Investigation of Dichloroethylene Isomers

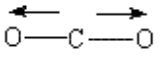


cis –1,2-dichloroethylene



trans –1,2-dichloroethylene

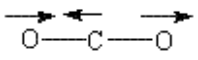
Raman and IR specroscopy are complementary techniques used for fingerprinting molecules. An electromagnetic field consists of an oscillating electric field that interacts with the charges (electrons and protons) in a molecule. The Raman and IR spectra come from changes in vibrations of the molecules due to these forces. Raman spectroscopy comes from measuring the scattered light by vibrating molecues. IR spectroscopy instead comes from measuring the absorption of light by vibrating molecules. For molecules having a center of inversion, such as *trans*-1,2-dichloroethylene, special rules apply. Only those vibration modes which result in changes in the molecule's dipole moment are IR active. The vibrational modes which result in the changes in polarizability are Raman active. This is called the **Mutual Exlusion Principle.** A simple molecule which obeys this principle is CO2, which has an inversion center. The following are its normal modes of vibrations. The IR and raman active modes are indicated below each type of vibration.



Symmetrical stretch

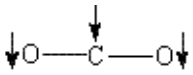
No change in dipole moment therefore IR inactive

There is change in polarisability therefore Raman active

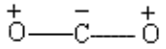


Asymmetrical stretch

There is change in dipole moment therefore IR active but Raman inactive



In plane bending



Out of plane bending

The deformation vibrations of CO_2 are degenerate and appear at the same region (666 cm^{-1}) in the IR spectrum of CO_2. There is no change in polarisability therefore these vibrations are Raman inactive.

For molecules without centers of inversion this complementarity is absent, but one does see differences in peak intensity depending on whether the vibrational modes are mostly changing the dipole moment or the polarizability. In this part of the experiment you will compare the spectral behavior of molecules with and without a center of inversion by acquiring Raman spectra of both *cis*- and *trans*-1,2-dichloroethylene. The IR spectra of these molecules has previously been recorded and you will import them to Jupyter for comparison.

1) Acquisition of Background Blank

Since the *cis*- and *trans*-1,2-dichloroethylene solutions are also contained in similar glass vials as the acetone solutions, we can use the background blank that we acquired with the empty vial for our background subtraction here.

2) Acquisition of Dichloroethylene Solution Spectra

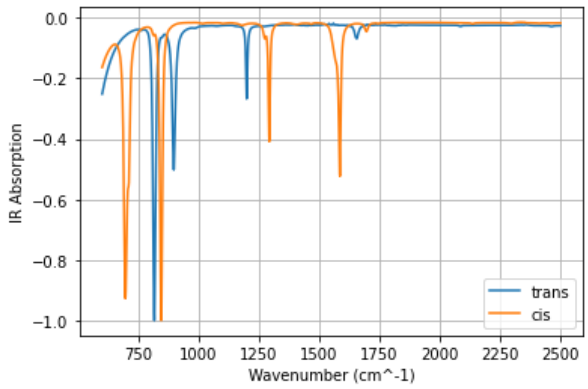
Place the *cis*-1,2-dichloroethylene (solution 4) onto the sample block within the circle, again this should leave about 1/3rd of the vial face extending over the focal line. Align the vial using the same procedure for the blank vial. In the CCDOPS program, click the "Grab" icon and set the exposure time to 90 seconds; click "OK" to acquire a Raman spectrum. Save this spectrum with FILE → Save As… as an ASCII (.txt) file. Name the file cisDCE. Repeat this procedure for the Raman spectrum of the *trans*-1,2-dichloroethylene (solution 5), naming this file transDCE. Load the spectra into your Jupyter notebook, and plot them versus wavenumbers.

3) Import the IR spectra for comparison. The IR data is in "IR_data.csv" which should be on the desktop and on BrightSpace.

```
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np

df = pd.read_csv('IR_data.csv')
#print(df)
IR_trans = df["trans"].to_numpy()
IR_cis = df["cis"].to_numpy()
IR_wavenumber = df["wavenumber"].to_numpy()

# Plot both graphs
plt.plot(IR_wavenumber, IR_trans, label="trans")
plt.plot(IR_wavenumber, IR_cis, label="cis")
plt.xlabel('Wavenumber (cm^-1)')
plt.ylabel('IR Absorption')
plt.grid()
plt.legend()
plt.show()
```



POSTLAB QUESTIONS:

Start a textcell and title it '# Postlab Questions' and answer these questions. Label each problem.

1) What are the frequencies of the peaks that are common in the IR and Raman spectra of *trans*-1,2-dichloroethylene?
2) Does this make sense that trans-DCE should have similar peaks in both IR and Raman spectra? Provide arguments to support your conclusion.
3) What are the frequencies of the peaks that are common in the IR and Raman spectra of *cis*-1,2-dichloroethylene?
4) Does this make sense that cis-DCE should have similar peaks in both IR and Raman spectra? Provide arguments to support your conclusion.

THIS IS THE END OF WEEK 1. UPLOAD YOUR NOTEBOOK TO BRIGHTSPACE AS A PDF BY THE END OF THE DAY.