

Texas Tech University
 Chemistry 3108
 Section _____

Name _____
 Partners Name _____
 Group Number _____

Experiment 35: Raman Spectroscopy Worksheet

If additional pages are needed to complete this worksheet, be sure to attach them to this worksheet. Each student must complete in a group must complete his/her own worksheet.

Part A: Raman Spectroscopy of Carbon Tetrachloride

1) After obtaining the Raman spectra for CCl_4 , complete the following table for all the peaks in the spectra. Attach your spectrum with this worksheet.

(Attach your spectra to this worksheet. You will have to use Excel to plot them out.)

Wavenumber (cm^{-1})	I^*	ΔI^{**}	Polarized (P) Or Depolarized (DP)

*Intensity relative to baseline. These are the intensities of the peaks of the spectrum.

Minus if peak points down, plus if peak points up. ΔI is obtained by clicking **Polarization on the acquisition window.

1. Assignment of Lines

Note that the subscript i on the wavenumber $\tilde{\nu}_i$ does not correspond to the order of the lines in the Raman spectrum but instead corresponds to the label of the vibrational mode as indicated in Table 1 in the textbook.

a) Give the wavenumbers of the peaks associated with the doublet. Calculate the average wavenumber of the peaks. (This average wavenumber will be used in the assignment of the vibrational modes.)

b) Give the wavenumbers of the stretching modes.

c) Give the wavenumbers of the bending modes.

d) Based on the polarization measurement, what are the wavenumbers of the $\tilde{\nu}_1$ -mode and $\tilde{\nu}_3$ -mode? Briefly explain your reasoning for these assignments.

d) What are the wavenumbers of the $\tilde{\nu}_2$ -mode and the $\tilde{\nu}_4$ -mode?

e) Which combination of $\tilde{\nu}_1$, $\tilde{\nu}_2$, and $\tilde{\nu}_4$ is involved in the Fermi resonance that gives rise to the doublet? Explain your answer.

2. Calculation of vibrational force constants .

(Attach separate pages to this worksheet showing your calculations)

a) Using Equations 12 and 13 on p. 389, calculate the force constants k and $k_8/\text{Å}^2$. (Make sure you are using the correct units for frequencies and masses (see p 390).)

b) Using Equations 14 and 15 on p. 389, calculate the force constants k and $k_8/\text{Å}^2$. (Make sure you are using the correct units for frequencies and masses (see p 390).)

c) How do the values of k and $k_8/\text{Å}^2$ obtained with Equations 12 and 13 compare with the values of k and $k_8/\text{Å}^2$ obtained with Equations 14 and 15. If there are discrepancies, give possible reasons for the discrepancies.

PART B: Analysis of Unknown using Raman Spectroscopy

In this part of the experiment, the Raman spectra will be taken of several common solvents. After analysis, the spectra will be used to determine the components of an unknown sample.

Procedure

a) Take the Raman spectra of neat acetone, methanol, acetonitrile, chloroform, and 1,3-dichlorobenzene and the Raman spectrum of your unknown. Set the integration time on the instrument to 10 seconds and don't forget to take a reference spectrum,. Attach your spectra at the end of this worksheet.

b) Fill in the table below noting the wavenumbers of up to six of the most prominent peaks in the spectrum

Solvent	Peak #1 (cm^{-1})	Peak #2 (cm^{-1})	Peak #3 (cm^{-1})	Peak #4 (cm^{-1})	Peak #5 (cm^{-1})	Peak #6 (cm^{-1})
acetone						
acetonitrile						
chloroform						
1,3-dichlorobenzene						
methanol						

c) List the peaks in your the Raman spectrum of your unknown:

d) Using the information in the above table, determine the components of your unknown. Explain your reasoning.

References

1. Ferraro, J. R.; Nakamoto, K. *Introduction to Raman Spectroscopy*, Academic Press, Inc.: San Diego, CA, 1994.
2. Dollish, F. R.; Fateley, W. G.; Bentley, F. F. *Characteristic Raman Frequencies of Organic Compounds*; John Wiley & Sons: New York, NY 1974.