Chemistry 14CL

Infrared Spectroscopy Computer Lab

Group Work and Report (Only one set of Worksheet per Group)

Instructions for filling out the Infrared Spectroscopy Worksheets:

(1) One of your group members will need to log on to the computer by using the UCLA login name. Password is the student's ID.

(2) Now open the specified molecules with PC Spartan '14 software. To open the file in the **CHEM IR** folder:

(i) Go to the desktop and open the "**Shared Coursework Files"** folder

(ii) Right click on the "**CHEM IR**" and select *COPY*

(iii) Open "**My Computer**" on the desktop and *PASTE* the **CHEM IR** folder in your *Z:* drive

The CHEM IR folder should now be in the *Z:* drive as a folder

- Now open SPARTAN '14. Within SPARTAN open **Carbon dioxide (STO3G)** molecule file.
- On the tools bar, click on "**Display**", select "**Spectra**" and select "**IR**".
- Start from the highest wavenumber (i.e., start from the bottom of the list. You may need to use the scroll bar) and work your way up to the smallest wavenumber.

There is no need to convert the wavenumber on the screen to frequency. Simply copy the wavenumbers on the worksheets.

Read the procedures on page 86-88 before you start working. You should go through all the molecules and fill out the Infrared worksheets on the following pages in the following order:

Carbon Dioxide (STO3G), Carbon Dioxide (PM3), Acetic Acid, Propionamide and Allyl Benzoate

Use a **separate** Infrared worksheet for **each** molecule. **Do not re-save any molecule.** When you completed one molecule, it is important for you to remember to close the file and open a new file for the new molecule.

All the instructions are listed on page (**Please read them!**) The following are only the changes:

For the **caffeine** molecule, only measure the bond length and angles by using PC SPARTAN. Your group will also need to analyze the infrared spectrum of caffeine for the post-lab (no need to use PC SPARTAN). The literature infrared spectrum is attached as the last page in this handout.

For **allyl benzoate**, you only need to find out where the aromatic rind stretch begins and ends. In other words, find the range where the C-H and C=C stretches begins and ends.

Important: The completed infrared worksheets are only part of your post-lab for this assignment. Check the course website for the complete detailed guidelines before you turn in anything to the teaching assistant.

Name of the Group Members: _____

TA: _____

Name of Compound: **Carbon Dioxide (STO3G)** Empirical Formula: _____

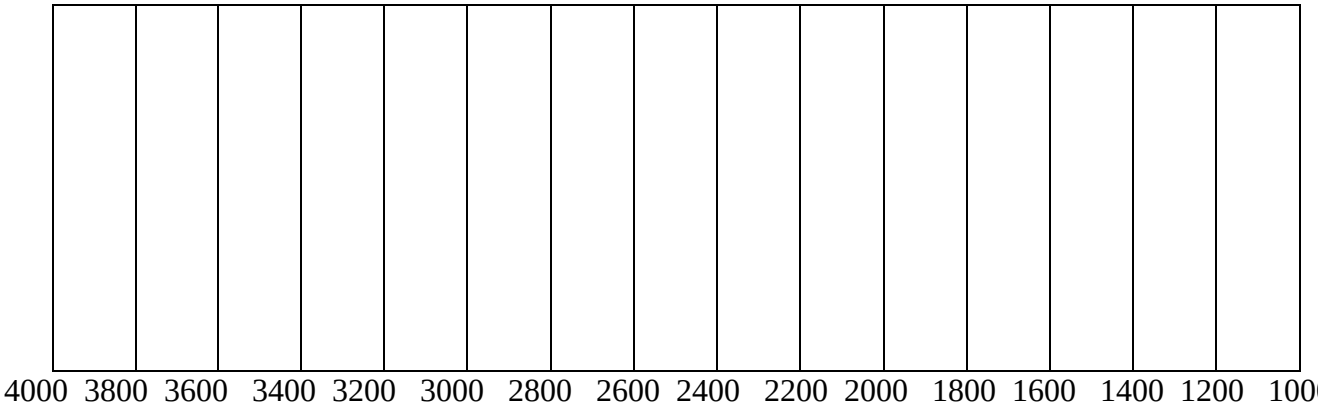
Degree of Unsaturation: _____

Use the PC SPARTAN software and fill out the following information (Refer to the lecture guide for specific types of vibrations. Use the back of the page for more space)

Wavenumber (cm^{-1})	Atoms involved (**Be Specific**)	Types of Vibration (**Be Specific**)

_____
_____
_____
_____
_____
_____
_____
_____
_____
_____
_____
_____

Complete the following IR chart by drawing a vertical line at the appropriate location for EACH of the wavenumber (only focus on the ones between 1000-4000 cm^{-1}) you just completed on this worksheet. Once you draw all lines, identify the lines by GROUPING them according to the various vibrational motions of the functional groups (i.e., OH stretch, CH_3 symmetric, etc.)



Name of the Group Members: _____

TA: _____

Name of Compound: **Carbon Dioxide (PM3)** Empirical Formula: _____

Degree of Unsaturation: _____

Use the PC SPARTAN software and fill out the following information (Refer to the lecture guide for specific types of vibrations. Use the back of the page for more space)

Wavenumber (cm^{-1})	Atoms involved (**Be Specific**)	Types of Vibration (**Be Specific**)

_____
_____
_____
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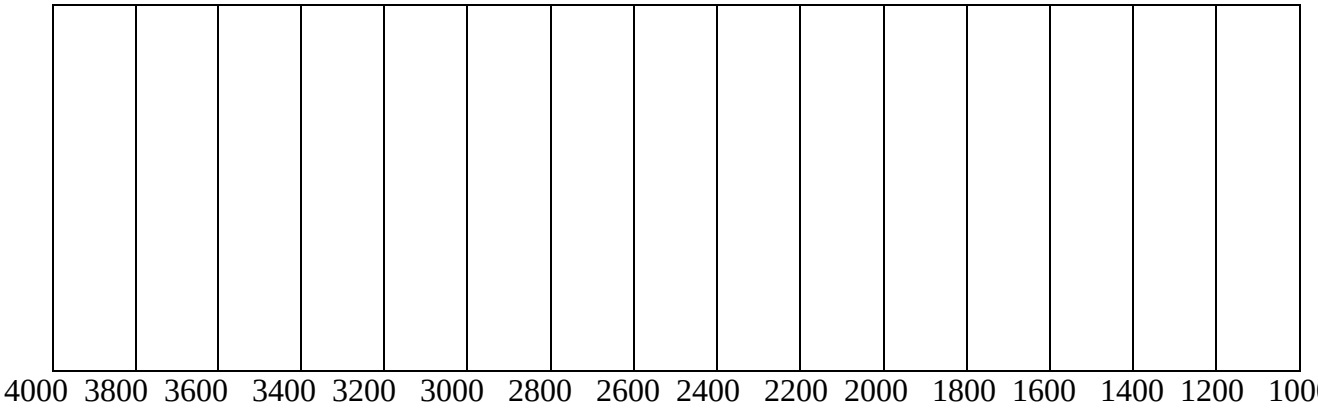
_____
_____
_____
_____

Complete the following IR chart by drawing a vertical line at the appropriate location for EACH of the wavenumber (only focus on the ones between 1000-4000 cm^{-1}) you just completed on this worksheet. Once you draw all lines, identify the lines by GROUPING them according to the various vibrational motions of the functional groups (i.e., OH stretch, CH_3 symmetric, etc.)



Name of the Group Members: _____

TA: _____

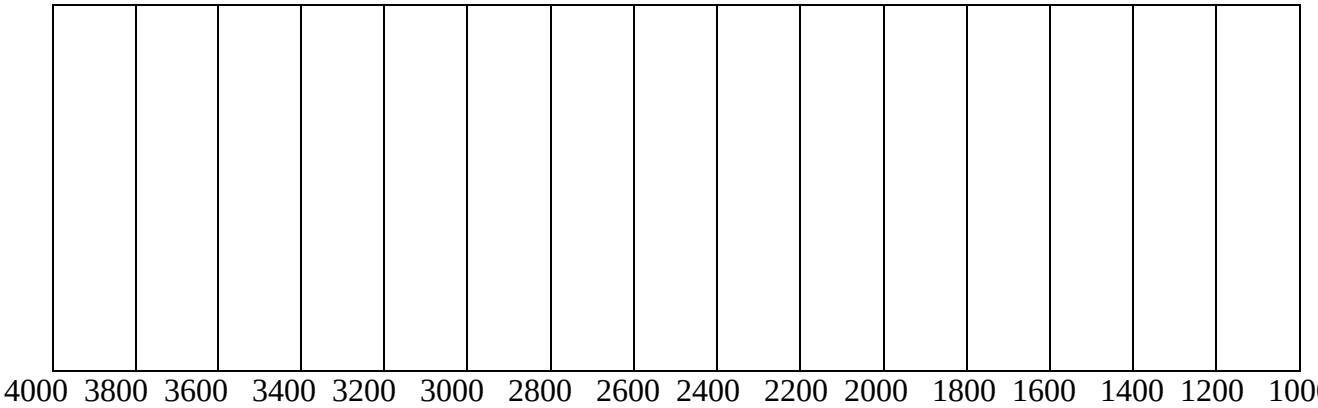
Name of Compound: **Acetic Acid** Empirical Formula: _____

Degree of Unsaturation: _____

Use the PC SPARTAN software and fill out the following information (Refer to the lecture guide for specific types of vibrations. Use the back of the page for more space)

Wavenumber (cm^{-1})	Atoms involved (**Be Specific**)	Types of Vibration (**Be Specific**)

Complete the following IR chart by drawing a vertical line at the appropriate location for EACH of the wavenumber (only focus on the ones between 1000-4000 cm^{-1}) you just completed on this worksheet. Once you draw all lines, identify the lines by GROUPING them according to the various vibrational motions of the functional groups (i.e., OH stretch, CH_3 symmetric, etc.)



Name of the Group Members: _____

TA: _____

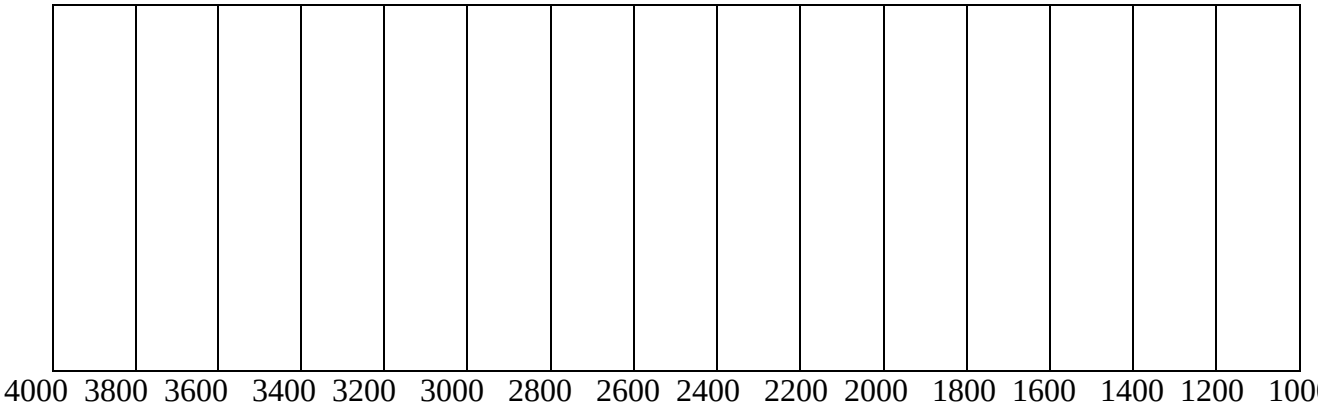
Name of Compound: **Propionamide** Empirical Formula: _____

Degree of Unsaturation: _____

Use the PC SPARTAN software and fill out the following information (Refer to the lecture guide for specific types of vibrations. Use the back of the page for more space)

Wavenumber (cm^{-1})	Atoms involved (**Be Specific**)	Types of Vibration (**Be Specific**)

Complete the following IR chart by drawing a vertical line at the appropriate location for EACH of the wavenumber (only focus on the ones between 1000-4000 cm^{-1}) you just completed on this worksheet. Once you draw all lines, identify the lines by GROUPING them according to the various vibrational motions of the functional groups (i.e., OH stretch, CH_3 symmetric, etc.)



Name of the Group Members: _____

TA: _____

Name of Compound: **Allyl Benzoate** Empirical Formula: _____

Degree of Unsaturation: _____

Use the PC SPARTAN software and fill out the following information (Refer to the lecture guide for specific types of vibrations. Use the back of the page for more space)

Wavenumber (cm^{-1})	Atoms involved (**Be Specific**)	Types of Vibration (**Be Specific**)

_____
_____
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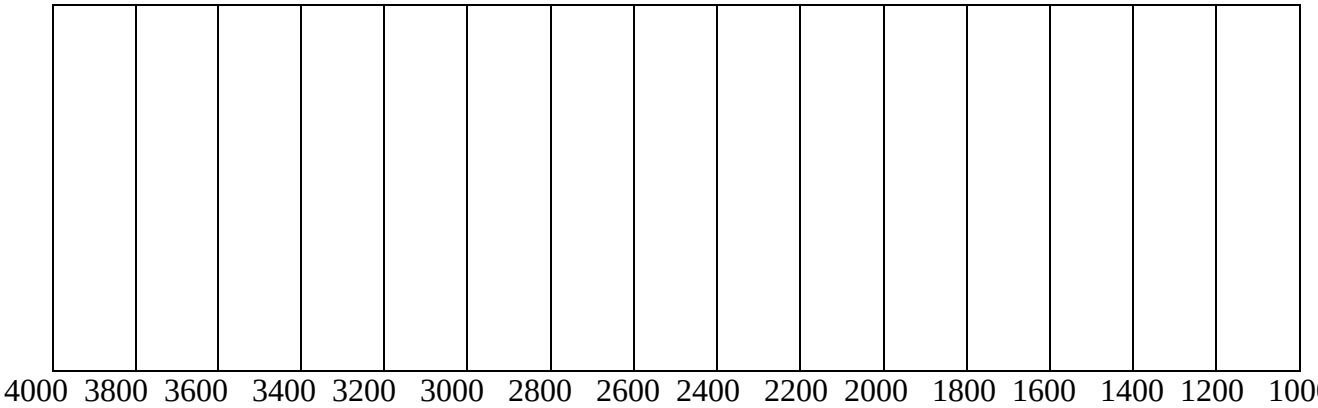
_____

Complete the following IR chart by drawing a vertical line at the appropriate location for EACH of the wavenumber (only focus on the ones between 1000-4000 cm^{-1}) you just completed on this worksheet. Once you draw all lines, identify the lines by GROUPING them according to the various vibrational motions of the functional groups (i.e., OH stretch, CH_3 symmetric, etc.)

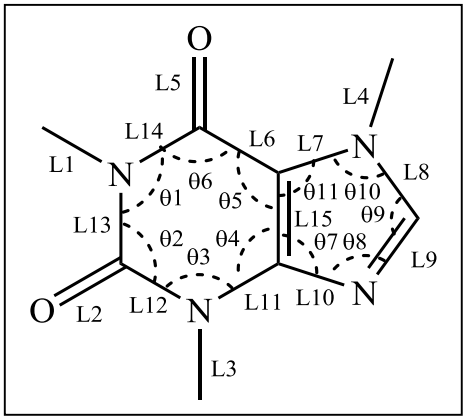


Use this worksheet to fill out the bond length, the bond angles and the strain energy of the caffeine molecule.

(1) **Strain Energy of Caffeine**: _____
(Ask your teaching assistant for assistance if you do not know how to find the strain energy on PC SPARTAN '14)

(2) Complete the following table by using PC SPARTAN to measure the specified bond lengths and bond angles in the caffeine (refer to the diagram shown below)

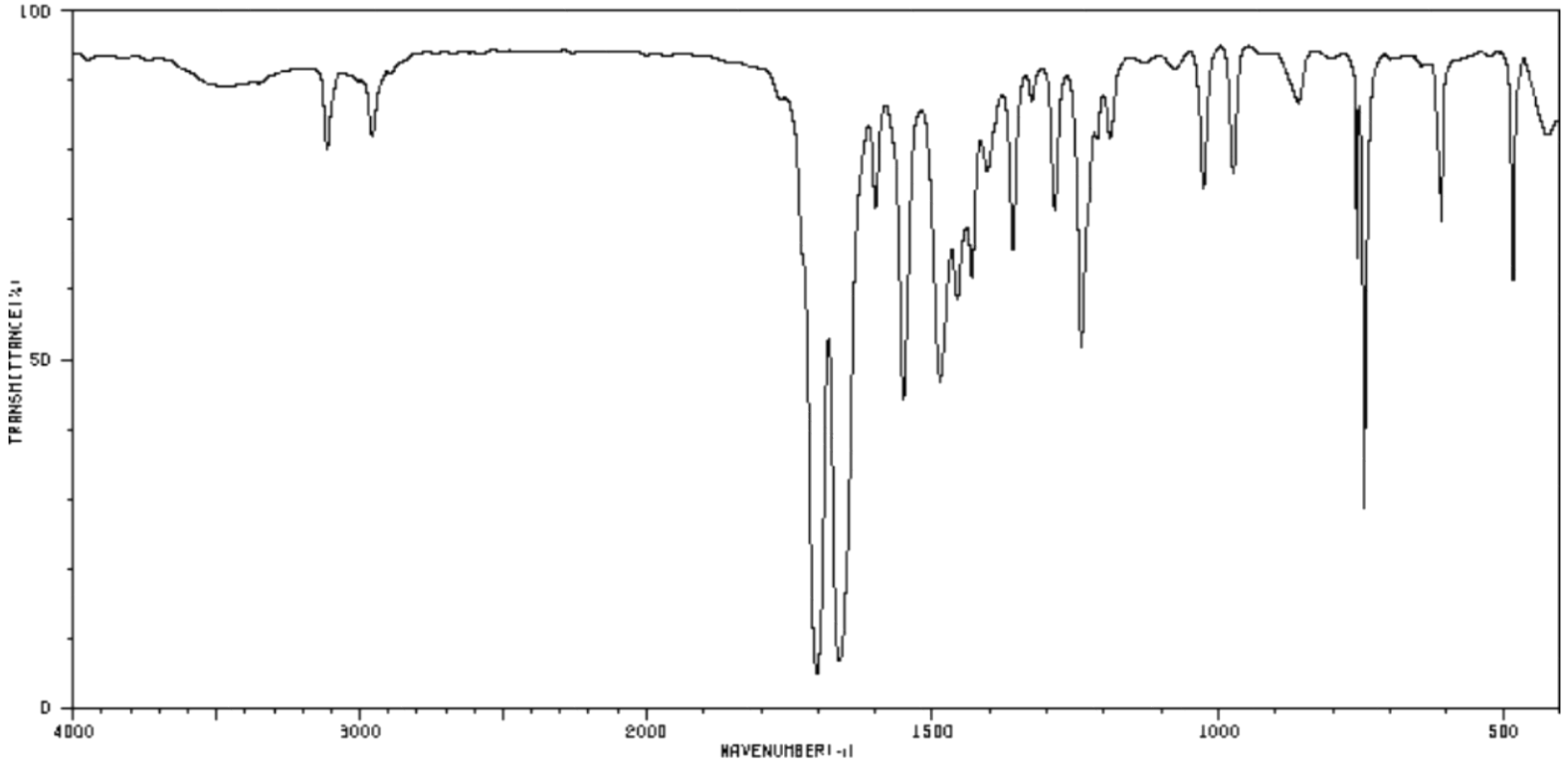
	Bond Length		**Bond Angles**
L 1		Θ 1	
L 2		Θ 2	
L 3		Θ 3	
L 4		Θ 4	
L 5		Θ 5	
L 6		Θ 6	
L 7		Θ 7	
L 8		Θ 8	
L 9		Θ 9	
L 10		Θ 10	
L 11		Θ 11	
L 12			
L 13			
L 14			
L 15			



HIT-NO=1705	SCORE= ( )	SDBS-NO=1898	IR-NIDA-62055 : KBR DISC

CAFFEINE

$C_8H_{10}N_4O_2$



3114	77	1466	67	1213	79	610	66
2955	79	1431	58	1190	79	482	58
1702	4	1405	74	1026	72		
1662	6	1360	64	974	74		
1600	68	1327	84	861	84		
1551	42	1287	68	759	82		
1487	44	1241	60	746	27