New Fellow Education Transfer Plan
Cover Sheet

Title of ETP	Infrared Spectroscopy
Name of IISME Fellow	Daniel Quach
Fellow's year-round email	dquach@offramp.org
Sponsor Company	Lockheed Martin Missiles and Space
Name of Mentor	Andrew Green; SEIT/SBIRS Director
National Board Certificate Area	Adolescence and Young Adulthood Science
I, the IISME **Fellow** named above, affirm that the ETP I am submitting is my own work, that I acknowledged sources where appropriate, and that I avoided including any proprietary information of the Sponsor Company. By my submission I am assigning to IISME my entire copyright in the ETP. I understand IISME is simultaneously granting me a license to use the ETP for pedagogical purposes. Signature ______________________ Date ______________	

Category	**Curriculum: Chemistry** Subject: Math Technology _________ Level: Elem Middle Other **Staff Development** *Describe*___________________________ *Other* *Describe*___________________________
Objectives	To teach students about infrared spectroscopy
Abstract (50 words or less)	Students will investigate the fundamentals of infrared spectroscopy through their basic knowledge of molecular structure and functional groups of organic compounds. Students will learn how to draw structural formulas of organic compounds, analyze and interpret infrared spectroscopy graphs, and infrared spectroscopy applications.
Describe how your ETP aligns with the National Board Standard stated in your proposal.	• Use a variety of instructional strategies to expand student's understandings of major ideas of science. • Translate difficult content into terms more available to students through a repertoire of verbal and visual aids.
Describe the connection between your ETP and the Summer Fellowship.	Qualitative and quantitative using analytical chemistry methods is vital when dealing with failure analyses of materials. The use of spectroscopy as well as other technology plays an important role in determining the causes of failures of connector cables and solar array panels on space satellites.

D4

Resources Needed	Molecular model of CO_2 Internet access (optional)
Evaluation/Assessment Measures Used	▪ Student-centered, teacher facilitated class and group discussions ▪ Completion of worksheet/activity ▪ Unit Exam
Formatting specifications	PC _X_ or Mac____ **(Must be in Word or Text Format)** Software used _Microsoft Word_
Submitted Copy	***Soft and hard copy due to peer coach by the end of the summer fellowship. Also, a copy of the cover sheet signed by a school site administrator submitted to IISME Oct.1, 2003 to receive $300 grant.***

I, the **Mentor** named above [please select one of the following],

- ❑ have read the attached ETP, and my comments, if any, appear below.
- ❑ have read the attached ETP, and, as outlined in the IISME-Company Fellowship Agreement, have reviewed it on behalf of the Sponsor Company, and have determined that the ETP does not contain any Sponsor-proprietary information. My additional comments, if any, appear below.

Comments:

Signature _______________ Date _______________

Administrator's comments:

Signature _______________ Date _______________

Infrared Spectroscopy

IISME Fellow – Summer 2003: Daniel Quach; dquach@offramp.org
Sponsor Company: Lockheed Martin Missiles and Space
Mentor: Andrew Green; SEIT/SBIRS Director
IISME Category: Science Curriculum (Chemistry) Development for High School

Description of Lesson and Intended Student Body

Infrared spectroscopy can be applied to fundamental chemistry concepts taught in a high school general chemistry course. A brief description of the three lessons are given below followed by the California State Standards they address.

Lesson I: HONC 1234 and Structural Formulas
Students learn the fundamentals of chemical bonding using the HONC 1234 rule to build structural formulas of organic compounds.

Chemistry Standard 10 (b)-Organic Chemistry and Biochemistry

b. The bonding characteristics of carbon that result in the formation of a large variety of structures ranging from simple hydrocarbons to complex polymers and biological molecules.

Lesson II: Functional Groups
Students build on their knowledge of chemical bonding by investigating groups of bonded atoms called functional groups. Students explore six different functional groups (alcohol, alkane, amine, carboxylic acid, ester, and ketone) and discover functional groups can lead to certain chemical properties.

Chemistry Standard 10 (e)-Organic Chemistry and Biochemistry

e. Identify the functional groups that form the basis of alcohols, ketones, ethers, amines, esters, aldehydes, and organic acids.

Lesson III: Infrared Spectroscopy
Students apply what they learned in Lesson I & II to infrared spectroscopy. Students learn how infrared spectroscopy works and investigate and interpret infrared spectra of different organic compounds.

Content Standard K-12 (a, d, l) – Investigation and Experimentation

a. Select and use appropriate tools and technology (such as computer-linked probes spreadsheets, and graphing calculators) to perform tests, collect data, analyze relationships, and display data.

d. Formulate explanations by using logic and evidence.

l. Analyze situations and solve problems that require combining and applying concepts from more than one area of science.

These lessons are intended for four 50-minute class periods or two block periods. The assessment at the end of this unit should be given in another 50-minute class period or the remaining portion of a block period. Extra time should be scheduled for Lesson II since the worksheet for that lesson is three pages.

Any student enrolled in a chemistry course should be able to complete this set of assignments. Students should also be familiar with Internet searches and use information obtained from the World Wide Web.

Educational Transfer Plan Rubric

Outcomes	**National Science Standard VIII** Throughout the three lessons I have incorporated the concepts, ideas, and evaluation strategies discussed in the National Science Standard VIII: "*Accomplished science teachers use a variety of instructional strategies to expand students' understanding of the major ideas of science*." I have adopted a student-centered teacher facilitated approach in teaching these three lessons. Students begin with initial ideas to build solid fundamental chemistry concepts through whole-class, group, and individual discussion. By mastering the fundamentals, students are able to explore more advanced topics such as infrared spectroscopy. This approach exemplifies the statement, "*…teachers translate difficult content into terms more available to their students. They know the best analogies and demonstrations to use in presenting difficult science concepts and are constantly expanding their repertoire of these verbal and visual aids*."
Assessment Procedure	Assessing and evaluating student learning fall under three categories: 1) **Making Sense Discussion** – Each lesson includes a "**Making Sense Discussion**" section that highlights the major topics discuss in that lesson and what students are expected to know by the end of the activity. Teacher facilitates a whole class discussion on the expected outcomes from that lesson at the end of the day. 2) **Activity/Worksheet** – Students are expected to complete all assignments. Students work in cooperative learning groups to discuss concepts and ideas with their group members. This classroom model promotes communication and invested student learning. 3) **Unit Exam** – Students will be assessed individually by completing a unit exam. Students will apply their knowledge and understanding of fundamental chemistry concepts and infrared spectroscopy in a real-world application of infrared spectroscopy. Student's grade for this unit is based on the total points on the worksheets/activity and the unit exam. Extra credit may be given for further research on infrared spectroscopy.
Ability to Replicate	The student handout, unit exam, and teacher's guide can be copied and distributed. The teacher's guide will aid teachers in leading group discussion, providing pertinent information, check for understanding, and how to assess assignments.
Identification of Resources	▪ Molecular model of CO_2 (for Lesson III) ▪ Internet access (optional)

Acknowledgements:

Lockheed Martin Missiles and Space
Andrew Green – SEIT/SBIRS, Program Director
David Lis – SEIT/SBIRS, Systems Engineer
John Aston – SEIT/SBIRS, Systems Specialty Engineer
Chris Rubke – Lockheed Martin Missiles and Space, Hardware Engineer
Norbert Ching – Materials and Processes, Materials Engineer

Industry Initiatives for Science and Math Educators (IISME)
Deborah Frazier – IISME Peer Coach

References:

Coates, John. “Interpretation of Infrared Spectra, A Practical Approach.” *Encyclopedia of Analytical Chemistry*. 2000.

Jones, Anita. “Infrared Spectroscopy Outline.” University of Edinburgh. 2002.

“Living By Chemistry.” Lawrence Hall of Science, UC Reagents of the University of California, Berkeley. 2001.

NIST Standard Reference Database Number 69. S.E. Stein, "Infrared Spectra" in NIST Chemistry WebBook, NIST Standard Reference Database Number 69, Eds. P.J. Linstrom and W.G. Mallard, March 2003. <http://webbook.nist.gov>.

Lesson I - HONC 1234 & Structural Formulas

Exploring the Topic

In this lesson students begin to understand the rationale for molecular structures. They are introduced to the HONC 1234 rule, which reminds students of the bonding tendencies of hydrogen, oxygen, nitrogen, and carbon. These bonding tendencies are consistent with the octet rule. Students will use this rule to create structural formulas from molecular formulas.

Introduction

Display the transparency for students to complete individually. If they have not learned what structural formulas are tell them a structural formula is a drawing or diagram that a chemist uses to show how the atoms in a molecule are connected.

Use the following guiding questions to discuss students' initial ideas.

- What patterns do you see?
- How many connections did each of the elements make with other atoms?
  Hydrogen? (1) **O**xygen? (2) **N**itrogen? (3) **C**arbon? (4)

Student Notes
Explain the HONC 1234 rule to students. Have them write the rule down in their notes.

HONC 1234 – A simple phrase that reminds chemists about the bonding of hydrogen, oxygen, nitrogen, and carbon. It tells us how many bonds each element usually makes within a molecule.

Double and triple bonds – Double and triple bonds still follow the HONC 1234 rule. The double bonded oxygen in the menthone molecule is bonded twice to carbon and therefore follows the guidelines. The same is true for the triple bonded nitrogen in the diisobutylamine molecule.

Activity

Explain the procedure. Write the following molecular formulas on the board and ask the students to work individually to create possible structural formulas for each one.

Procedure:

1. Start with the carbon, oxygen, and nitrogen atoms – connect them to each other.
2. Fill in with the hydrogen atoms.
3. Problem solve until you have the correct number of bonds for each element.

C_3H_8 C_3H_8O C_3H_9N

Making Sense Discussion

Ask students to come to the board and draw their structural formulas. More than one student can draw each molecule because there are several possible orientations and structures for each molecular formula. It may be more straightforward to draw and process one molecule at a time. Focus on the fact that a single molecular formula can represent more than one structural formula.

Assist students in summarizing what they learned in today's class.

- The HONC 1234 rule tells us how many times hydrogen, oxygen, nitrogen, and carbon like to bond.
- When a molecule is oriented differently in space it is still the same molecule.
- A molecular formula can be associated with more than one distinct structural formula.

Homework (optional)

1. Use the HONC 1234 rule to create possible molecules with the following molecular formulas. Remember it is easiest to start with the carbon atoms.
   $C_3H_8O_2$ $C_4H_{11}N$ C_4H_{10} $C_5H_{12}O$
2. From what you have seen so far, what <u>is</u> a structural formula?
3. Are the following structural formulas correct? If not, specify what is wrong with them.

H **H** **H H H**

| | | | |

$C - H - O - H - C$ $C - O - C$

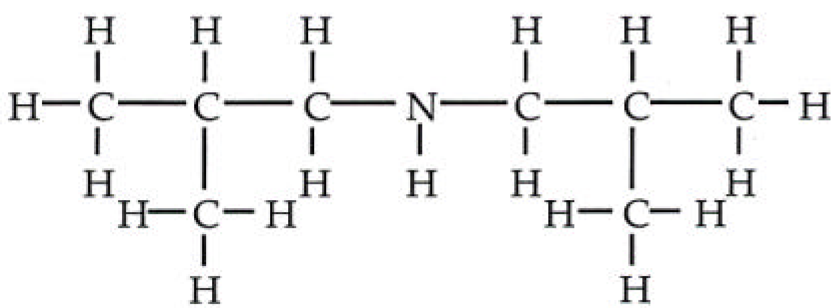
| | | | |

H H H H H

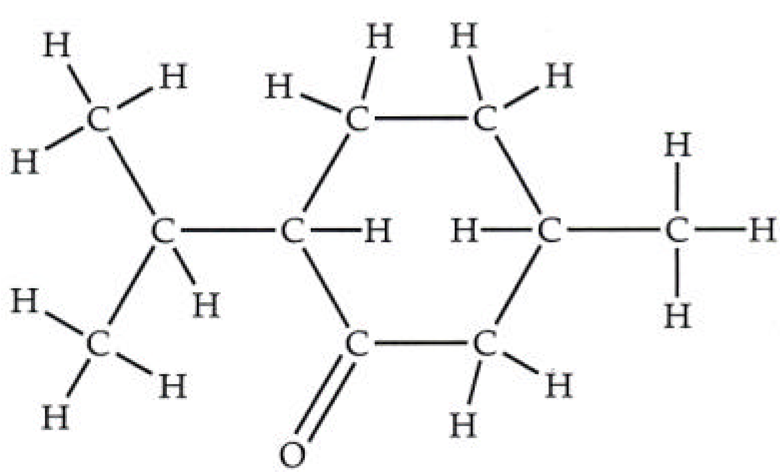
Transparency for Lesson I

What patterns do you see in the bonding of hydrogen, oxygen, nitrogen, and carbon?

diisobutylamine



menthone



Lesson II – Functional Groups

Exploring the Topic

In the last lesson students used the HONC 1234 rule to draw structural formulas. In this lesson they will investigate how certain groups of atoms appear frequently in molecules, which seem to account for some of their properties. This leads to an introduction to functional groups and infrared spectroscopy.

Introduction

Display the transparency (or make a class set of handouts) with the following infrared spectra. Point out to students that they are looking at how much infrared light certain molecules can absorb and transmit at different wavelengths in the infrared spectrum. Have students focus on any patterns they see.

Use the following guiding questions to discuss students' initial ideas.

- What patterns do you see?
- Do all the peaks occur at the same wavelength?
- Do certain molecules create sharp peaks while other molecules create broad peaks?
- What peaks do all the alcohol molecules have in common? What about all the alkane molecules?

Student Notes
Explain to students that chemists are able to characterize molecules by certain groupings of atoms they have in common.

Functional groups – Structural features that show up repeatedly in molecules and seem to account for some of their chemical properties (i.e. boiling point, melting point, amount of light it can absorb).

O **‖** **- C -** **ketone functional group**	**O** **‖** **– C – O – H** **carboxylic acid functional group**	**O** **‖ |** **- C – O – C -** **|** **ester functional group**
| **- C – N -** **| |** **amine functional group**	**| |** **- C – C -** **| |** **alkane functional group**	**|** **– C – O – H** **|** **alcohol functional group**

Activity

Hand out the Functional Groups worksheet. Explain to your students the purpose of this activity is to have them identify the functional group in each molecule. They are encouraged to use their notes. The last part of this activity is for students to recognize that the nomenclature of molecules is based on its functional group (i.e. molecules with an alcohol functional group end in –ol, like methan**ol** and ethan**ol**).

Making Sense Discussion

Once students have had a chance to work on the worksheet gather the whole class together to investigate their findings. Be sure to focus on the following:

- Students are able to identify different functional groups in a molecule.
- Students are able to draw the structural formula of a molecule with a specific functional group.
- Students discover patterns between the name of the molecule, its functional group, etc.

Homework (optional)

Students who did not finish the worksheet should finish it for homework.

Transparency for Lesson II

Look at the infrared spectra for the two alkane molecules and the two alcohol molecules.

- What do the two alkane molecules and two alcohol molecules have in common?

- What is different between the alkane molecules and the alcohol molecules?

Alkanes

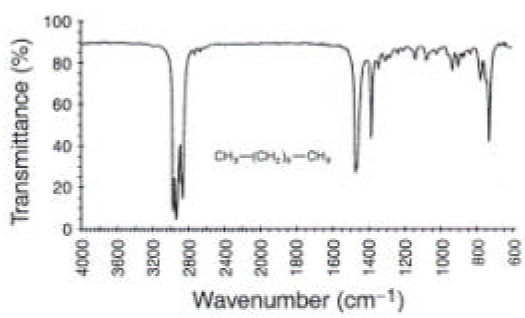


Figure 3 Attenuated total reflectance (ATR) spectrum of *n*-heptane. Copyright Coates Consulting.

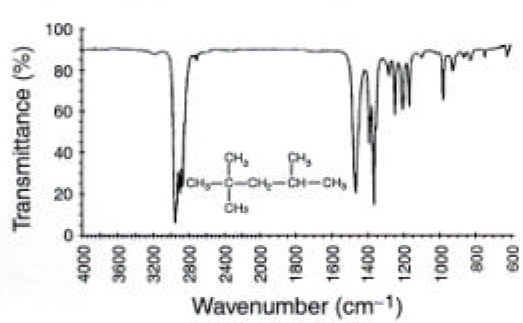


Figure 4 ATR spectrum of 2,2,4-trimethylpentane (isooctane). Copyright Coates Consulting.

Alcohols

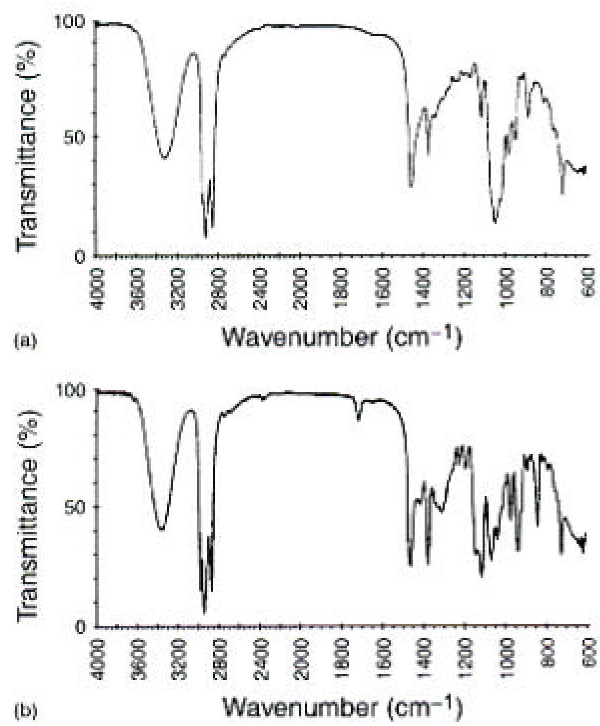
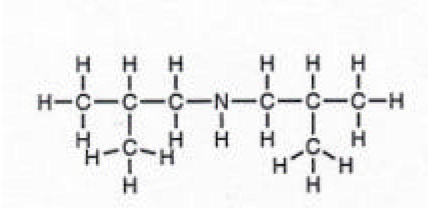
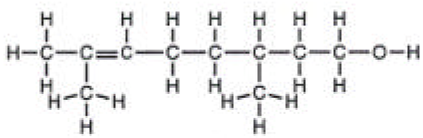
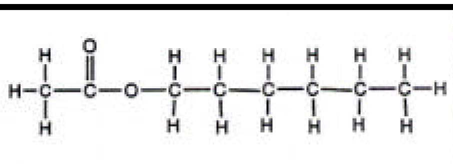
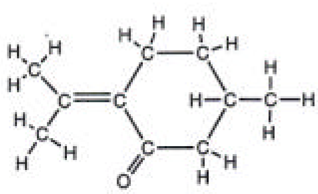
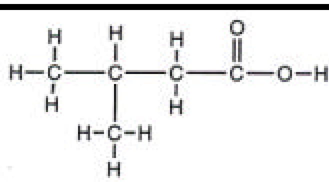
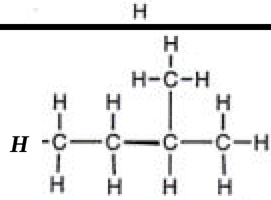


Figure 8 ATR spectra of (a) primary (1-octanol) and (b) secondary (2-octanol) alcohols. Copyright Coates Consulting.

Functional Groups Name ____________________
[30 points] Date ______________ Per __

Part I: Circle the functional group for each molecule. Write down the name of the functional group in the left column. Use your notes to help you. [12pt]

Molecule	**Name of the Functional Group**
	
	
	
	
	
	

Part II: Here is your chance to draw some more structural formulas! On the back of this sheet draw a molecule that contains at least three carbons and an alcohol functional group. Next, draw a molecule that contains three carbons and an ester functional group. Do the same for all the other functional groups. HINT: Use HONC 1234 to remind you how many bonds each element makes. [6pt]

Part III: For each group write down any patterns you see between the name of the molecule, molecular formula, and functional group. The first one is done for you as an example. [10pt]

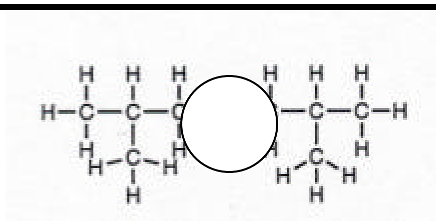
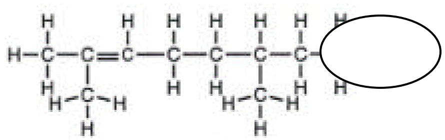
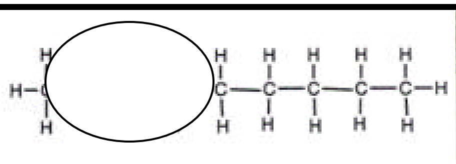
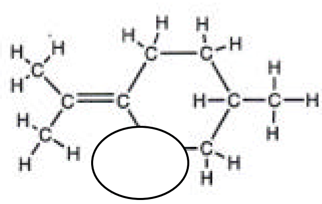
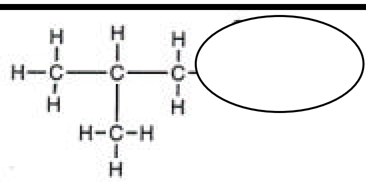
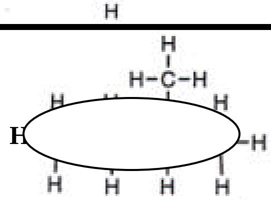
Name	Molecular Formula	Functional Group	Patterns
phenylethylamine diisobutylamine ethylamine	$C_8H_{11}N$ $C_8H_{11}N$ C_2H_7N	amine	• Amines contain N • Molecules with amine functional groups end in -amine
1-carvone menthone pulegone	$C_{10}H_{14}O$ $C_{10}H_{18}O$ $C_{10}H_{16}O$	ketone	
isoamyl acetate ethyl valerate amyl propionate	$C_7H_{14}O_2$ $C_7H_{14}O_2$ $C_8H_{16}O_2$	ester	
methane ethane octane	CH_4 C_2H_6 C_8H_{18}	alkane	
methanol ethanol octanol	CH_3OH C_2H_5OH $C_8H_{17}OH$	alcohol	
butyric acid isopentanoic acid hexanoic acid	$C_4H_8O_2$ $C_5H_{10}O_2$ $C_6H_{12}O_2$	carboxylic acid	

Based on the patterns you see, are there any rules you can come up with for each functional group? You should be able to come up with at least two. If you find more you will receive one extra credit point for each rule that works! [2pt]

Example: All esters contain 2 oxygens is **NOT** a rule because carboxylic acids also contain 2 oxygens. However, all alkanes contain only carbons and hydrogens is a very good rule!

Functional Groups (Answer Sheet) Name ___________________
[30 points] Date ______________ Per __

Part I: Circle the functional group for each molecule. Write down the name of the functional group in the left column. Use your notes to help you. [12pt]

Molecule	**Name of the Functional Group**
	**amine**
	**alcohol**
	**ester**
	**ketone**
	**carboxylic acid**
	**alkane**

Part II: Here is your chance to draw some more structural formulas! On the back of this sheet draw a molecule that contains at least three carbons and an alcohol functional group. Next, draw a molecule that contains three carbons and an ester functional group. Do the same for all the different functional groups. HINT: Use HONC 1234 to remind you how many bonds each element makes. [6pt] **There are many answers for each molecule. Check to see student structures follow HONC 1234**

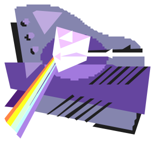
Part III: For each group write down any patterns you see between the name of the molecule, molecular formula, and functional group. The first one is done for you as an example. [10pt]

Name	Molecular Formula	Functional Group	Patterns
phenylethylamine diisobutylamine ethylamine	$C_8H_{11}N$ $C_8H_{11}N$ C_2H_7N	amine	• Amines contain N • Molecules with amine functional groups end in -amine
1-carvone menthone pulegone	$C_{10}H_{14}O$ $C_{10}H_{18}O$ $C_{10}H_{16}O$	ketone	• **Ketones end in –one** • **Ketones contain one oxygen**
isoamyl acetate ethyl valerate amyl propionate	$C_7H_{14}O_2$ $C_7H_{14}O_2$ $C_8H_{16}O_2$	ester	• **Esters contain 2 oxygens** • **Esters end in –ate**
methane ethane octane	CH_4 C_2H_6 C_8H_{18}	alkane	• **Alkanes contain only C and H** • **Alkanes end in -ane**
methanol ethanol octanol	CH_3OH C_2H_5OH $C_8H_{17}OH$	alcohol	• **Alcohols end in –ol** • **Alcohols contains OH in the molecular formula**
butyric acid isopentanoic acid hexanoic acid	$C_4H_8O_2$ $C_5H_{10}O_2$ $C_6H_{12}O_2$	carboxylic acid	• **Acids contain two oxygens** • **They have acids in the name**

Based on the patterns you see, are there any rules you can come up with for each functional group? You should be able to come up with at least two. If you find more you will receive one extra credit point for each rule that works! [2pt]

Example: All esters contain 2 oxygens is **NOT** a rule because carboxylic acids also contain 2 oxygens. However, all alkanes contain only carbons and hydrogens is a very good rule!

- **Ketones end in –one**
- **Esters end in –ate**
- **Alkanes end in –ane**
- **Alcohols end in –ol**



Lesson III – Infrared Spectroscopy

Exploring the Topic

Students will investigate in greater depth the infrared spectra they first saw in the previous lesson. The purpose of this lesson is to provide students with a basic understanding of infrared spectra and its applications in the world around them. Students will first understand how infrared spectroscopy works and use the working knowledge they obtain to interpret infrared spectra by locating key functional group transmittance. Finally, students will have the opportunity to independently research infrared spectra to locate applications of infrared spectroscopy in industry, the health profession, and in their daily lives.

Introduction

Display the transparency for students to study. The purpose of this activity is to have students study the infrared spectra in greater detail.

Use the following guiding questions to discuss students' initial ideas. Encourage students to share ideas and welcome all suggestions.

- What do you think you are looking at?
- Look at the labels for the x-axis and y-axis. What are they measuring?
- How is the molecule behaving?
- What happens at different wavelengths of light?

Student Notes

Tell students that they are looking at infrared spectra for different molecules. Molecules behave differently as infrared light passes through them.

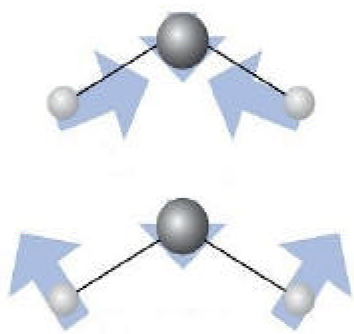
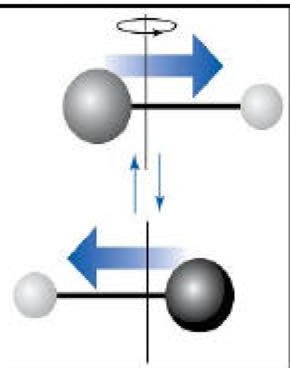
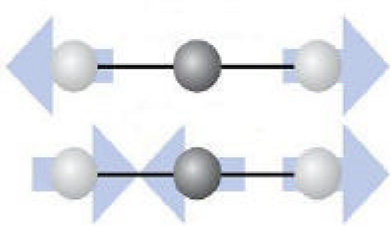
Infrared Spectroscopy – The production and investigation of spectra in the infrared spectrum (radiation having a wavelength between about 700 nanometers and 1 millimeter) due to the vibrational energy of molecules.

Activity

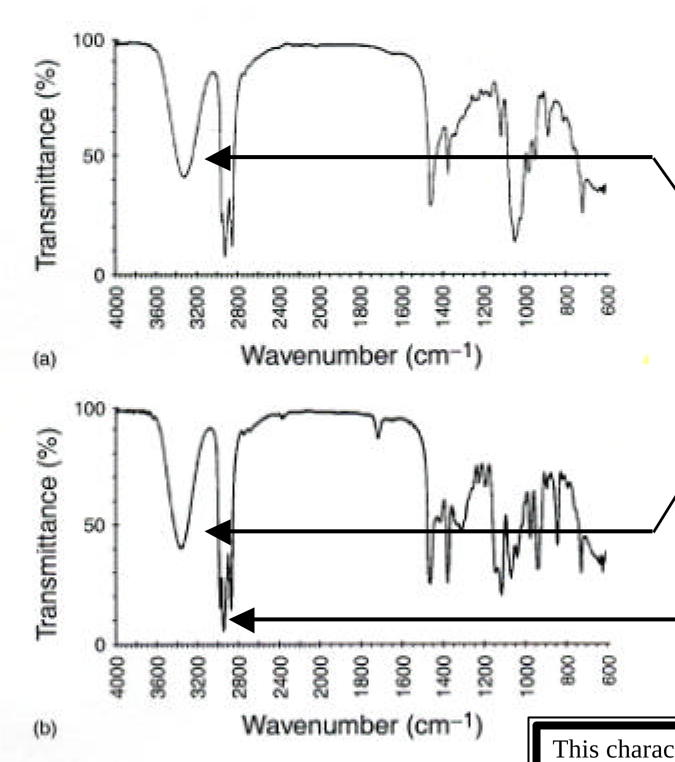
Before class, build a ball and stick model of carbon dioxide. Hand out the student worksheet. Have the students follow along on their worksheet as you demonstrate how infrared spectroscopy works using a ball and stick model. Use the CO_2 model to demonstrate how the molecule can bend, stretch, and rotate while the students follow along with their worksheet.

Origins of the Infrared Spectrum

The infrared spectrum is formed as a consequence of the absorption of electromagnetic radiation at frequencies relating to the vibration of specific sets of chemical bonds from within a molecule (i.e. functional group). When molecules are heated they begin to move faster. They can wiggle, jiggle, and bounce. Chemists have specific terms for each one! There are different types of energy a molecule exhibits:

Energy	Diagram	Explanation
vibrational (bending)		**The bonds between the atoms bend**
rotational		**The whole molecule rotates in 3-dimensional space**
translational (stretching)		**The bonds between the atoms stretch**

Direct students to the sample infrared spectra on their worksheet. Pass out the infrared spectra characteristic absorption chart. Point out the key ideas as illustrated below.



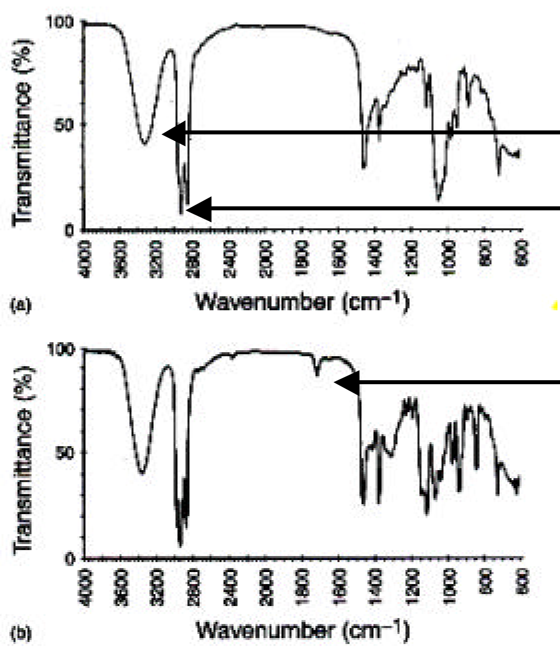
Notice the characteristic peak that appears at approximately 3500 cm^{-1}. On the table of absorbencies, locate the alcohol characteristic peak absorbance. Does it match with the infrared spectra shown here?

Also notice that this peak is **broad** while the other ones are **sharp**.

It is also important that you can exclude molecules in the absence of characteristic peaks. For example, if this peak were not there, then you would be able to exclude alcohol as a possibility.

This characteristic peak is called the alkyl C – H stretch. This peak is common in all organic compounds so it is less useful in determining structure. However if that is the only peak you see, the compound will most likely be an alkane.

Have students try to identify the functional group and molecule on their worksheet. **(alcohol)**



Size does matter! The top arrow is pointing to a medium **(m)** peak, the middle arrow is pointing a strong **(s)** peak, and the bottom arrow is pointing to a weak **(w)** peak. Look on your table of absorbencies. You will notice that these abbreviations are written next to the wavenumber.

NOTE: Students may experience some frustration identifying characteristic peaks and its respective functional group. Encourage students to help each other and discuss the different possibilities. Explain to students that forensic scientists (scientists in general often consult their peers as well) consult with other scientists about different possibilities when trying to identify an unknown compound. This is common practice among professionals and therefore should be common practice in the classroom.

Depth of Investigation: Depending on how extensive you want this unit to become you may add other topics to supplement this unit.

- Lewis dot structures
- Molecular motion
- Electronegativity and polarity
- Electromagnetic radiation and energy

Making Sense Discussion

Once students have had the opportunity to work on the worksheet go over these key ideas that will help them identify infrared spectra.

- Infrared spectroscopy is built upon the idea that molecules exhibit vibrational, rotational, and translational energy.
- Identifying functional groups can be made by matching characteristic peaks with a table of absorbencies.
- Identification can also be made by excluding molecules by the absence of characteristic peaks.
- Applications of IR spectroscopy
    - Analyses of polymers and rubbers
    - Vibrational spectroscopy of carbon and silicon materials
    - Detection of cancer
    - Imaging for biomedical applications
    - IR spectroscopy of proteins
    - Vibrational spectroscopy of lipids, nucleic acids, carbohydrates, and sugars.
    - Forensic science: Identifying chemicals involved in a crime scene investigation

Homework (optional)

Students may research applications of IR spectroscopy in groups and have them present their findings to the class. This can be a simple online research or something more involved (i.e. interviewing professionals, visiting a lab, PowerPoint presentation, etc.) depending on the amount of time available.

Characteristic Infrared Absorption Frequencies

Functional Group	**Characteristic Absorption(s) (cm^{-1})**	**Notes**
Alkyl C-H Stretch	2950 - 2850 (m or s)	Alkane C-H bonds are fairly ubiquitous and therefore usually less useful in determining structure.
Alkenyl C-H Stretch Alkenyl C=C Stretch	3100 - 3010 (m) 1680 - 1620 (v)	Absorption peaks above 3000 cm^{-1} are frequently diagnostic of unsaturation
Alkynyl C-H Stretch Alkynyl C≡C Stretch	~3300 (s) 2260 - 2100 (v)	
Aromatic C-H Stretch Aromatic C-H Bending Aromatic C=C Bending	~3030 (v) 860 - 680 (s) 1700 - 1500 (m,m)	
Alcohol/Phenol O-H Stretch	3550 - 3200 (broad, s)	
Carboxylic Acid O-H Stretch	3000 - 2500 (broad, v)	
Amine N-H Stretch	3500 - 3300 (m)	Primary amines produce two N-H stretch absorptions, secondary amides only one, and tertiary none.
Nitrile C≡N Stretch	2260 - 2220 (m)	
Aldehyde C=O Stretch Ketone C=O Stretch Ester C=O Stretch Carboxylic Acid C=O Stretch Amide C=O Stretch	1740 - 1690 (s) 1750 - 1680 (s) 1750 - 1735 (s) 1780 - 1710 (s) 1690 - 1630 (s)	The carbonyl stretching absorption is one of the strongest IR absorptions, and is very useful in structure determination as one can determine both the number of carbonyl groups (assuming peaks do not overlap) but also an estimation of which types.
Amide N-H Stretch	3700 - 3500 (m)	As with amines, an amide produces zero to two N-H absorptions depending on its type.

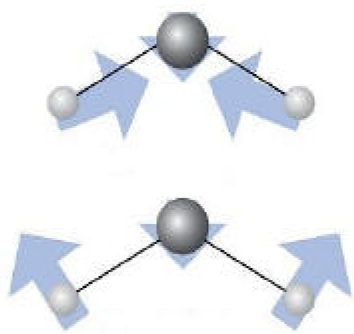
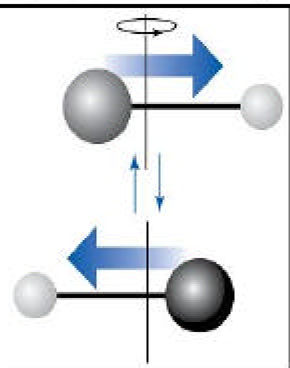
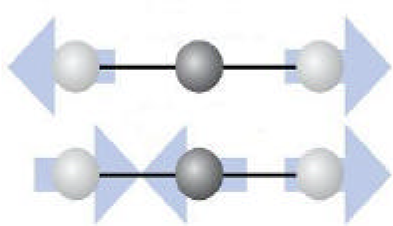
v - variable, m - medium, s - strong, w - weak

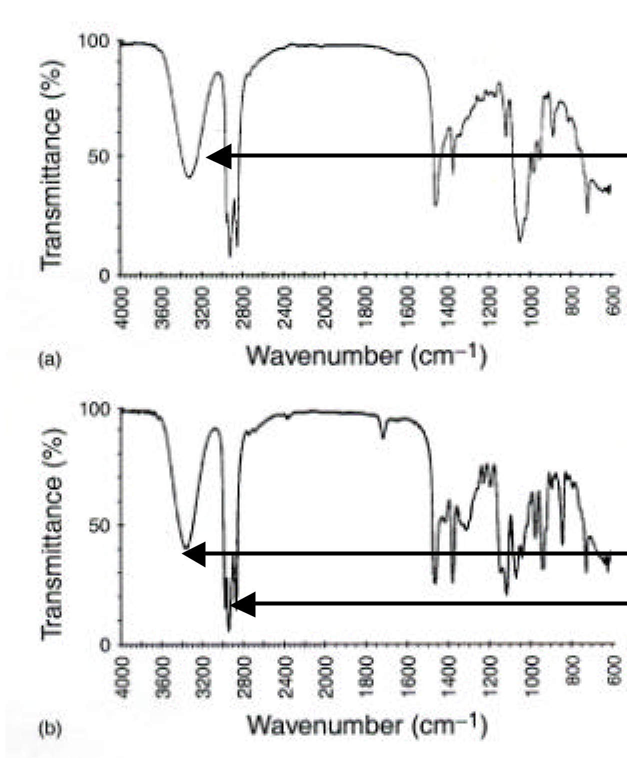
All figures are for the typical case only -- signal positions and intensities may vary depending on the particular bond environment.

Infrared Spectroscopy
Student Handout

Infrared Spectroscopy – The production and investigation of spectra in the infrared spectrum (radiation having a wavelength between about 700 nanometers and 1 millimeter) due to the vibrational energy of molecules.

The infrared spectrum is formed as a consequence of the absorption of electromagnetic radiate at frequencies relating to the vibration of specific sets of chemical bonds from within a molecule (i.e. functional group). When molecules are heated they begin to move faster. They can wiggle, jiggle, and bounce. Chemists have specific terms for each one! There are different types of energy a molecule exhibits:

Energy	Diagram	Explanation
vibrational (bending)		**The bonds between the atoms bend**
rotational		**The whole molecule rotates in 3-dimensional space**
translational (stretching)		**The bonds between the carbon and oxygen stretch and contracts**



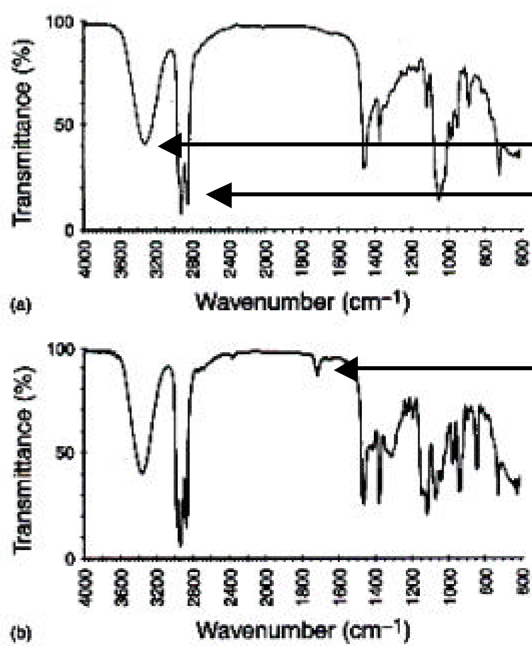
Notice the characteristic peak that appears at approximately 3500 cm^{-1}. On the table of absorbencies, locate the alcohol characteristic peak absorbance. Does it match with the infrared spectra shown here?

Also notice that this peak is **broad** while the other ones are **sharp**.

It is also important that you can exclude molecules in the <u>absence</u> of characteristic peaks. For example, if this peak were not there, then you would be able to exclude alcohol as a possibility.

This characteristic peak is called the alkyl C – H stretch. This peak is common in all organic compounds so it is less useful in determining structure. However if that is the only peak you see, the compound will most likely be an alkane.

Example: Look at the spectra above. Can you identify the functional group of this molecule?



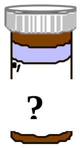
Size does matter! The top arrow is pointing to a medium **(m)** peak, the middle arrow is pointing a strong **(s)** peak, and the bottom arrow is pointing to a weak **(w)** peak. Look on your table of absorbencies. You will notice that these abbreviations are written next to the wavenumber.

Note: Infrared spectroscopy is often times used in conjunction with other spectroscopy techniques such as mass spectrometry, NMR, and UV spectroscopy. For example, if you want to identify an unknown compound you would use IR spectroscopy and mass spectrometry to validate the mass and arrangement of atoms of that particular compound.

Applications of Infrared Spectroscopy

There are many uses of IR spectroscopy in the real world. From identifying unknown compounds to determining the behavior of proteins in the human body, IR spectroscopy has proven to be an important source of information. Here are some more examples of how IR spectroscopy is used today:

- Analyses of polymers and rubbers
- Vibrational spectroscopy of carbon and silicon materials
- Detection of cancer
- Imaging for biomedical applications
- IR spectroscopy of proteins
- Vibrational spectroscopy of lipids, nucleic acids, carbohydrates, and sugars
- Forensic science: Identifying chemicals involved in a crime scene investigation



Infrared Spectroscopy
Student Worksheet [20 points]

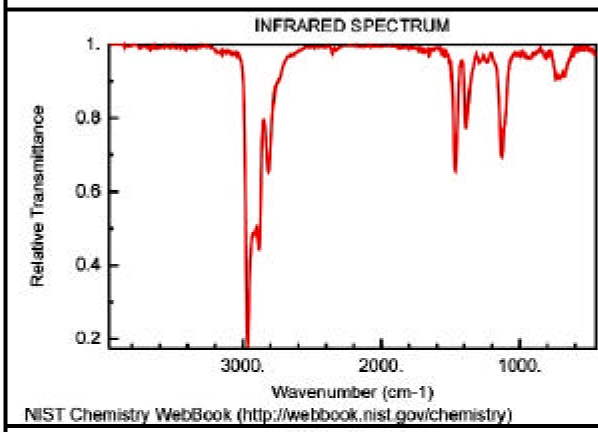
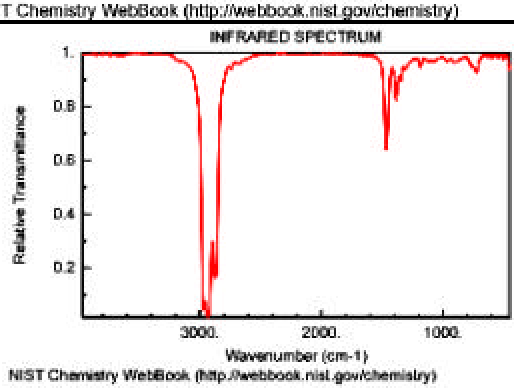
Name ________________
Date ____________ Per __

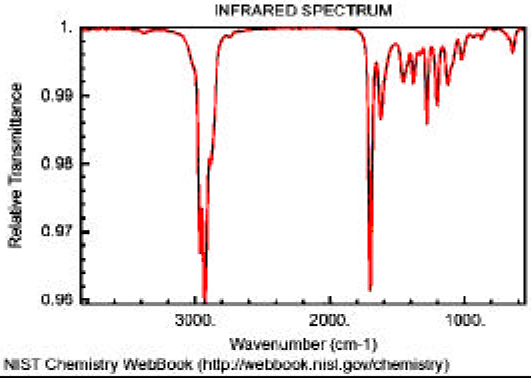
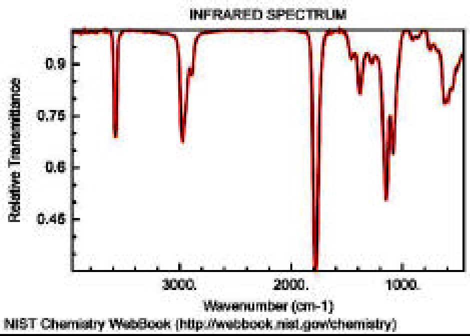
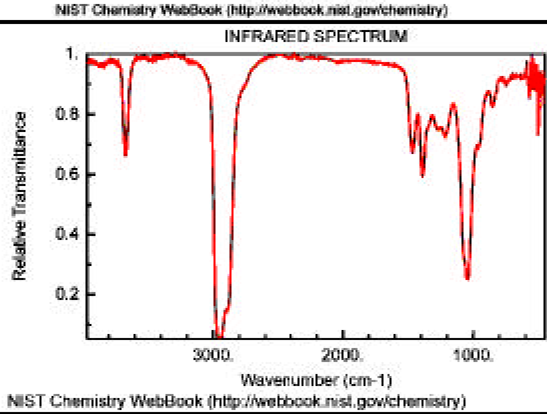
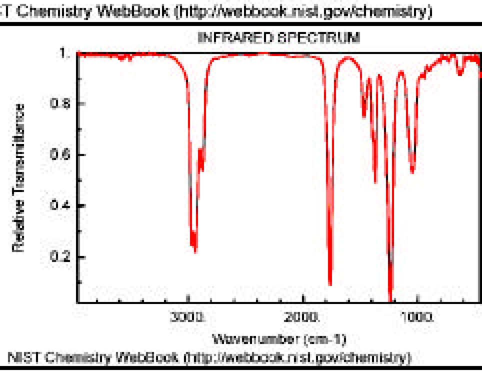
The Case of the Fallen Chemical Labels

Early one morning you arrive in your chemistry laboratory to find that some of the labels on your bottles have fallen off! This is a serious problem because adding unknown chemicals in an experiment can be dangerous, if not deadly. Each of these six chemicals is a clear liquid at room temperature with their own distinct chemical properties. Just then, like Archemides, you proclaim, "Eureka! I've got it." You decide to use infrared spectroscopy to help you identify the chemicals in each bottle and correctly replace the labels.

Use the infrared spectra below and the naming patterns you discovered in Lesson II to help you identify the substance in each bottle. Then correctly match the labels listed below with its compound.

butanol	**butyric acid**	**diisobutylamine**
hexyl acetate	**octane**	**pulegone**

Infrared Spectra	Characteristic Functional Group	Compound Name
		
		

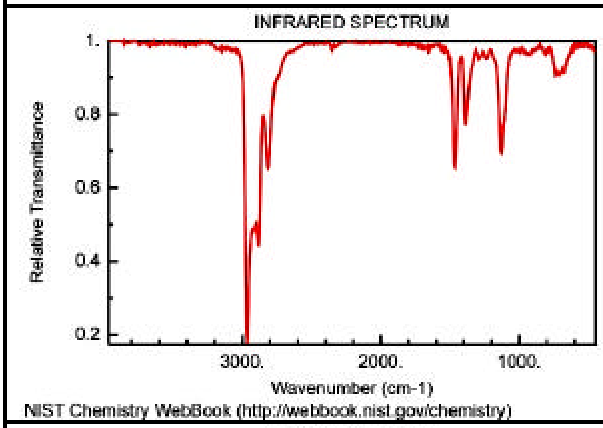
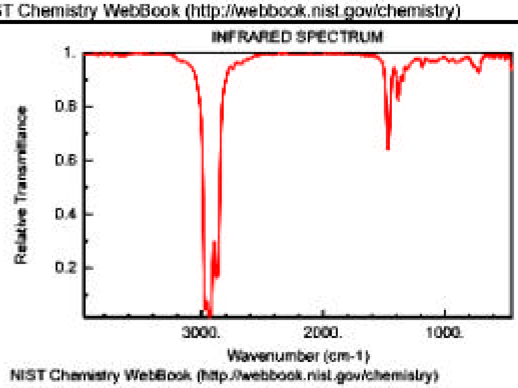
Infrared Spectra	Characteristic Functional Group	Compound Name
		
		
		
		

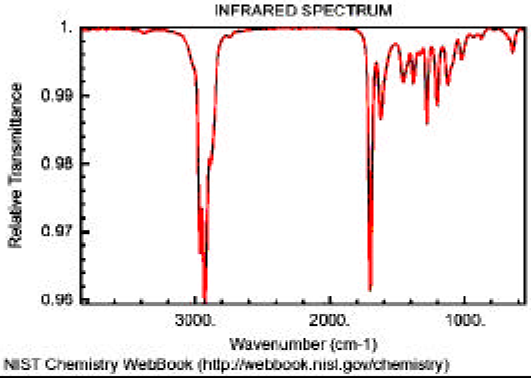
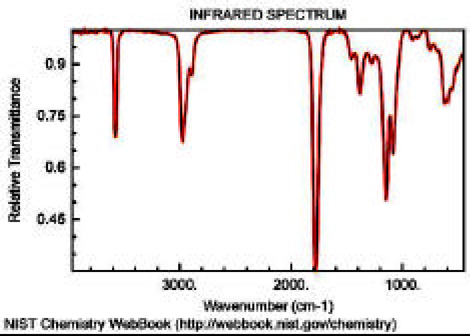
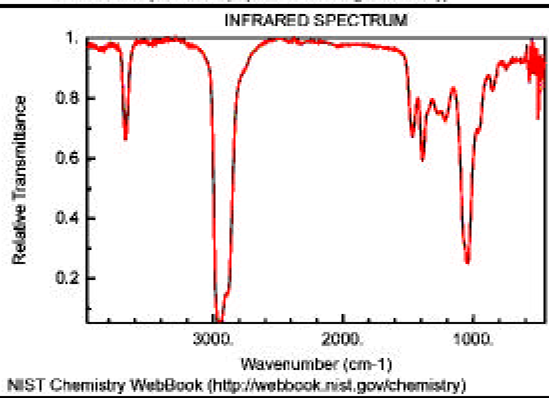
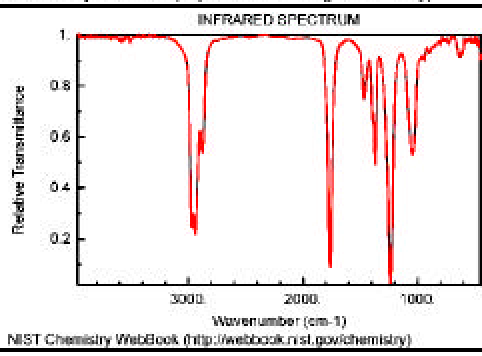
The Case of the Fallen Chemical Labels

Early one morning you arrive in your chemistry laboratory to find that some of the labels on your bottles have fallen off! This is a serious problem because adding unknown chemicals in an experiment can be dangerous, if not deadly. Each of these six chemicals is a clear liquid at room temperature with their own distinct chemical properties. Just then, like Archemides, you proclaim, "Eureka! I've got it." You decide to use infrared spectroscopy to help you identify the chemicals in each bottle and correctly replace the labels.

Use the infrared spectra below and the naming patterns you discovered in Lesson II to help you identify the substance in each bottle. Then correctly match the labels listed below with its compound.

butanol	**butyric acid**	**diisobutylamine**
hexyl acetate	**octane**	**pulegone**

Infrared Spectra	Characteristic Functional Group	Compound Name
	**amine 3500-3000 (m)**	**diisbutylamine**
	**alkane 2950-2850 (m)**	**octane**

Infrared Spectra	Characteristic Functional Group	Compound Name
	**ketone** **1750-1680 (s)**	**pulegone**
	**carboxylic acid** **1780-1710 (s)** **3000-2500 (broad,v)**	**butyric acid**
	**alcohol** **3550-3200 (broad,s)**	**butanol**
	**ester** **1750-1735 (s)**	**hexyl acetate**

Transparency for Lesson III

Study the infrared spectra below.

- Look at the x-axis and y-axis. What are they measuring?
- What do you think the molecule is doing?
- What happens at different wavelengths of light?

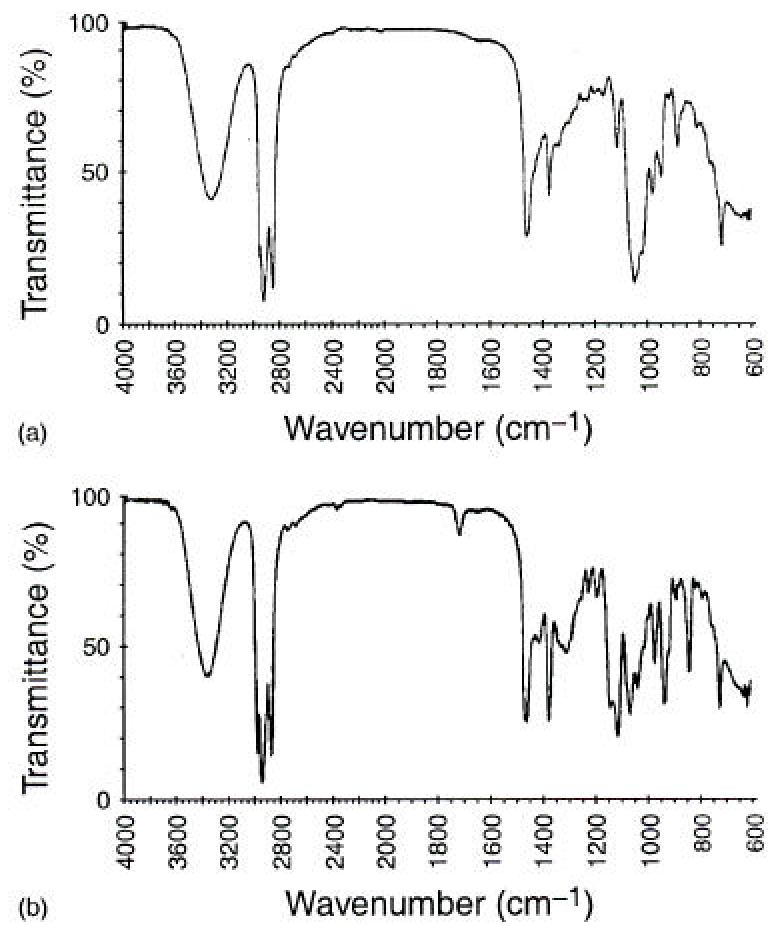


Figure 8 ATR spectra of (a) primary (1-octanol) and (b) secondary (2-octanol) alcohols. Copyright Coates Consulting.

Crime Scene Investigation Name ________________________

Chemistry Date _________________ Per ____

GRADING		Score	Out Of
Lab Courtesy	You were silent and focused when you did your lab.		10
Data	Your data table is complete.		25
Results	Your evidence matches your data.		30
Identity of Unknown	You correctly determined which compound caused the poisoning		5
Conclusion	You answered the questions completely and accurately.		20
Clean-Up	You cleaned up your work area and returned the materials you obtained from your instructor		10
	TOTAL SCORE		100

Directions Follow the instructions below to perform the following experiment **individually**. If you have any questions, raise your hand. Make sure that you clean up when you are finished.

Purpose

Detective Watson just returned from a crime scene where a young man was poisoned. You are world famous for your work with infrared spectroscopy and Detective Watson needs your help to determine what caused the poisoning. There are three possibilities:

1. pentanoic acid, $C_5H_{10}O_2$
2. butamine, $C_4H_{11}N$
3. octanol, $C_8H_{17}OH$

Materials

- Infrared Spectra you retrieved from your machine
- Table of Characteristic Absorbencies
- Periodic Table of Elements

Procedure

1. Obtain an infrared spectra print-out, a Table of Characteristic Absorbencies, and a Periodic Table from your instructor.
2. Write the unknown letter of your spectra on your data table.
3. Study the infrared spectra and complete the data table.
4. Answer the conclusion questions
5. Return the materials to your instructor.

Data

Unknown Letter	Functional Group	Identity of the Compound

What is the identity of the unknown substance that poisoned the young man? What evidence will you provide Detective Watson?

Conclusions **Be sure to provide evidence for your results.**

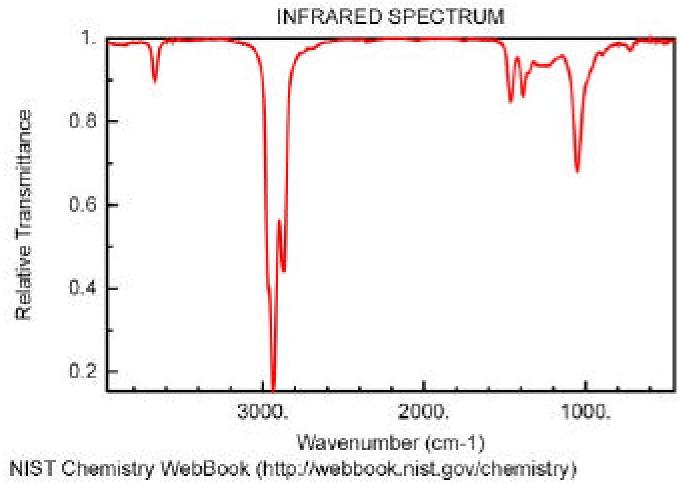
1. Draw a possible structural formula for the compound you obtained above.

2. You have two completely different molecules with different chemical properties. However, they have the same molecular formula, $C_4H_8O_2$. How can these two different molecules have the same molecular formula? Use drawings to help you answer this question.

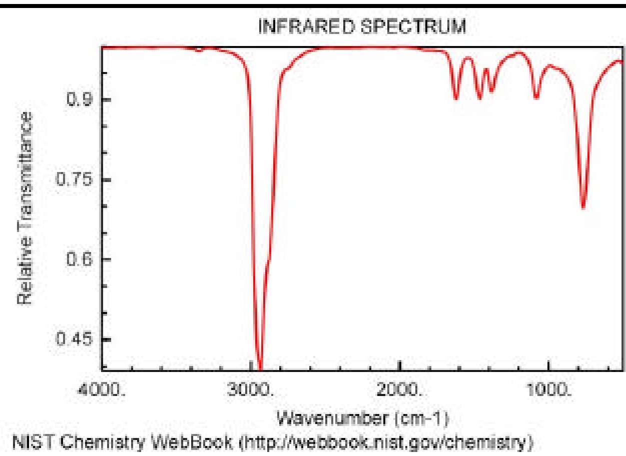
Give each student one of the unknowns.

A = octanol
B = butamine
C = pentanoic acid

A



B



C