

Author(s): MELO 3D Project Team, 2011

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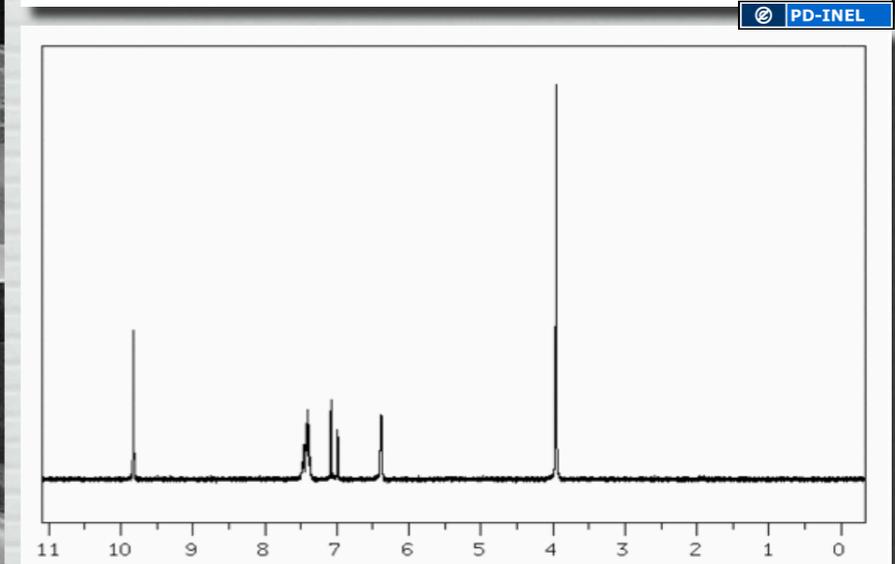
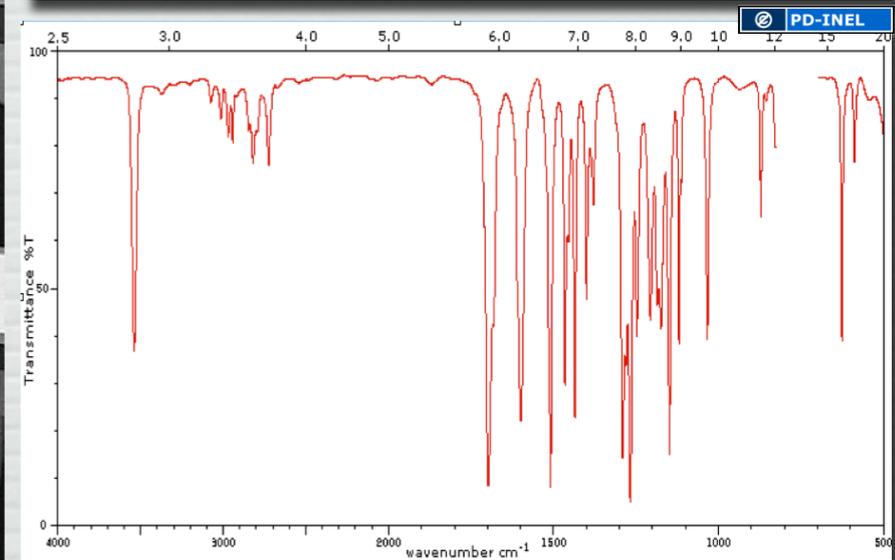
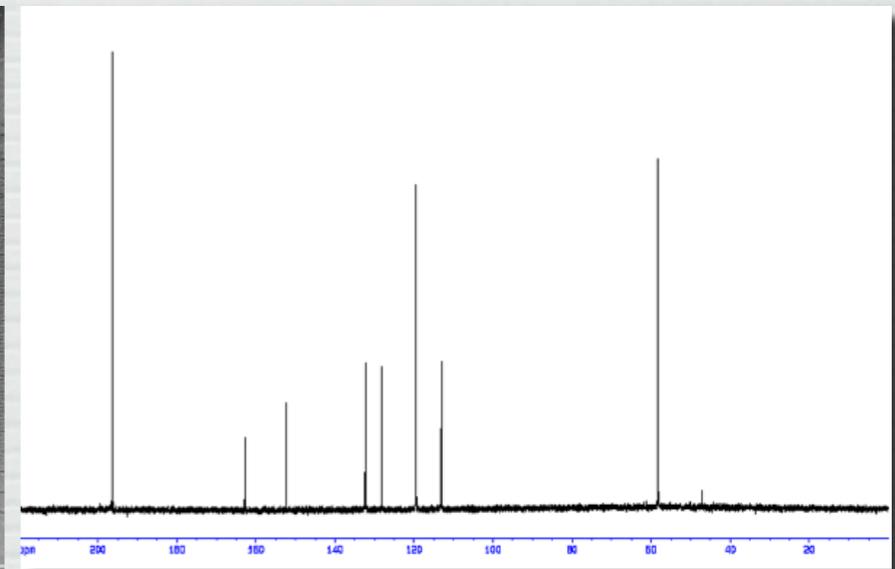
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Spectroscopy

❖ Chemistry 216

MELO3D Update
February 7, 2012

From Last Term:

- ❧ Implemented two types of LOs to 48 students:
 - ❧ Problem solving
 - ❧ VoiceThread
- ❧ Students accessing LOs multiple times per week
- ❧ Improvement in performance seen on first exam
- ❧ Lots of data to sort through
 - ❧ CTools analytics
 - ❧ Beginning and end-of-term surveys

This Term:

- ❧ Implemented in an entire lecture section (~300 students)
 - ❧ Large scale has lead to some challenges with communication to students and GSIs
 - ❧ Advantage is we can now discuss LOs in lecture and not just rely on individual GSIs
- ❧ Surveys now collected using Qualtrix instead of hard copies
 - ❧ Makes data collection much easier

Learning Objects

[Options](#)

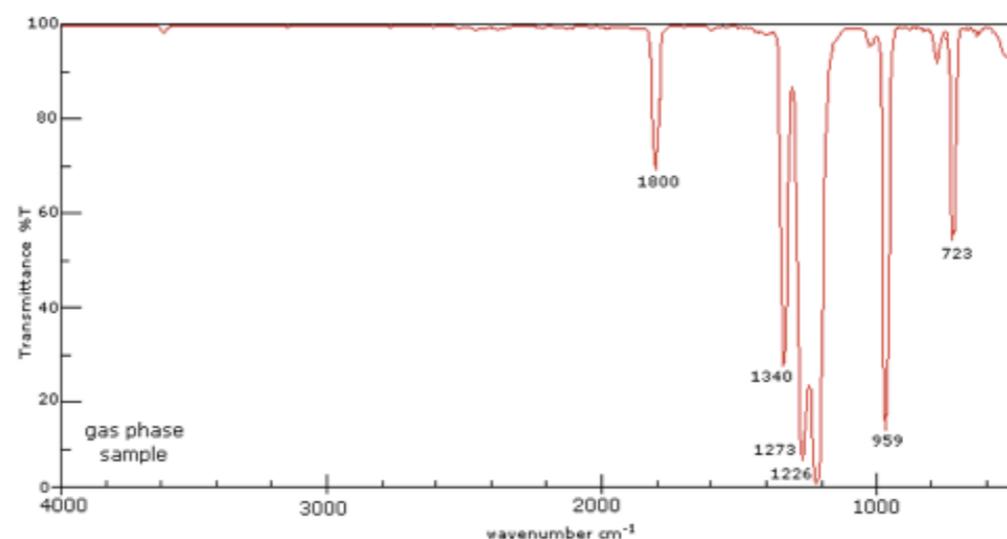
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Help

For your prelab this week, complete Problem 2. Explain in your own words how you arrived at your answer. Write as if you were explaining how to solve the problem to a classmate. Feel free to draw on or label the spectra.

To gain experience with infrared spectroscopy, try out some of the practice problems below. It may be helpful to print out this page in order to review multiple spectra at once. Please refresh the page if some spectra have not loaded properly.

Infrared Spectroscopy is covered in Chapter 12 of Organic Chemistry (Ege) on pages 453-466 as well as in Appendix B of your lab manual. Refer to page 456 in Ege for a table of Characteristic Infrared Absorption Frequencies to help you solve the spectra below.

Problem 1: Below is a spectrum of a colorless gas that condenses at $-26\text{ }^{\circ}\text{C}$. It contains six fluorines. Interpret the spectrum below and identify the compound, matching the main peaks to the functionalities present in the compound. Using a chemical database determine if the compound you have identified is consistent with the physical data provided.

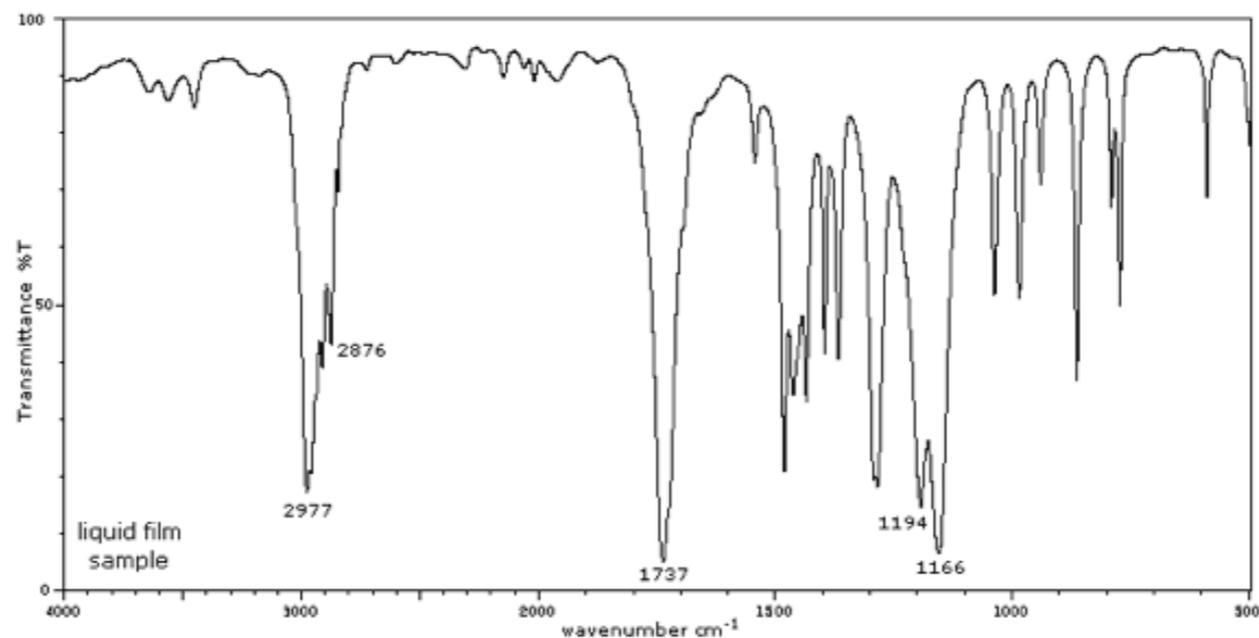


Problem 2: Five isomers with the molecular formula $\text{C}_4\text{H}_8\text{O}$ are presented. Match the structure to its corresponding spectrum below.

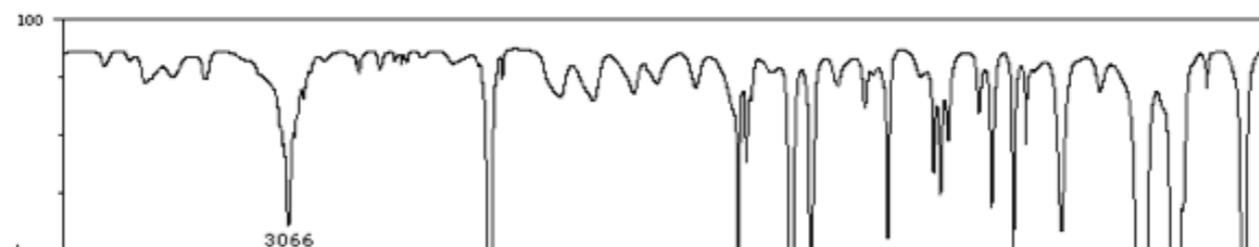
Pre-Lab Problem

Turn in answer to assigned problem to their GSI as part of their pre-lab assignment.

Below is a spectrum of a pleasant-smelling liquid with a boiling point of 101 °C and a molecular formula of $C_6H_{12}O_2$. Interpret the spectrum, matching the main peaks to the functionalities present in the compound. Using a chemical database determine if the compound identified is consistent with the physical data provided.



Below is a spectrum of an oily liquid having a boiling point of 191 °C, a melting point of -13 °C and a molecular formula of C_7H_5N . Interpret the spectrum and identify the compound, matching the main peaks to the functionalities present in the compound. Using a chemical database determine if the compound identified is consistent with the physical data provided. To hear a GSI solve this problem, [click here](#).



Problem Solving Help

say more

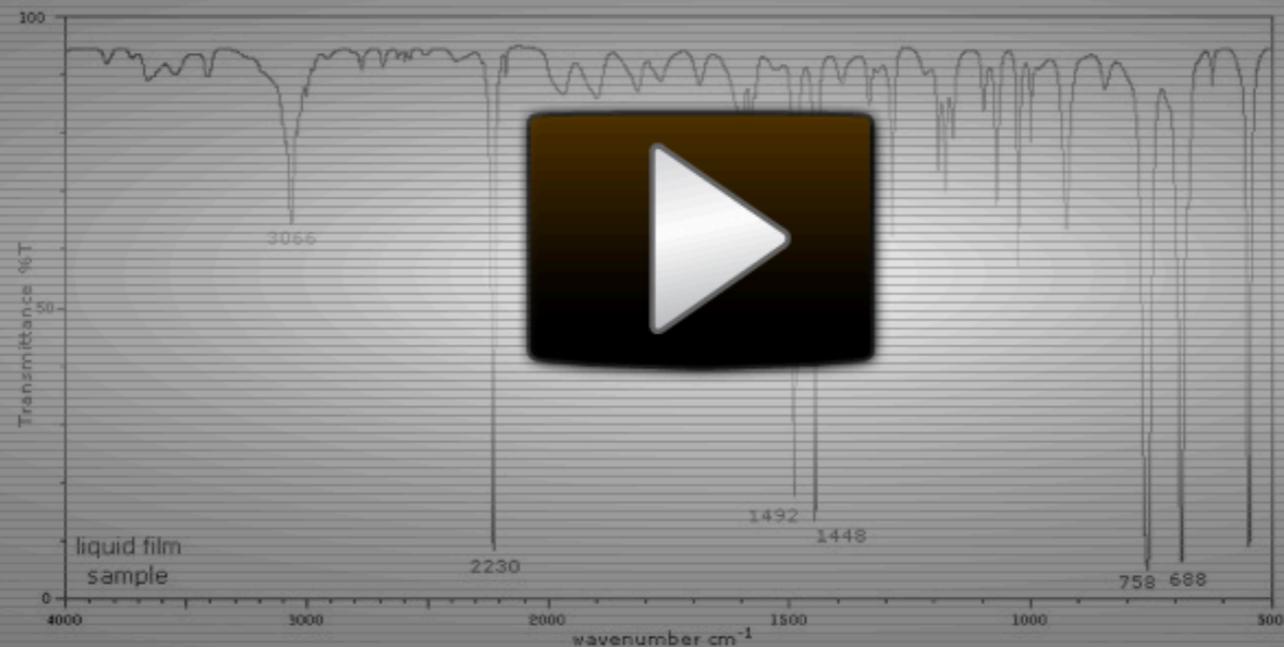
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Spectrum of an oily liquid having a boiling point of 191 °C, a melting point of -13 °C and a molecular formula of C_7H_5N . Interpret the spectrum and assign the main peaks to the functionalities present in the compound. Using a chemical database determine if the compound you have identified



FAIR USE

Problem Solving Help

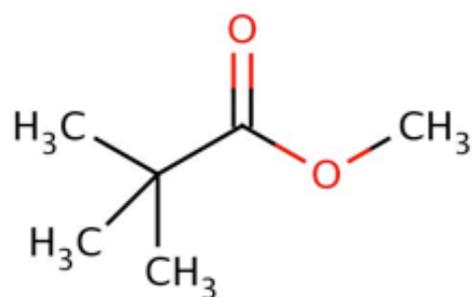
“Learning objects were useful in getting me to think about IR and NMR spectra and study them in advance...they could be improved by **having access to answers afterwards.**”

--Ian, former CH216 MELO3D student



Week 2: Problem 2: Week 2 problems can be found [here](#) for reference.

Calculating units of unsaturation with the molecular formula reveals only one unit of unsaturation. This could be a ring, an alkene or a carbonyl. Looking at the IR spectrum, the first thing you likely noticed is a strongly absorbing carbonyl peak in the center of the spectrum. Carbonyl stretching at 1737 cm^{-1} and C-O stretching at 1194 cm^{-1} and 1166 cm^{-1} are consistent with an ester functionality. Lack of C-H absorption above 3000 cm^{-1} indicates no C-C unsaturation, which makes sense. The ester is what gives this compound its one unit of unsaturation and the ester contains both of the oxygens, so determining the rest of the structure is mostly trial and error. You likely drew out many different linear or branched esters. By checking their physical properties, you would have determined that the compound is methyl 2,2-dimethylpropanoate, shown below.



Week 1: Problem 4: Week 1 problems can be found [here](#) for reference.

a) Which compound contains an aromatic ring?

C-H alkene stretches show up with medium intensity around $3080\text{-}3020\text{ cm}^{-1}$.

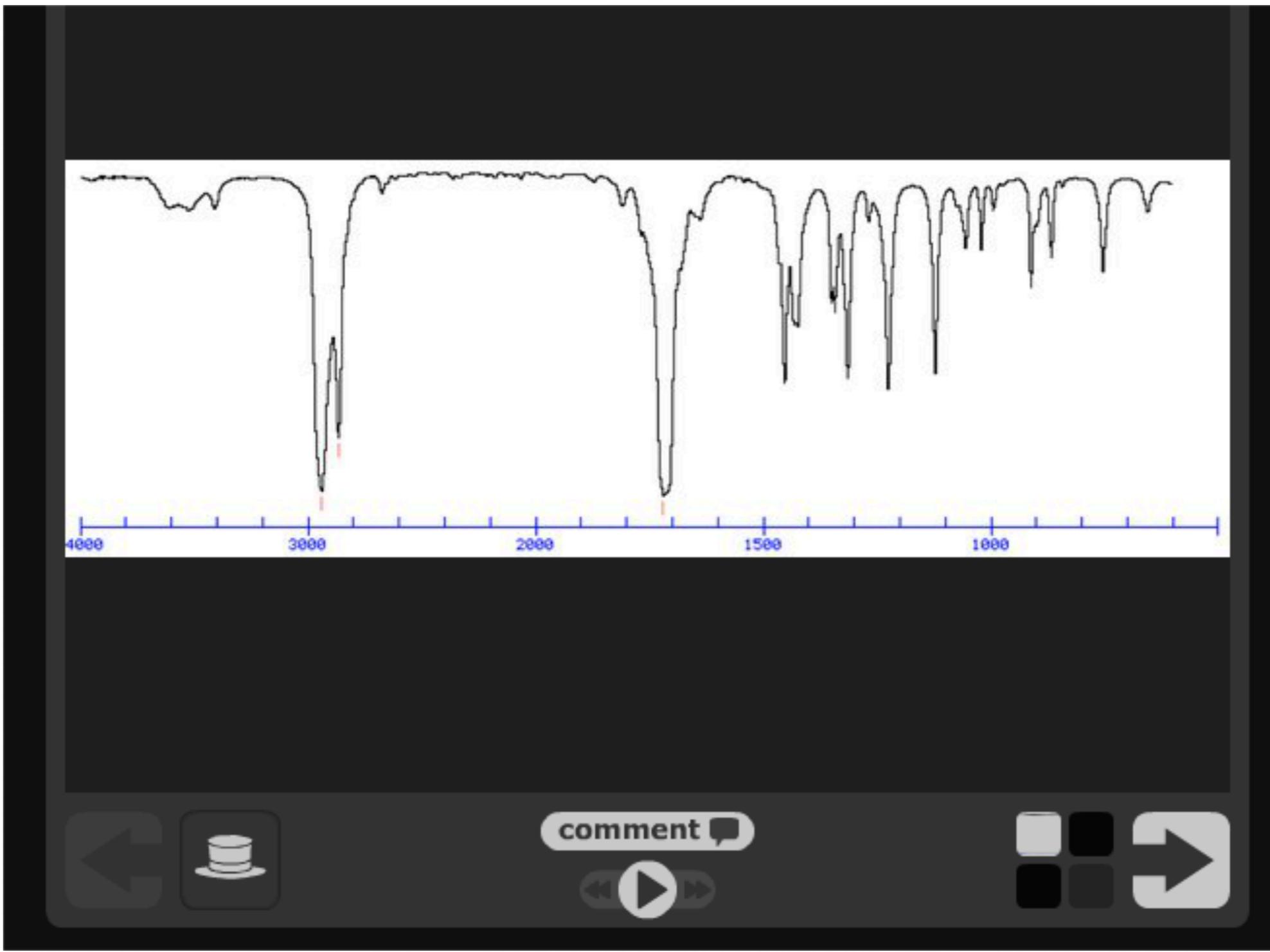
C-H alkene bending shows up with strong absorptions between $1000\text{-}675\text{ cm}^{-1}$. C=C aromatic stretches show up around $1680\text{-}1450\text{ cm}^{-1}$ with variable intensity.

Using this data, we can propose 3, 6, or 7 has an aromatic ring.

b) Which compound would be reduced by NaBH_4 (in EtOH/NaOH)?

You know that NaBH_4 reduces most carbonyls like ketones and aldehydes, though typically not amides, carboxylic acids or esters.

You should be looking for spectra with a carbonyl peak. These would be:



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VoiceThread

1	Electromagnetic spectrum	1	2	3	4
2	Infrared light and its relative energy	1	2	3	4
3	The relationship between energy and wavelength	1	2	3	4
4	The relationship between wavelength and wavenumber	1	2	3	4
5	The interaction of light with matter	1	2	3	4
6	Molecular vibrations	1	2	3	4
7	<u>Wavenumbers</u>	1	2	3	4
8	Significance and origin of the units of <u>wavenumbers</u> (cm^{-1})	1	2	3	4
9	Spectrum / spectra	1	2	3	4
10	Functional group region	1	2	3	4
11	Fingerprint region	1	2	3	4
12	Stretch	1	2	3	4
13	Band	1	2	3	4
14	What type of information that can be determined from an IR spectrum	1	2	3	4
15	What type of information that cannot be determined from an IR spectrum	1	2	3	4
16	The difference between Infrared and NMR spectroscopy	1	2	3	4
17	The effect of hydrogen bonding on the position and shape of an alcohol stretch	1	2	3	4
18	The effect of molecular structure on the position of a carbonyl stretch	1	2	3	4

Knowledge Probe

Indicate your familiarity with the following infrared spectroscopy terms and topics:

#	Question	Mean	Mean
1	Electromagnetic spectrum	3.23	3.28
2	Infrared light and its relative energy	3.28	3.17
3	The relationship between energy wavelength	3.26	3.35
4	The relationship between wavelength and wavenumber	3.02	3.12
5	The interaction of light with matter	2.96	3.00
6	Molecular vibrations	3.04	3.23
7	Wavenumbers	3.11	3.16
8	Significance and origin of the units of wavenumbers (cm-1)	2.96	2.96
9	Spectrum / spectra	3.57	3.60
10	Functional group region	3.70	3.77
11	Fingerprint region	3.53	3.60
12	Stretch	3.53	3.57
13	Band	3.38	3.40
14	What type of information that can be determined from an IR spectrum	3.81	3.74
15	What type of information that cannot be determined from an IR spectrum	3.72	3.57
16	The difference between Infrared and NMR spectroscopy	3.77	3.73
17	The effect of hydrogen bonding on the position and shape of an alcohol stretch	3.43	3.28
18	The effect of molecular structure on the position of a carbonyl stretch	3.30	3.26
	Average:	3.367	3.377

Infrared Spectroscopy Survey shows little difference, however...

- ❧ Problem (lower degree of difficulty)
 - ❧ LO students scored 8/8
 - ❧ Non-LO students scored 7.3/8

- ❧ Problem (higher degree of difficulty)
 - ❧ LO students scored 10/12
 - ❧ Non-LO students scored 6.9/12

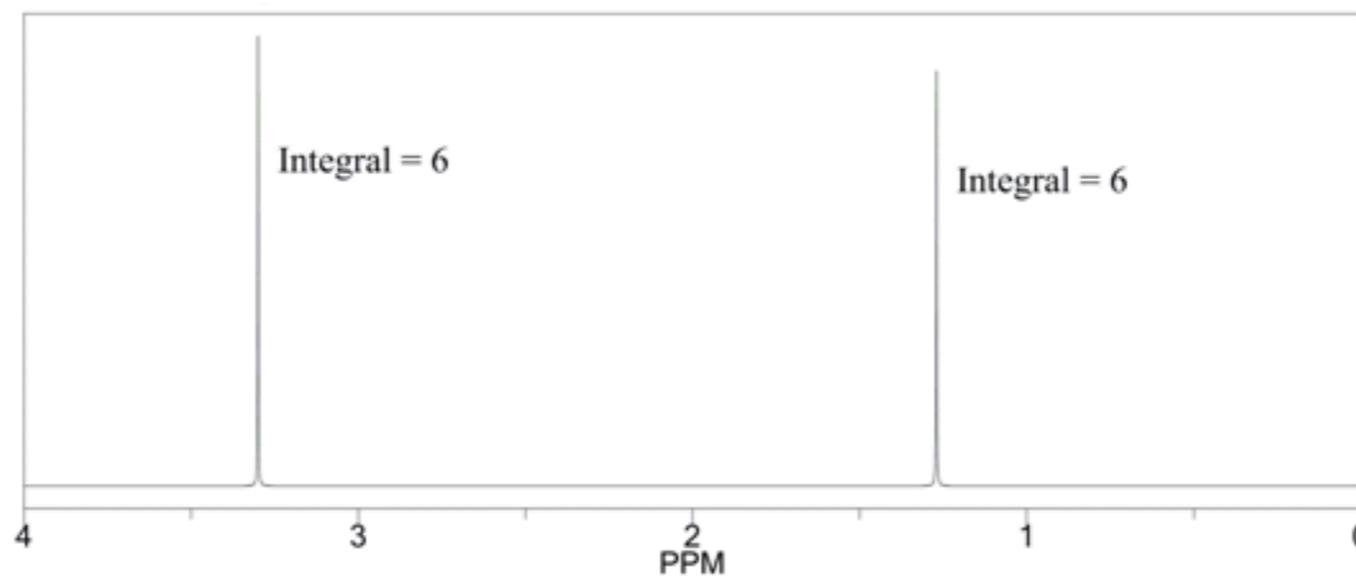
Indicate your familiarity with the following nuclear magnetic resonance (NMR) spectroscopy terms and topics:

#	Topic	LO Mean	Non-LO Mean
1	Nuclear spin	2.72	2.68
2	Significance and origin of parts per million (ppm) units	2.70	2.81
3	Significance and origin of Sigma (σ)	2.40	2.44
4	What type of information that can be determined from an NMR spectrum	3.62	3.61
5	What type of information can not be determined from an NMR spectrum	3.45	3.37
6	Integration	3.40	3.22
7	Chemical equivalency	3.57	3.36
8	Chemical shift	3.49	3.31
9	Splitting	3.61	3.31
10	Coupling	2.98	3.04
11	^1H -NMR compared to ^{13}C -NMR (similarities and differences)	3.28	3.11
12	Isotopes	2.83	2.89
13	NMR silent	2.38	2.26
14	NMR active	2.36	2.31
15	Upfield shifted	3.49	3.16
16	Downfield shifted	3.49	3.16
	Average:	3.110625	3.0025

NMR Problem

1. Draw the structure of a molecule with the formula $C_5H_{12}O_2$ that corresponds to the following NMR spectrum.

1H NMR 300 MHz



2. Explain, in your own words, how you arrived at your answer. Write as if you were explaining how to solve the problem to classmate. Feel free to draw on or label the spectrum above.

NMR Answers

Score #	Definition	LO Response	LO %	Non-LO	Non-LO%
1	Did Not Attempt	6	13%	19	13%
2	Attempted, Wrong Answer	11	23%	61	43%
3	Attempted, Correct Answer	30	64%	61	43%
	Total	47	100%	141	100%

Statistic	LO Sections	Non-LO Sections
Min Value	1	1
Max Value	3	3
Mean	2.51	2.30
Variance	0.52	0.48
Standard Deviation	0.72	0.69
Total Responses	47	141

NMR Explanations

Score	Answer	LO Response	LO %	Non-LO	Non-LO %
1	Did Not Explain	8	17%	40	28%
2	Explained Poorly	14	30%	67	48%
3	Explained Well	25	53%	34	24%
	Total	47	100%	141	100%

Statistic	LO Sections	Non-LO Sections
Min Value	1	1
Max Value	3	3
Mean	2.36	1.96
Variance	0.58	0.53
Standard Deviation	0.76	0.73
Total Responses	47	141

Chemistry 216: Synthesis and Characterization of Organic Compounds

last edited by  Chem216 1 week, 4 days ago

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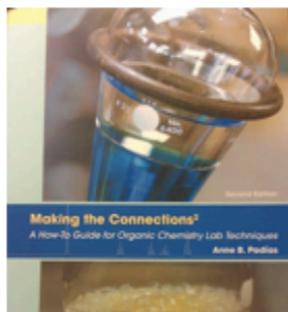
Syllabus:

Please review the syllabus for the CH216 course prior to attending your first lab. Familiarizing yourself with the resources on this site will allow you to utilize it as a resource throughout the entire term.

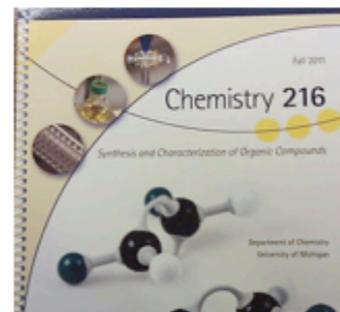
Attendance is absolutely critical. Students are expected to sign in each day and complete all 9 experiments. E-mail both [Dr. Shultz](#) and your GSI in advance in the event of an absence.



Required Materials:



- Text: Padias "Making the Connections; A How-To Guide for Organic Chemistry Lab Techniques" 2nd Edition, Hayden McNeil: Plymouth, MI; 2011 (ISBN: 978-0-7380-4135-3)
- Lab Manual: Department of Chemistry, University of Michigan, Synthesis and Characterization of Organic Compounds, 2012 (ISBN: 9780738042831)



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Navigator

 Chem216 Syllabus 

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