SI Organic Chemistry - Full Discipline Demo

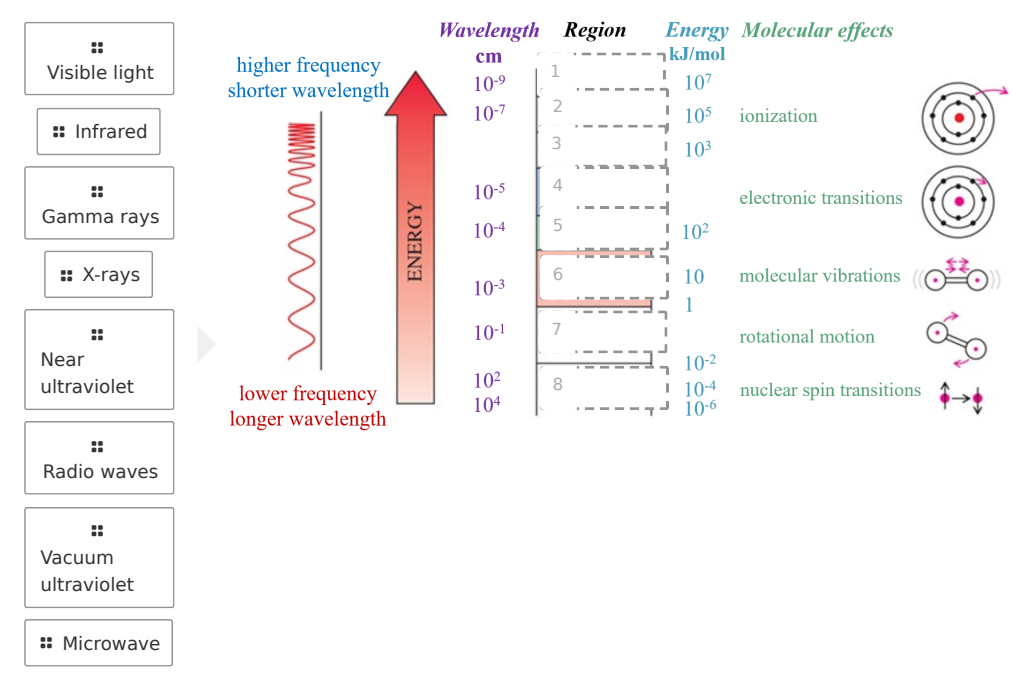
Infrared Spectroscopy

Final Report - Answer Guide

Institution	Science Interactive University
Session	SI Organic Chemistry - Full Discipline Demo
Course	SI Organic Chemistry - Full Discipline Demo
Instructor	Sales SI Demo

Test Your Knowledge

Label the diagram with the wavelength categories.



Correct answers:

1 Gamma rays 2 X-rays 3 Vacuum ultraviolet 4 Near ultraviolet

5 Visible light 6 Infrared 7 Microwave 8 Radio waves

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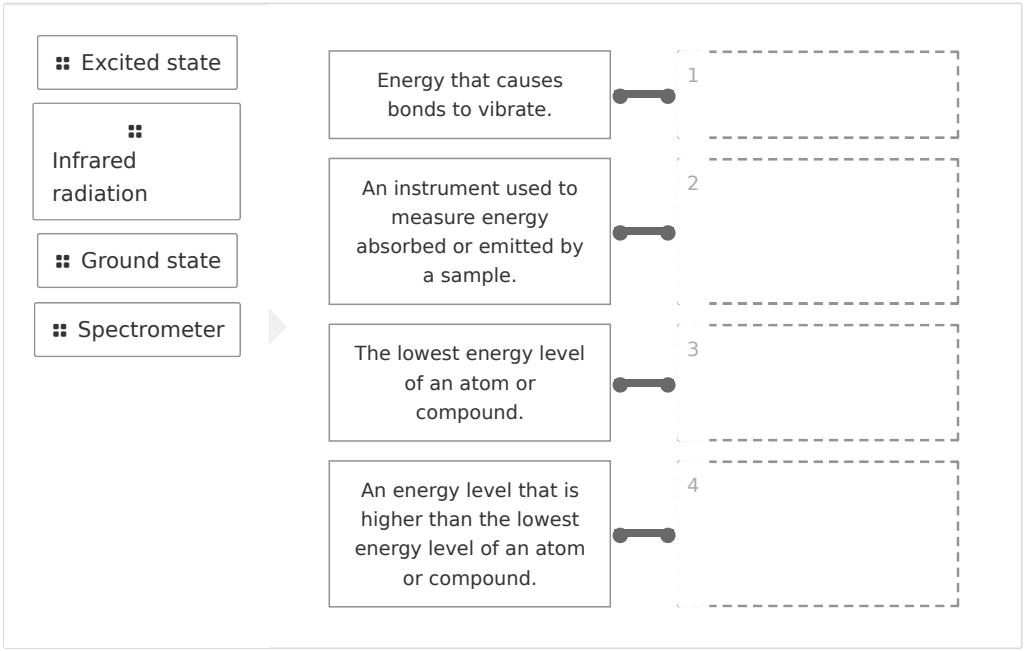
Match each term to the best description.



Correct answers:

1 Infrared radiation 2 Spectrometer 3 Ground state

4 Excited state

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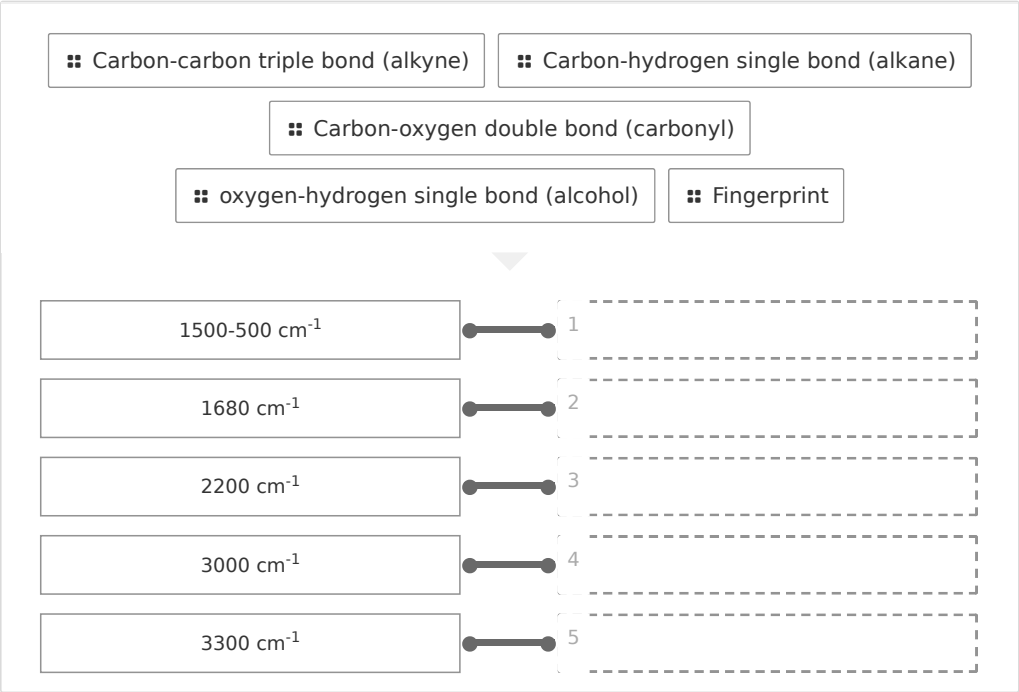
Match each functional group to the appropriate stretching frequency.



Correct answers:

1 Fingerprint 2 Carbon-oxygen double bond (carbonyl)

3 Carbon-carbon triple bond (alkyne) 4 Carbon-hydrogen single bond (alkane)

5 oxygen-hydrogen single bond (alcohol)

Exploration

Spectroscopy utilizing infrared light provides information related to the _____ of a compound.

- chemical environment
- vibrational energy ✔
- molecular weight
- All of the above

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An infrared-active molecule must have a dipole moment.

- True ✔
- False

A carbon-carbon triple bond requires more energy to vibrate than a carbon-carbon double bond.

- True ✔
- False

The most common frequency in organic chemistry is the _____.

- carbon-carbon double bond
- carbon-carbon single bond
- carbon-oxygen single bond
- None of the above ✔

A carbon-carbon double bond stretching frequency is in the _____ cm^{-1} range.

- 3200-3000
- 1800-1600 ✔
- 1500-1000
- None of the above

Electron withdrawing groups weaken bonds, causing a decrease in the measured wavenumber.

- True ✔
- False

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If an aliphatic C=O peak is located at about 1715 $cm,^{-1}$ its aromatic counterpart would be located at _____ $cm.^{-1}$

- 1745
- 1715
- 1685 ✔
- 1615

A(n) _____ is the functional group indicated by a strong, sharp peak at 2155 and an additional peak at 3305.

- nitrile
- carboxylic acid
- aldehyde
- terminal alkyne ✔

Exercise 1

Explain why infrared spectroscopy cannot be used to tell structural isomers apart.

Infrared spectroscopy is a qualitative technique used to identify the functional groups present rather than connectivity. This is why two isomers would be indistinguishable in infrared spectroscopy.

Explain how infrared spectroscopy is used to differentiate between an alkene and a ketone.

Alkenes will produce a peak between 1620–1680 cm-1, whereas ketones have a peak between 1680–1750 cm-1.

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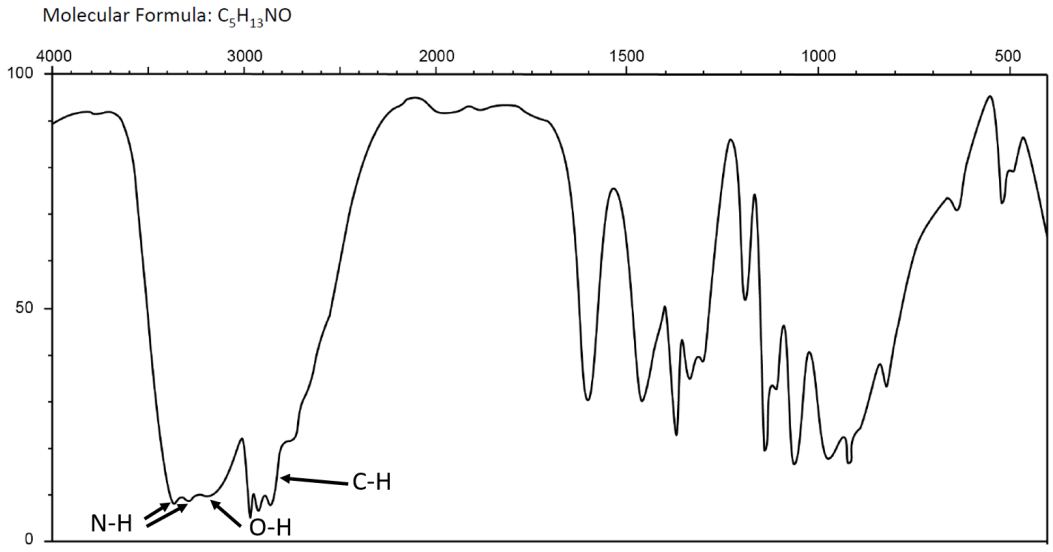
How would the stretching frequency of an O-H change if the oxygen was bonded to an alkane (alcohol) vs. a carbonyl (carboxylic acid)?

The O-H stretch would be higher in energy for an alcohol than a carboxylic acid because the carbonyl would weaken the O-H bond due to resonance. The observed effect would be a shift in the IR frequency to a lower frequency for the carboxylic acid.

Photo 1: Infrared Spectra 1
(SAMPLE ANSWER BELOW)



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Data Table 1: Peak Assignments for Infrared Spectra 1

(SAMPLE ANSWER BELOW)

Peak (cm^{-1})	Bond	Functional Group
3300, 3350	N-H	amine (1°)
3200-3400	O-H	alcohol
2950	C-H	alkane

Photo 2: Circle Structure(s) that Match the Spectra

(SAMPLE ANSWER BELOW)

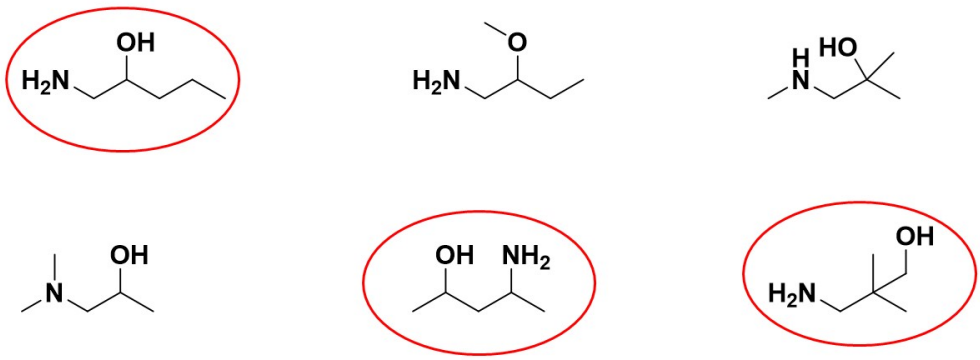

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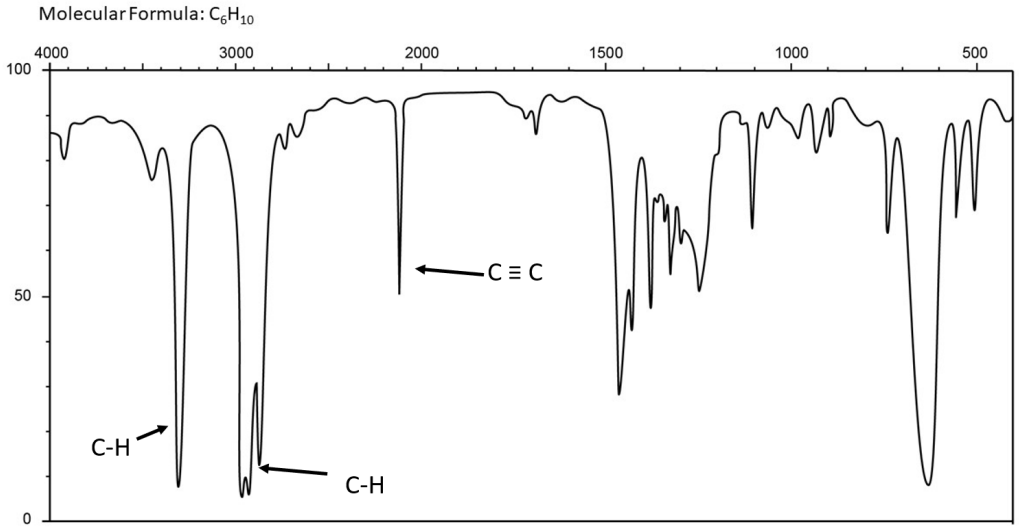
Photo 3: Infrared Spectra 2

(SAMPLE ANSWER BELOW)



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Data Table 2: Peak Assignments for Infrared Spectra 2
(SAMPLE ANSWER BELOW)

Peak (cm^{-1})	Bond	Functional Group
3300	C-H	alkyne
3000-2800	C-H	alkane
2150	C-C	triple bond

Photo 4: Circle Structure(s) that Match the Spectra
(SAMPLE ANSWER BELOW)

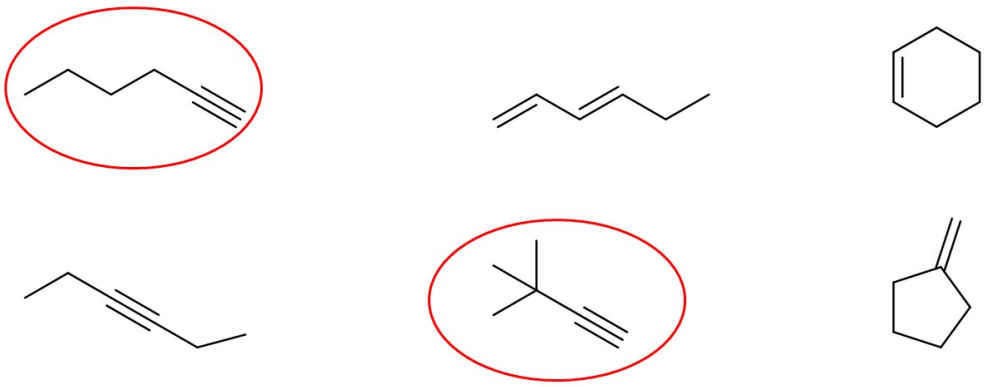

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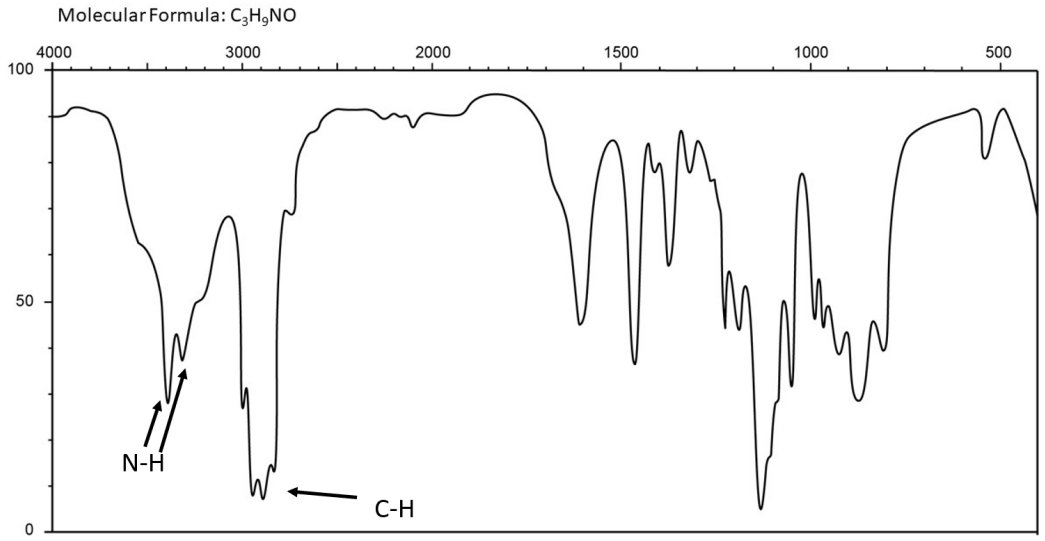
Photo 5: Infrared Spectra 3

(SAMPLE ANSWER BELOW)



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Data Table 3: Peak Assignments for Infrared Spectra 3
(SAMPLE ANSWER BELOW)

Peak (cm^{-1})	Functional group	Functional group
3400, 3300	N-H	amine 1°
2750-2900	C-H	alkane

Photo 6: Circle the Structure(s) that match the spectra
(SAMPLE ANSWER BELOW)

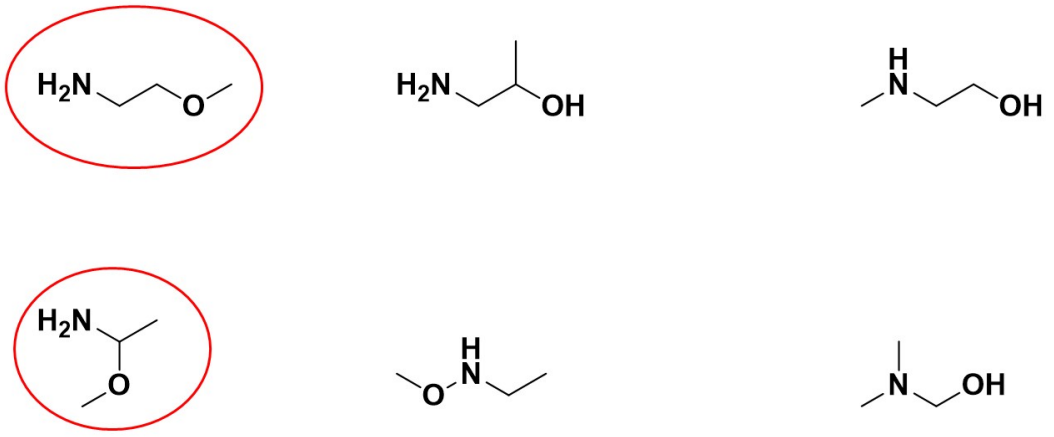

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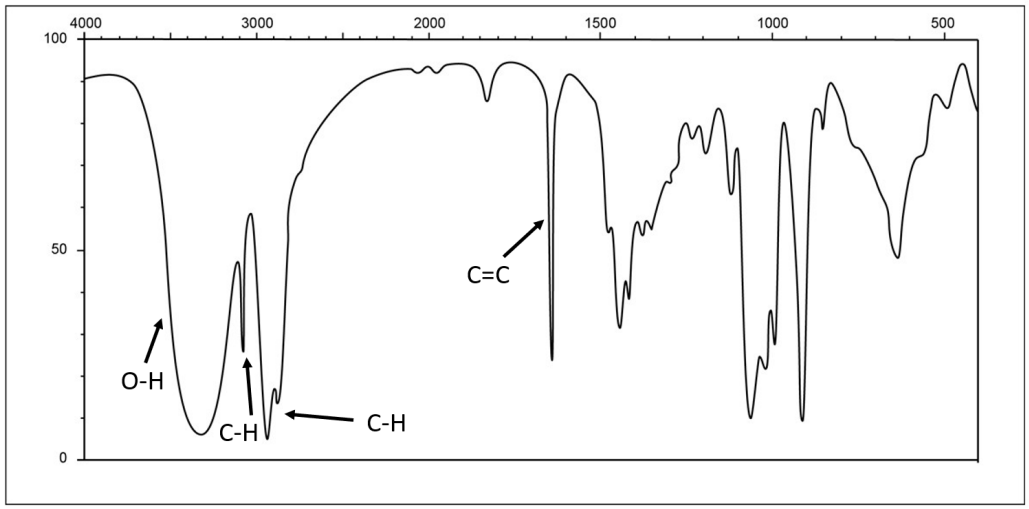
Photo 7: Infrared Spectra 4

(SAMPLE ANSWER BELOW)

Molecular Formula: $C_5H_{10}O$



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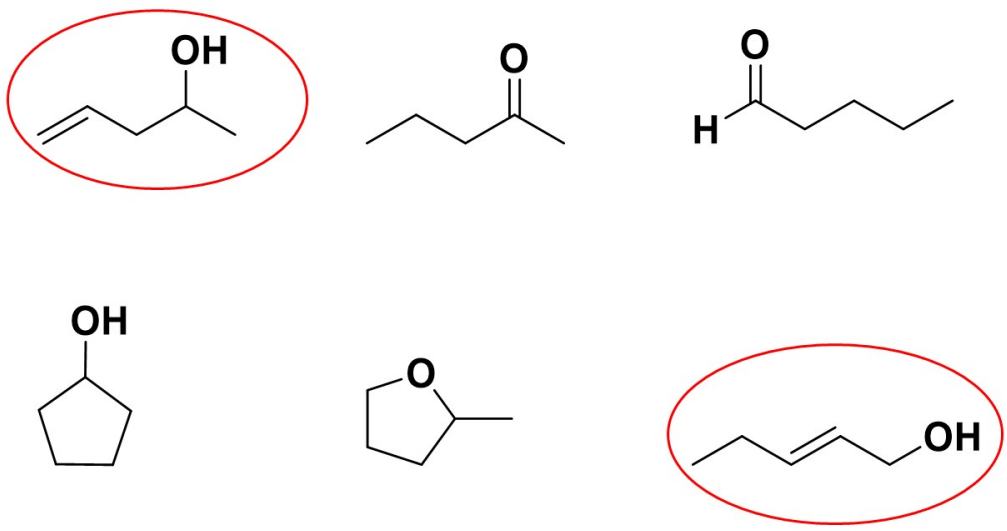
Data Table 4: Peak Assignments for Infrared Spectra 4

(SAMPLE ANSWER BELOW)

Peak (cm^{-1})	Functional Group
3100-3600	O-H (alcohol)
3000	C-H (alkene)
2800-2950	C-H (alkane)
1650	C=C (alkene)

Photo 8: Circle the Structure(s) that Match the IR spectra

(SAMPLE ANSWER BELOW)



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Exercise 2

What is the most productive place in an infrared spectrum for examining what kinds of functional groups are in the analyzed molecule? Explain your answer.

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What are the main differences in an infrared spectrum of an alkene vs. an alkane?

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What is the main giveaway that an infrared spectrum is of an aromatic ring instead of a simple alkene?

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Photo 9: Spectra A
(SAMPLE ANSWER BELOW)

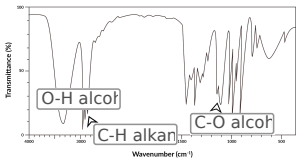


Photo 10: Spectra B
(SAMPLE ANSWER BELOW)

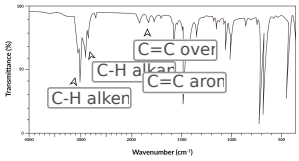
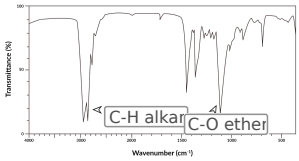


Photo 11: Spectra C
(SAMPLE ANSWER BELOW)



Data Table 5: Matching Spectra A-C
(SAMPLE ANSWER BELOW)

Spectra	Molecule Identity
A	2-butanol
B	toluene
C	dihexyl ether

Data Table 6: Spectra D Peaks
(SAMPLE ANSWER BELOW)

Peak (cm^{-1})	Bond	Functional Group
~3100	C-H	alkene
~2950	C-H	alkane

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~1650	C=C	alkene

Data Table 7: Spectra E Peaks
(SAMPLE ANSWER BELOW)

Peak (cm^{-1})	Bond	Functional Group
~2890	C-H	alkane

Data Table 8: Spectra F Peaks
(SAMPLE ANSWER BELOW)

Peak (cm^{-1})	Bond	Functional Group
~3300	C-H	alkyne
~2950	C-H	alkane
~2120	C≡C	alkyne

Data Table 9: Matching Spectra D-F
(SAMPLE ANSWER BELOW)

Spectra	Molecule Identity
D	2-methyl-2-pent
E	octane
F	1-hexyne

Exercise 3

The benzamide spectrum is highly unusual for an organic molecule. What peak is missing from its spectrum? Why is this so unusual in infrared spectrometry? Does it make sense given the molecule's structure?

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What common peak is shared by infrared spectra of carboxylic acids, aldehydes, ketones, and amides?

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What peaks easily differentiate between carboxylic acids, aldehydes, ketones, and amides?

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Photo 15: Spectra G
(SAMPLE ANSWER BELOW)

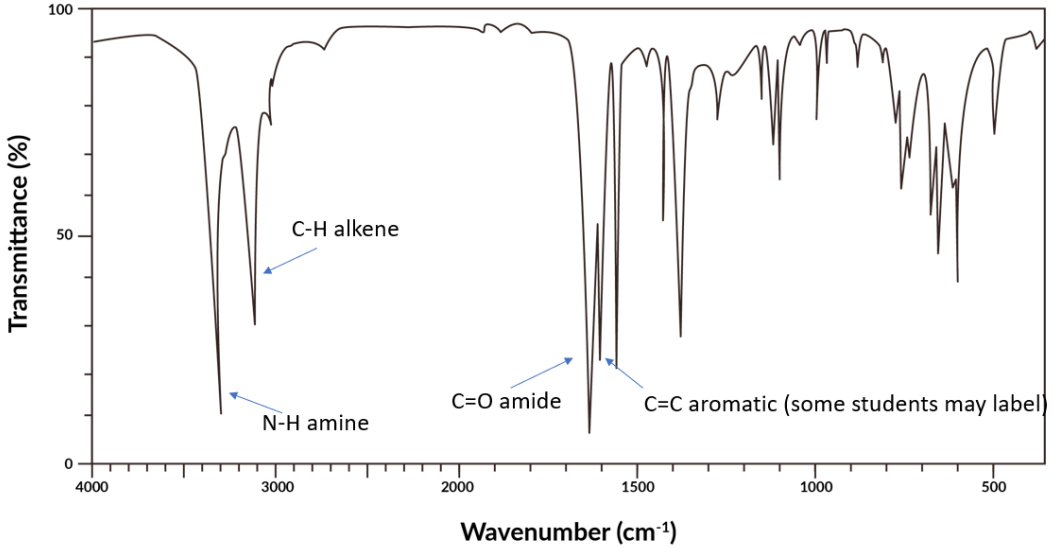

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Photo 16: Spectra H

(SAMPLE ANSWER BELOW)

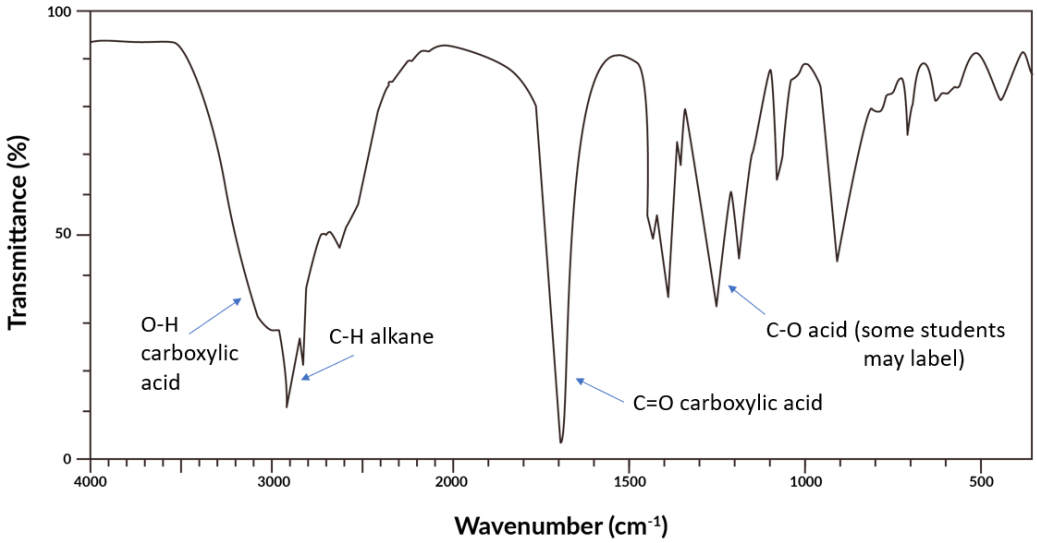

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Photo 17: Spectra I

(SAMPLE ANSWER BELOW)

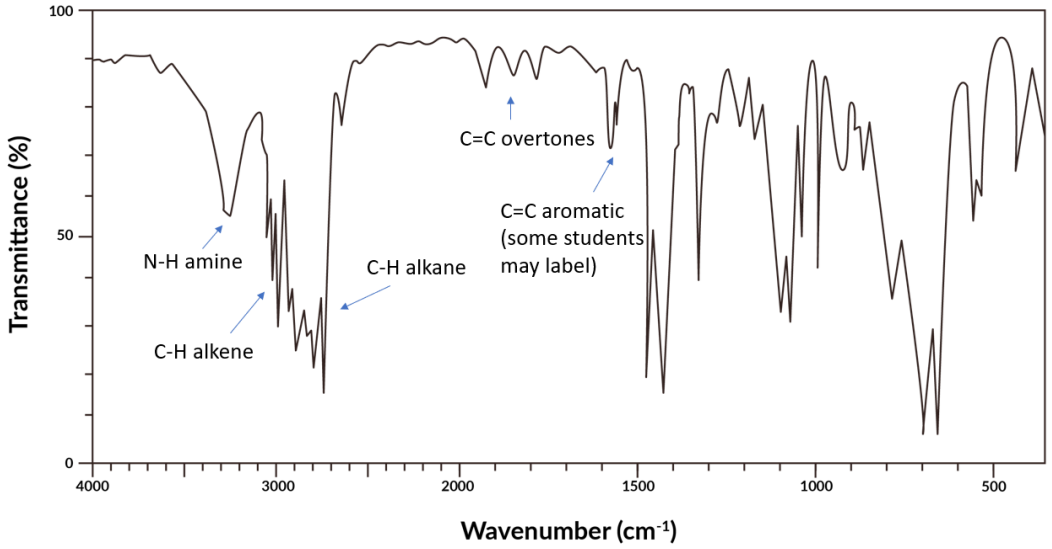

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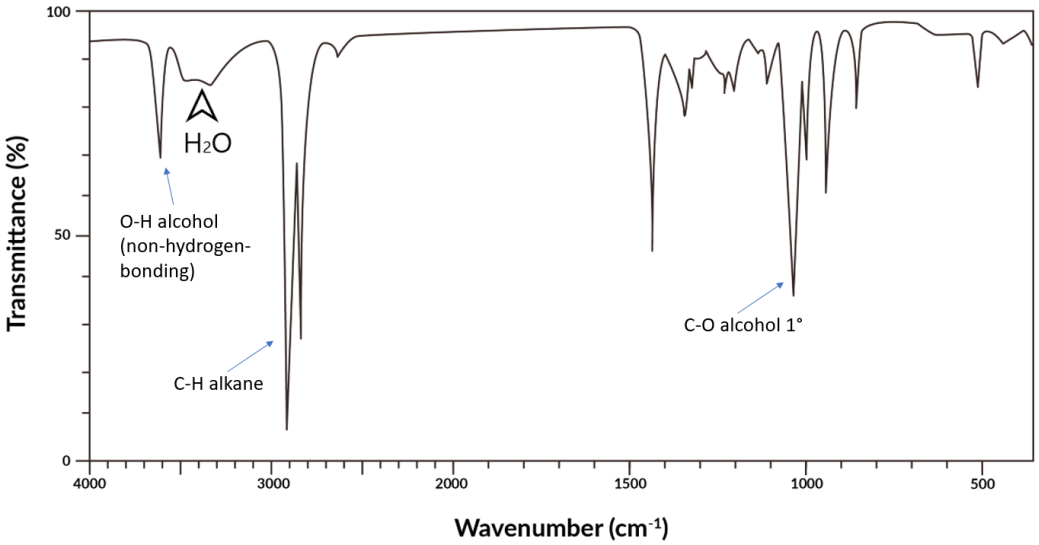
Photo 18: Spectra J

(SAMPLE ANSWER BELOW)



Data Table 10: Matching Spectra G-J

(SAMPLE ANSWER BELOW)

Spectrum	Molecule Identity

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G	benzamide
H	pentanoic acid
I	n-methyl-benzyl
J	cyclohexanol

Photo 19: Spectra K
(SAMPLE ANSWER BELOW)

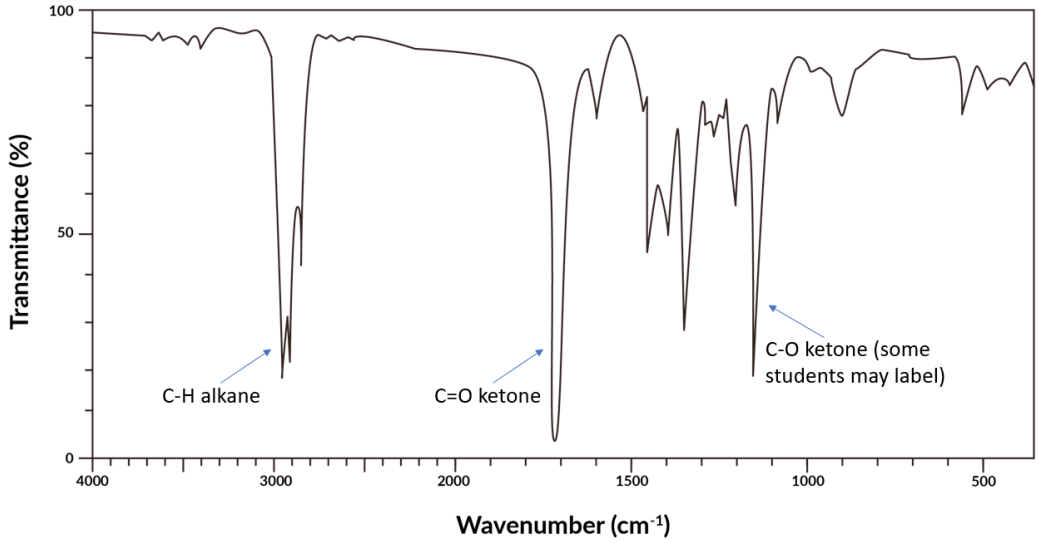

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Photo 20: Spectra L

(SAMPLE ANSWER BELOW)

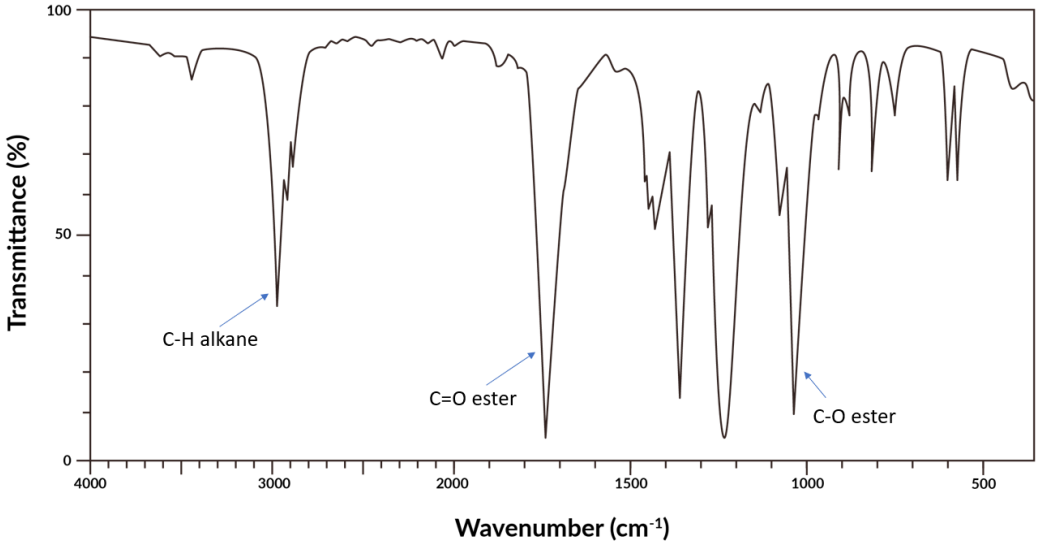

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Photo 21: Spectra M
(SAMPLE ANSWER BELOW)

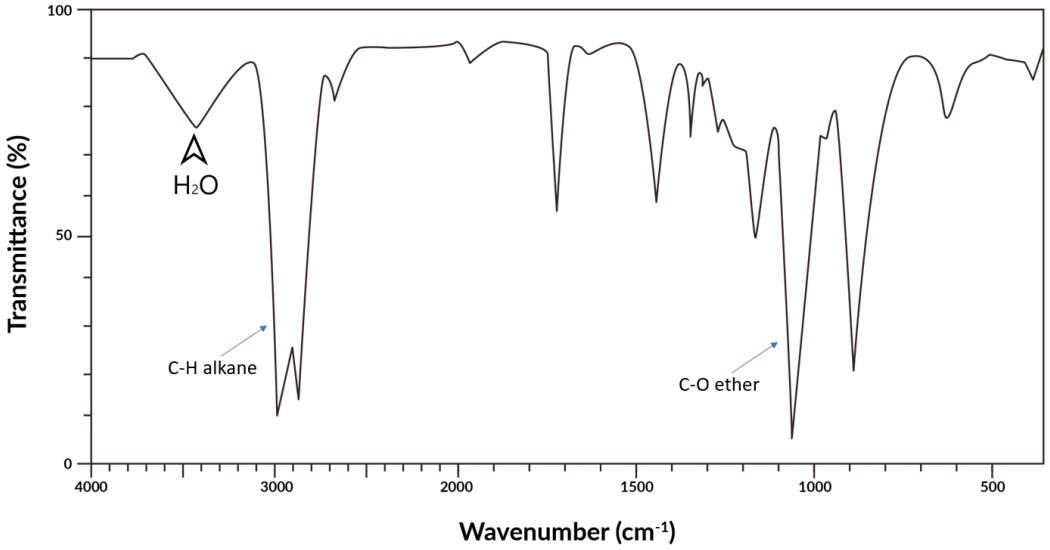

Photo 22: Spectra N
(SAMPLE ANSWER BELOW)

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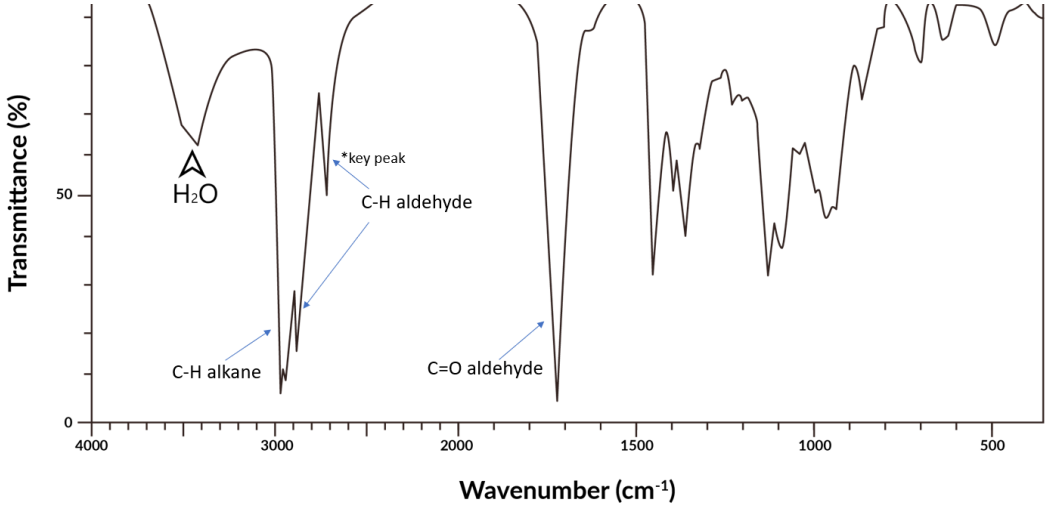

Data Table 11: Matching Spectra K-N

(SAMPLE ANSWER BELOW)

Spectrum	Molecule Identity
K	2-heptanone
L	ethyl acetate

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M	tetrahydrofuran
N	pentanal

Competency Review

Electromagnetic radiation located in the _____ region is required to vibrate covalent bonds.

- infrared ✔
- ultraviolet
- visible
- None of the above

Spectroscopy uses radiation from the electromagnetic spectrum to study its interactions with matter.

- True ✔
- False

The _____ functional group requires the most energy to vibrate the bond.

- alcohol (O-H) ✔
- alkane (C-H)
- amine (N-H)
- alkene (C-H)

A bond vibration frequency is directly proportional to the difference in _____ between the bonded atoms.

- molecular weight
- reduced mass ✔
- force constant
- None of the above

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The peak that corresponds to an O-H stretching frequency is described as broad.

- True ✔
- False

A primary amine (R-NH_2) will have only one stretching frequency in an infrared spectra.

- True
- False ✔

An infrared spectrum can be used to distinguish between two isomers.

- True
- False ✔

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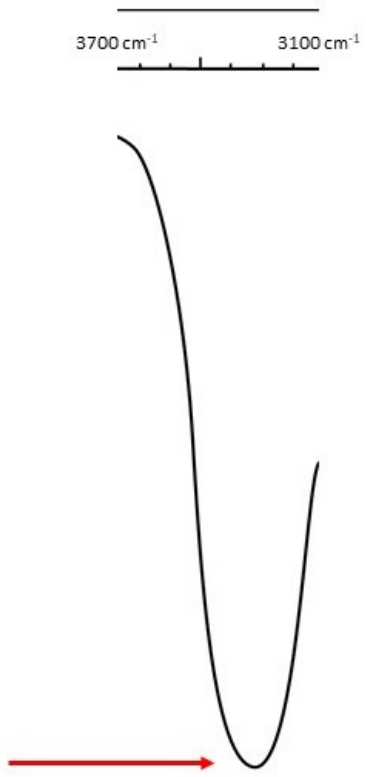
The peak represented in the image is a _____ stretching frequency.



- C-H (alkane)
- O-H ✔
- C=C (alkene)
- None of the above

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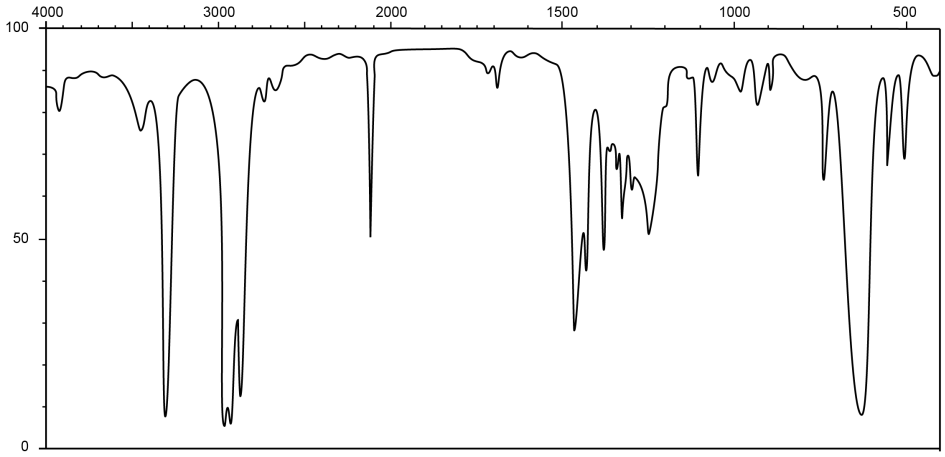
The infrared spectra in the image below contains a(n) _____ stretching frequency.



- alkyne
- C-H (alkyne)
- C-H (alkane)
- All of the above ✔

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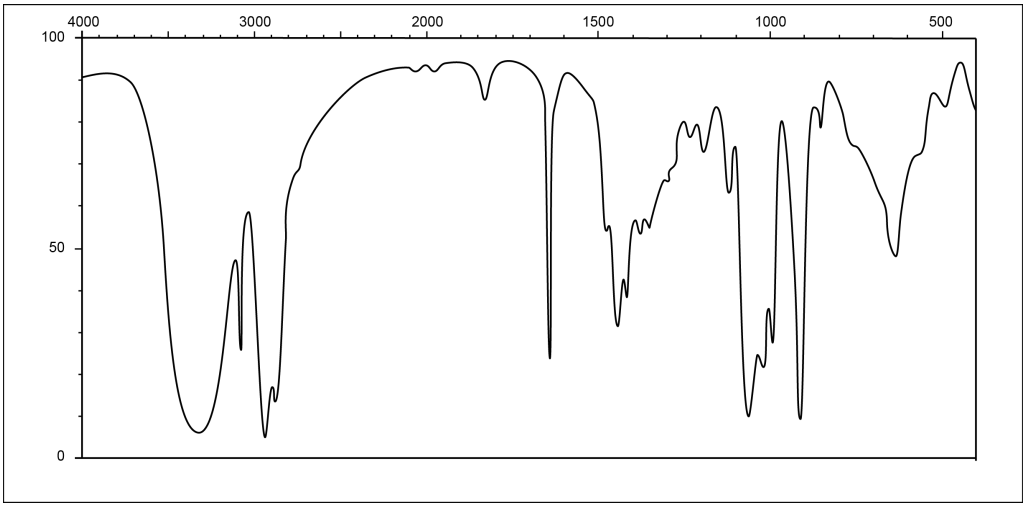
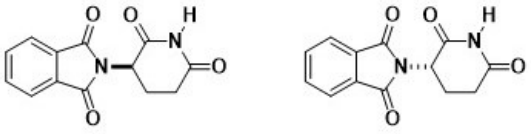
In the provided spectra below, the carbon-carbon double bond has a peak appearing at _____ cm^{-1}.



- 3350
- 2900
- 1680 ✔
- None of the above

Extension Questions

Thalidomide is a drug that exists as two enantiomers. See below for the structure of Thalidomide.



(*R*)-Thalidomide (*S*)-Thalidomide

A) If infrared spectra were obtained for both enantiomers, could you determine which structure matches which spectrum?
B) Predict the defining peaks present in an infrared spectrum of Thalidomide.

(SAMPLE ANSWER BELOW)

A) Infrared spectra of both (R) and (S) Thalidomide contain the same functional groups, and thus would not be able to be differentiated.

B) Thalidomide will have a C=O (amide) peak, C=C (aromatic) peaks with overtones, an N-H peak, and C-H (alkane and alkene) peaks.

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