

12.8: INFRARED SPECTRA OF SOME COMMON FUNCTIONAL GROUPS

OBJECTIVE

After completing this section, you should be able to use an infrared spectrum to determine the presence of functional groups, such as alcohols, amines and carbonyl groups, in an unknown compound, given a list of infrared absorption frequencies.

STUDY NOTES

In Chapter 12.7 you should have learned, in broad terms, where a few key absorptions occur. Otherwise, to find the characteristic infrared absorptions of the various functional groups, refer to [this IR table](#).

SPECTRAL INTERPRETATION BY APPLICATION OF GROUP FREQUENCIES

One of the most common application of infrared spectroscopy is to the identification of organic compounds. The major classes of organic molecules are shown in this category and also linked on the bottom page for the number of collections of spectral information regarding organic molecules.

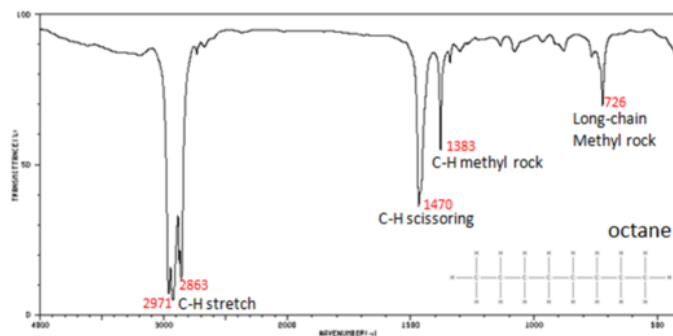
HYDROCARBONS

Hydrocarbons compounds contain only C-H and C-C bonds, but there is plenty of information to be obtained from the infrared spectra arising from C-H stretching and C-H bending.

In alkanes, which have very few bands, each band in the spectrum can be assigned:

- C-H stretch from $3000\text{--}2850\text{ cm}^{-1}$
- C-H bend or scissoring from $1470\text{--}1450\text{ cm}^{-1}$
- C-H rock, methyl from $1370\text{--}1350\text{ cm}^{-1}$
- C-H rock, methyl, seen only in long chain alkanes, from $725\text{--}720\text{ cm}^{-1}$

Figure 12.8.1 shows the IR spectrum of octane. Since most organic compounds have these features, these C-H vibrations are usually not noted when interpreting a routine IR spectrum. Note that the change in dipole moment with respect to distance for the C-H stretching is greater than that for others shown, which is why the C-H stretch band is the more intense.



12.8.1: Infrared Spectrum of Octane

In alkenes compounds, each band in the spectrum can be assigned:

- C=C stretch from $1680\text{--}1640\text{ cm}^{-1}$
- =C-H stretch from $3100\text{--}3000\text{ cm}^{-1}$
- =C-H bend from $1000\text{--}650\text{ cm}^{-1}$

Figure 12.8.2 shows the IR spectrum of 1-octene. As alkanes compounds, these bands are not specific and are generally not noted because they are present in almost all organic molecules.

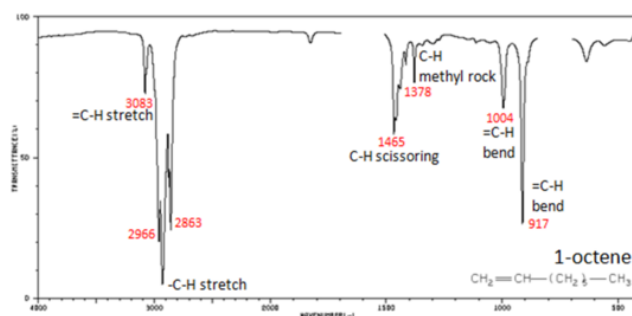


Figure 12.8.2: Infrared Spectrum of 1-Octene

In alkynes, each band in the spectrum can be assigned:

- $\text{C}\equiv\text{C}$ stretch from $2260\text{--}2100\text{ cm}^{-1}$
- $\text{C}\equiv\text{C}\text{--H}$: C–H stretch from $3330\text{--}3270\text{ cm}^{-1}$
- $\text{C}\equiv\text{C}\text{--H}$: C–H bend from $700\text{--}610\text{ cm}^{-1}$

The spectrum of 1-hexyne, a terminal alkyne, is shown below.

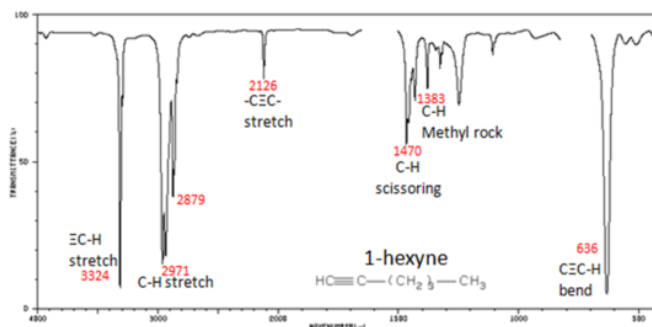


Figure 12.8.3: Infrared Spectrum of 1-Hexyne

In aromatic compounds, each band in the spectrum can be assigned:

- C–H stretch from $3100\text{--}3000\text{ cm}^{-1}$
- overtones, weak, from $2000\text{--}1665\text{ cm}^{-1}$
- C–C stretch (in-ring) from $1600\text{--}1585\text{ cm}^{-1}$
- C–C stretch (in-ring) from $1500\text{--}1400\text{ cm}^{-1}$
- C–H "oop" from $900\text{--}675\text{ cm}^{-1}$

Note that this is at slightly higher frequency than is the C–H stretch in alkanes. This is a very useful tool for interpreting IR spectra. Only alkenes and aromatics show a C–H stretch slightly higher than 3000 cm^{-1} . Figure 12.8.4 shows the spectrum of toluene.

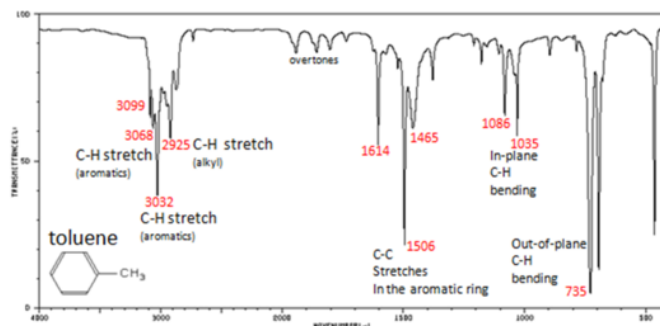


Figure 12.8.4: Infrared Spectrum of Toluene

FUNCTIONAL GROUPS CONTAINING THE C-O BOND

Alcohols have IR absorptions associated with both the O–H and the C–O stretching vibrations.

- O–H stretch, hydrogen bonded $3500\text{--}3200\text{ cm}^{-1}$
- C–O stretch $1260\text{--}1050\text{ cm}^{-1}$ (s)

Figure 12.8.5 shows the spectrum of ethanol. Note the very broad, strong band of the O–H stretch.

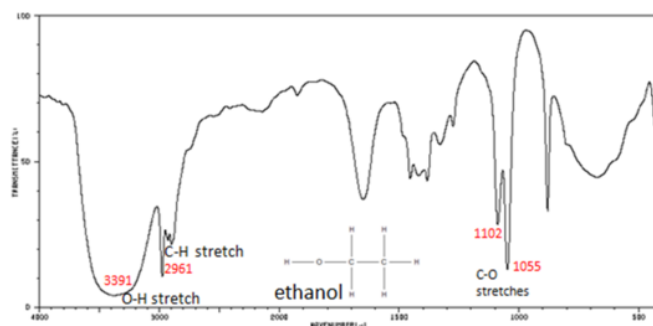


Figure 12.8.5: Infrared Spectrum of Ethanol

The carbonyl stretching vibration band C=O of saturated aliphatic ketones appears:

- C=O stretch - aliphatic ketones 1715 cm⁻¹
- α , β -unsaturated ketones 1685-1666 cm⁻¹

Figure 12.8.6 shows the spectrum of 2-butanone. This is a saturated ketone, and the C=O band appears at 1715.

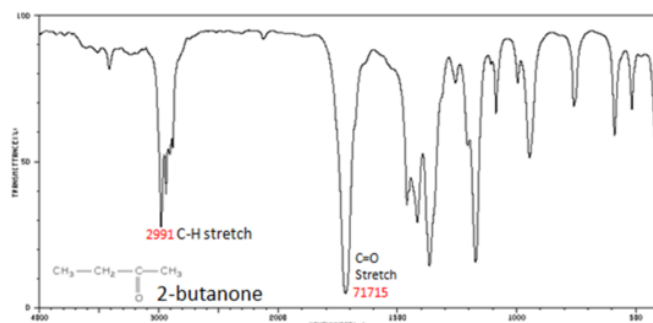


Figure 12.8.6: Infrared Spectrum of 2-Butanone

If a compound is suspected to be an aldehyde, a peak always appears around 2720 cm⁻¹ which often appears as a shoulder-type peak just to the right of the alkyl C-H stretches.

- H-C=O stretch 2830-2695 cm⁻¹
- C=O stretch:
 - aliphatic aldehydes 1740-1720 cm⁻¹
 - α , β -unsaturated aldehydes 1710-1685 cm⁻¹

Figure 12.8.7 shows the spectrum of butyraldehyde.

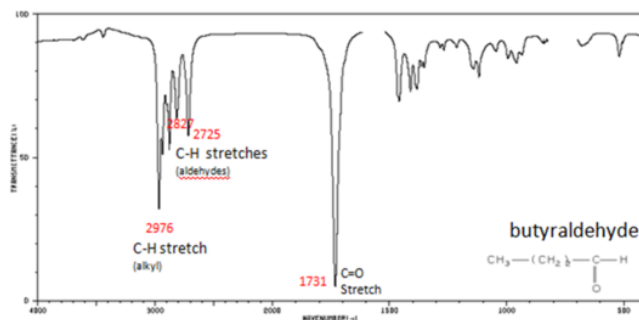


Figure 12.8.7: Infrared Spectrum of Butyraldehyde

The carbonyl stretch C=O of esters appears:

- C=O stretch
 - aliphatic from 1750-1735 cm⁻¹
 - α , β -unsaturated from 1730-1715 cm⁻¹

- C–O stretch from 1300-1000 cm^{-1}

Figure 12.8.8: shows the spectrum of ethyl benzoate.

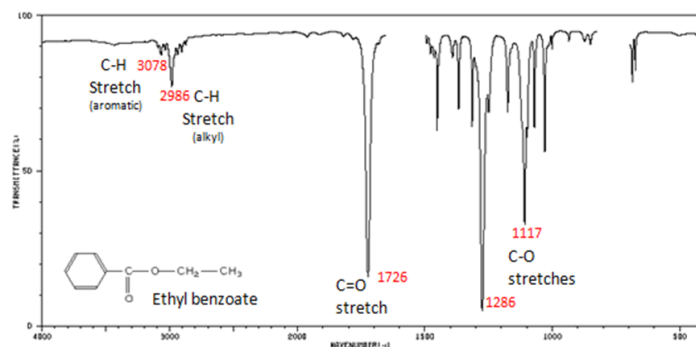


Figure 12.8.8: Infrared Spectrum of Ethyl benzoate

The carbonyl stretch $\text{C}=\text{O}$ of a carboxylic acid appears as an intense band from 1760-1690 cm^{-1} . The exact position of this broad band depends on whether the carboxylic acid is saturated or unsaturated, dimerized, or has internal hydrogen bonding.

- O–H stretch from 3300-2500 cm^{-1}
- $\text{C}=\text{O}$ stretch from 1760-1690 cm^{-1}
- C–O stretch from 1320-1210 cm^{-1}
- O–H bend from 1440-1395 and 950-910 cm^{-1}

Figure 12.8.9: shows the spectrum of hexanoic acid.

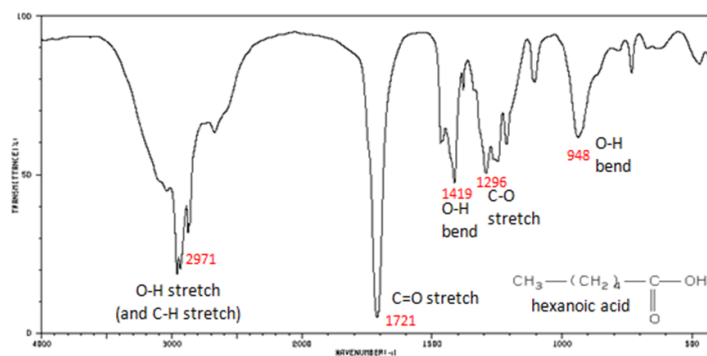


Figure 12.8.9: Infrared Spectrum of Hexanoic acid

ORGANIC NITROGEN COMPOUNDS

- N–O asymmetric stretch from 1550-1475 cm^{-1}
- N–O symmetric stretch from 1360-1290 cm^{-1}

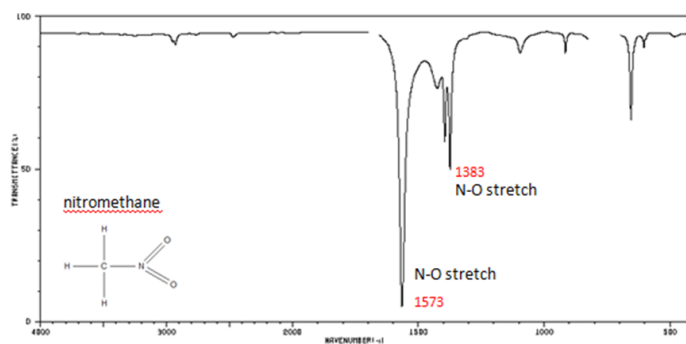


Figure 12.8.10 Infrared Spectrum of Nitromethane

ORGANIC COMPOUNDS CONTAINING HALOGENS

Alkyl halides are compounds that have a C–X bond, where X is a halogen: bromine, chlorine, fluorene, or iodine.

- C–H wag ($-\text{CH}_2\text{X}$) from $1300\text{--}1150\text{ cm}^{-1}$
- C–X stretches (general) from $850\text{--}515\text{ cm}^{-1}$
 - C–Cl stretch $850\text{--}550\text{ cm}^{-1}$
 - C–Br stretch $690\text{--}515\text{ cm}^{-1}$

The spectrum of 1-chloro-2-methylpropane are shown below.

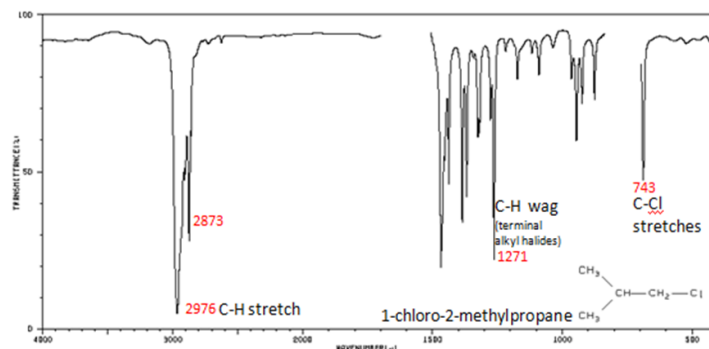


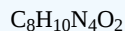
Figure 12.8.11: Infrared Spectrum of 1-chloro-2-methylpropane

For more Infrared spectra [Spectral database of organic molecules](#) is introduced to use free database. Also, the [infrared spectroscopy correlation](#) table is linked on bottom of page to find other assigned IR peaks.

? EXERCISE 12.8.1

Caffeine has a mass of 194.19 amu, determined by mass spectrometry, and contains C, N, H, O. What is a molecular formula for this molecule?

Answer



$$\text{C} = 12 \times 8 = 96$$

$$\text{N} = 14 \times 4 = 56$$

$$\text{H} = 1 \times 10 = 10$$

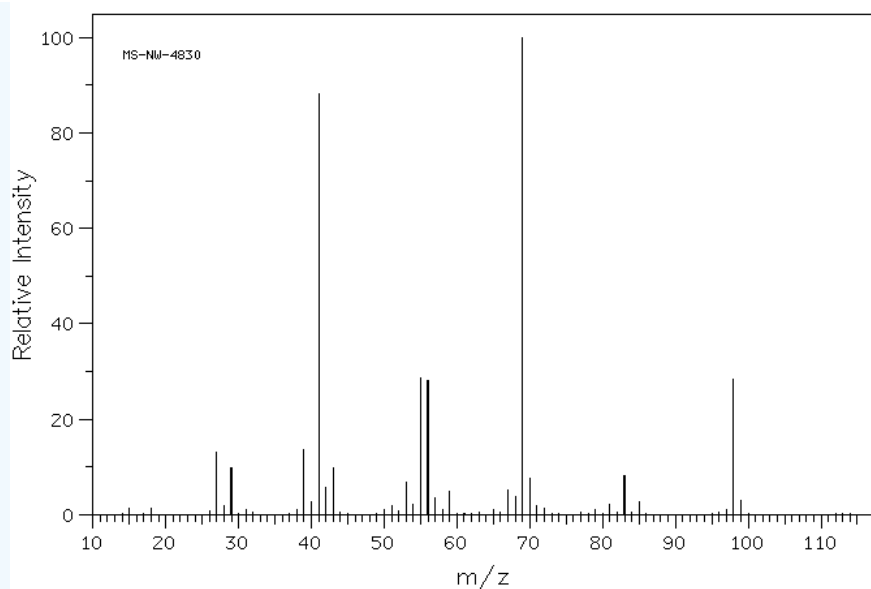
$$\text{O} = 2 \times 16 = 32$$

$$96 + 56 + 10 + 32 = 194 \text{ g/mol}$$

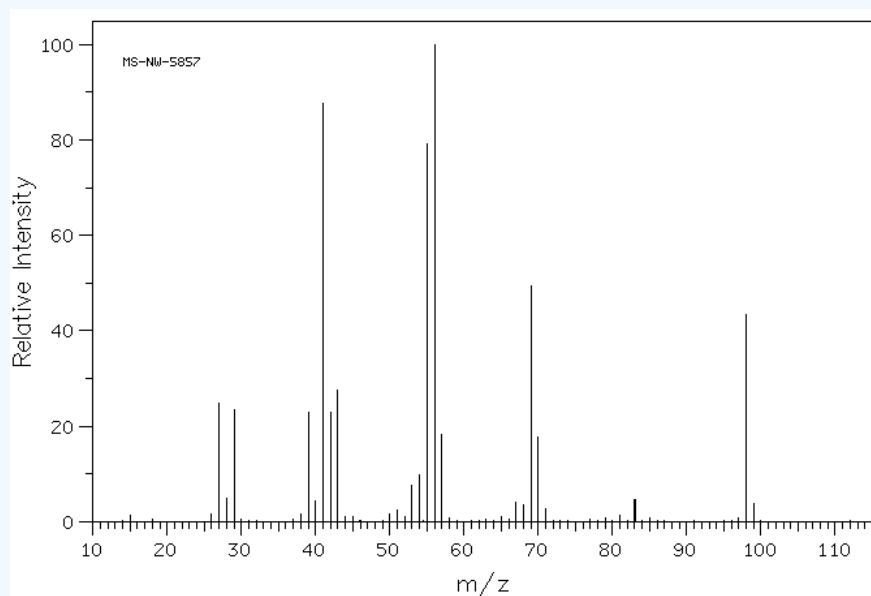
? EXERCISE 12.8.2

The following are the spectra for 2-methyl-2-hexene and 2-heptene, which spectra belongs to the correct molecule. Explain.

A:



B:



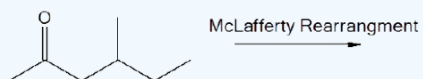
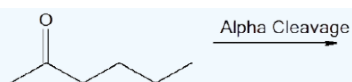
Source: SDBSWeb : <http://sdb.sdb.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, 2 December 2016)

Answer

The (A) spectrum is 2-methyl-2-hexene and the (B) spectrum is 2-heptene. Looking at (A) the peak at 68 m/z is the fractionated molecule with just the tri-substituted alkene present. While (B) has a strong peak around the 56 m/z , which in this case is the di-substituted alkene left behind from the linear heptene.

? EXERCISE 12.8.3

What are the masses of all the components in the following fragmentations?



Answer



? EXERCISE 12.8.4

Which of the following frequencies/wavelengths are higher energy

- $\lambda = 2.0 \times 10^{-6} \text{ m}$ or $\lambda = 3.0 \times 10^{-9} \text{ m}$
- $\nu = 3.0 \times 10^9 \text{ Hz}$ or $\nu = 3.0 \times 10^{-6} \text{ Hz}$

Answer

- $\lambda = 3.0 \times 10^{-9} \text{ m}$
- $\nu = 3.0 \times 10^9 \text{ Hz}$

? EXERCISE 12.8.5

Calculate the energies for the following;

- Gamma Ray $\lambda = 4.0 \times 10^{-11} \text{ m}$
- X-Ray $\lambda = 4.0 \times 10^{-9} \text{ m}$
- UV light $\nu = 5.0 \times 10^{15} \text{ Hz}$
- Infrared Radiation $\lambda = 3.0 \times 10^{-5} \text{ m}$
- Microwave Radiation $\nu = 3.0 \times 10^{11} \text{ Hz}$

Answer

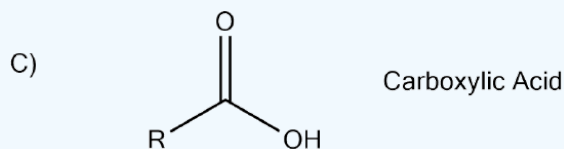
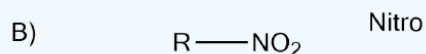
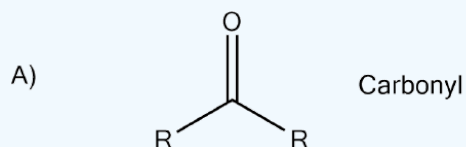
- a. 4.965×10^{-15} J
- b. 4.965×10^{-17} J
- c. 3.31×10^{-18} J
- d. 6.62×10^{-21} J
- e. 1.99×10^{-22} J

? EXERCISE 12.8.6

What functional groups give the following signals in an IR spectrum?

- a. 1700 cm^{-1}
- b. 1550 cm^{-1}
- c. 1700 cm^{-1} and $2510\text{-}3000 \text{ cm}^{-1}$

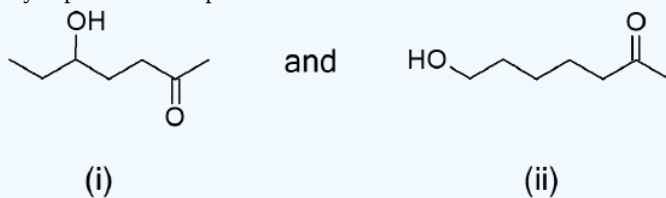
Answer



? EXERCISE 12.8.7

How can you distinguish the following pairs of compounds through IR analysis?

- a. CH_3OH (Methanol) and $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$ (Diethylether)
- b. Cyclopentane and 1-pentene.

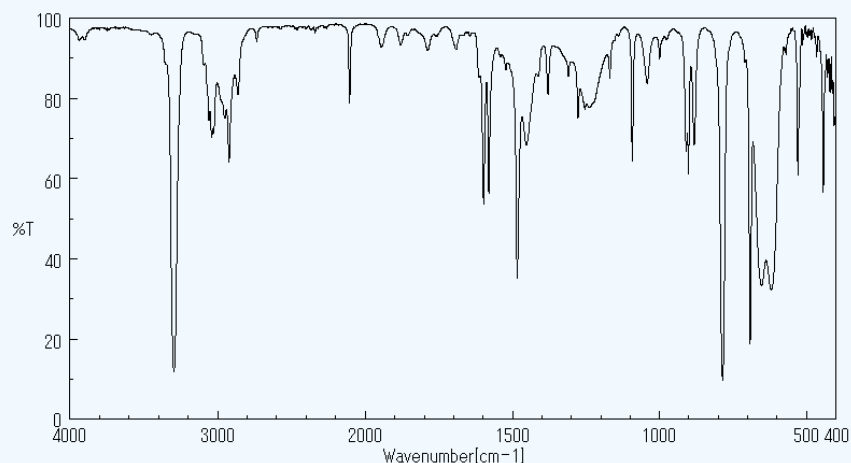
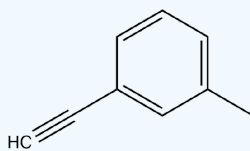


Answer

- a. A OH peak will be present around 3300 cm^{-1} for methanol and will be absent in the ether.
- b. 1-pentene will have an alkene peak around 1650 cm^{-1} for the $\text{C}=\text{C}$ and there will be another peak around 3100 cm^{-1} for the $\text{sp}^2 \text{ C-H}$ group on the alkene
- c. Cannot distinguish these two isomers. They both have the same functional groups and therefore would have the same peaks on an IR spectra.

? EXERCISE 12.8.8

The following spectra is for the accompanying compound. What are the peaks that you can identify in the spectrum?



Source: SDBSWeb : <http://sdb.s.db.aist.go.jp> (National Institute of Advanced Industrial Science and Technology, 2 December 2016)

Answer

Frequency (cm⁻¹) Functional Groups

3200 C≡C-H

2900-3000 C-C-H, C=C-H

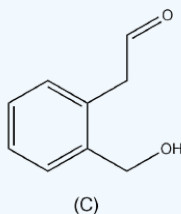
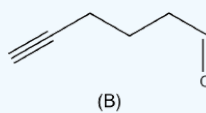
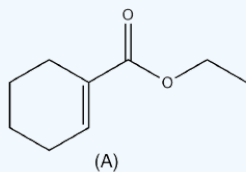
2100 C≡C

1610 C=C

(There is also an aromatic undertone region between 2000-1600 which describes the substitution on the phenyl ring.)

? EXERCISE 12.8.9

What absorptions would the following compounds have in an IR spectra?



Answer

A)

Frequency (cm⁻¹) Functional Group

2900-3000 C-C-H, C=C-H

1710 C=O

1610 C=C

1100 C-O

B)**Frequency (cm⁻¹) Functional Group**

3200 C≡C-H

2900-3000 C-C-H, C=C-H

2100 C≡C

1710 C=O

C)**Frequency (cm⁻¹) Functional Group**

3300 (broad) O-H

2900-3000 C-C-H, C=C-H

2000-1800 Aromatic Overtones

1710 C=O

1610 C=C

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