

## Infrared Spectroscopy (#1b)

In organic chemistry there are two types of spectroscopy that are important: infrared spectroscopy and nuclear magnetic resonance spectroscopy. A review of infrared spectroscopy is discussed here.

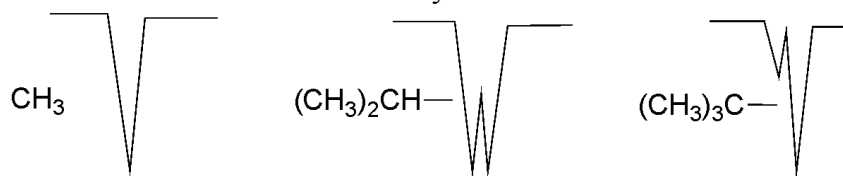
**Infrared spectroscopy** is used to gather information on the **functional groups** in a molecule. In infrared spectroscopy, the sample absorbs energy of a certain frequency. This absorption of energy causes the molecule to go from a lower energy (ground state) to a higher energy (excited state). Absorption of this energy causes vibrational energy changes. This is not enough energy to destroy the molecule. It only causes molecular motions, which means that bonds stretch and bend. Infrared radiation is absorbed when its frequency is the same as that of the vibrating bond. The normal range of infrared frequency used is  $4000\text{ cm}^{-1}$  to  $400\text{ cm}^{-1}$ ; " $\text{cm}^{-1}$ " is a new unit called a **wavenumber**. Completely nonpolar bonds do not absorb IR radiation. For example, the C-C bond in ethane does not absorb radiation, whereas the CH bond does. The intensity of the absorption increases with the polarity of the bond so a C-O stretching band is more intense than a C-H band. Also, intensity increases with the number of the bands. In general, stretching bands are more intense than bending bands. Bending includes such motions as "rocking," "twisting," and "wagging," which are more like molecular aerobics than bending motions!

When we take an IR spectrum of a sample we allow radiation to pass through the sample. If the sample absorbs the radiation then it does not go to the detector and we plot it on the paper as the amount transmitted, so we get downward deflections. The infrared radiation is varied from high frequency to low frequency and is on the x axis. In Chem 304L you will use a slightly different instrument called an **ATR IR spectrometer**. ATR uses a different method to collect the data on which frequencies of radiation are absorbed and which are transmitted through the sample. Your sample is placed on a diamond crystal and pressure may be applied to ensure it has good contact with the crystal surface. Then a beam of IR radiation penetrates into the sample for only a few micrometers. It bounces off the crystal surface and returns to a detector, and information on which frequencies are missing can be processed.

There are three regions that should be examined in an IR in the sequence given below.

- A.  $4000\text{-}1400\text{ cm}^{-1}$  is the functional group region and contains the **stretching** vibrations of the functional groups
- B.  $1000\text{-}600\text{ cm}^{-1}$  will tell you the substitution patterns for alkenes and aromatics; it is a **bending** region
- C.  $1400\text{-}1000\text{ cm}^{-1}$  is the **fingerprint region** which contains the bending vibrations of nonassignable peaks and is unique to each molecule. Methyl bending is found here as well as carbon-oxygen bending.

**Alkanes:** In alkanes there is always a C-H stretch at  $2970\text{-}2850\text{ cm}^{-1}$ , just below  $3000\text{ cm}^{-1}$ . Don't forget that every organic molecule has C-H in it. One other peak that is helpful sometimes is the bending for  $\text{CH}_3$  at  $1380\text{ cm}^{-1}$ . If an organic molecule does not have a  $\text{CH}_3$  then this will be absent. If an organic molecule has an isopropyl group in it then this band will appear as 2 bands. A tertiary butyl group in an organic molecule will have the two bands but they will be uneven so that one of them is small.



**Alkenes:** In alkenes there is  $sp^2$  C-H stretching at  $3100-3010\text{ cm}^{-1}$ , just above  $3000\text{ cm}^{-1}$ . Also there is C=C stretching at about  $1650\text{ cm}^{-1}$ . You can also tell the substitution pattern of your alkene and determine whether it is trisubstituted, disubstituted, cis, trans, etc. You can tell this by using the table. Do not memorize any of the numbers.

**Alkynes:** There is stretching for  $sp$ -hybridized C-H at  $3300\text{ cm}^{-1}$ . There is also a C-C triple bond stretch for terminal alkynes at  $2100-2140\text{ cm}^{-1}$ .

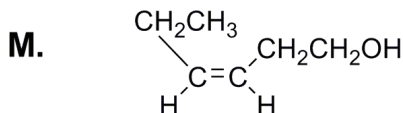
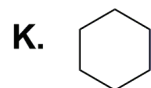
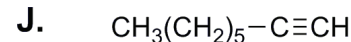
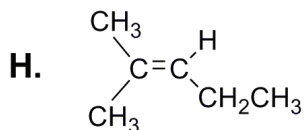
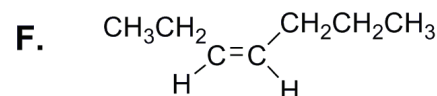
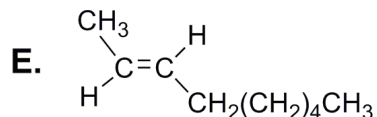
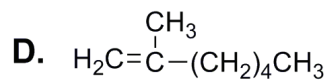
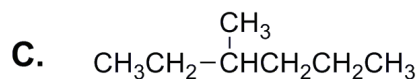
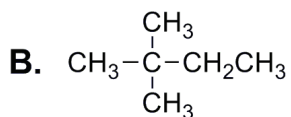
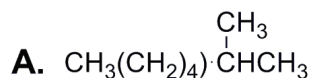
**Alcohols:** Alcohols have a very broad O-H stretch at  $3300-3350\text{ cm}^{-1}$ . You can also tell whether it is a primary, secondary or tertiary alcohol from the C-O stretch. Use the table.

**Carbonyl-Containing Compounds:** They all display a C=O stretching vibration in the IR. It will occur anywhere from  $1815$  to  $1650\text{ cm}^{-1}$ .

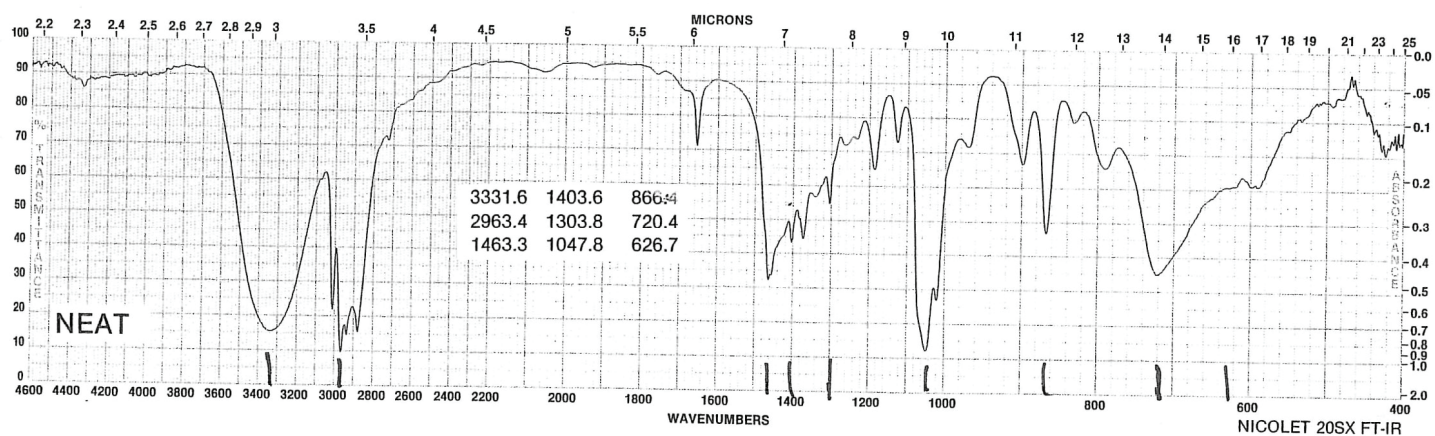
### Postlab:

You should complete the following assignment in your lab notebook as you would any postlab assignment. Include your name, the title of the assignment, and the date (1 pt) and a purpose statement clearly describing the objectives of this assignment (2 pts).

Below are the structures of compounds followed by 2 infrared spectra. Using the letters beside each structure, match the correct structure to its infrared spectrum. You must list at least **three important absorptions** that help identify your structure. A chart of IR absorptions is located on page 25.



Spectrum 1



Spectrum 2

