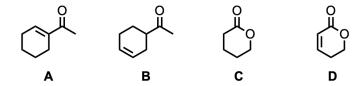
Infrared Spectroscopy Worksheet

Warm-Up Questions:

Watch the Khan Academy videos on IR spectroscopy.



All of the molecules shown above absorb IR radiation in the range between 1600 and 1850 cm⁻¹. In each molecule:

1) Label the functional groups that are present.

2) Identify the specific bond(s) responsible for the absorption(s) and predict the approximate wavenumber of absorption for each of these bonds.

Fundamental Vibrational Modes of Water:

Take screenshots of all three vibrational modes of water:

Bending	Symmetric Stretching	Antisymmetric Stretching

Take a screenshot of the predicted gas phase IR spectrum of water:

IR-active versus IR-inactive: Take screenshots of all seven vibrational modes of acetylene:

Take a screenshot of the predicted gas phase IR spectrum of acetylene:

Functional Groups and Trends:

1) Take a screenshot of stacked IR spectra for benzaldehyde, cyclohexanone, and acetonitrile:

2) Identify the frequencies of the following bonds:

a) The aldehyde C–H stretch in benzaldehyde:

b) The carbonyl stretch in cyclohexanone: _____

c) The CN triple bond stretch in acetonitrile: _____

3) Take a screenshot of stacked IR spectra for butane and 1-butene. What are the key differences between the butane and 1-butene spectra?

Resonance Effects:

1) Take a screenshot of stacked IR spectra for cyclohexanone and 2-cyclohexen-1-one:

2) Compare the key carbonyl vibrations for the two compounds. Which stretching frequency is lower? Can you explain why based on a simple Lewis structure approach?

Mass Effects:

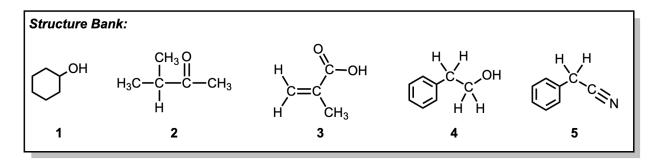
1) Take a screenshot of stacked IR spectra for acetylene and acetylene-d2.

2) What do you notice about the spectrum of the non-deuterated molecule as compared to the deuterated molecule? Why do you think this difference is observed? How can this be useful for a synthetic chemist?

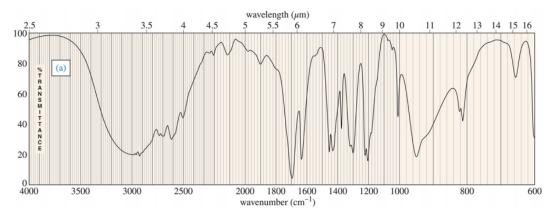
Individual Exercise:

Two infrared spectra are shown, corresponding to two of the following compounds. Match the corresponding structure to each IR spectrum by:

- 1) Identifying how the major peaks (above 1500 cm⁻¹) in each spectrum correspond to the structure you have chosen
- 2) Using molecular modeling to perform a vibrational analysis with Maestro to confirm your answers



IR Spectrum A:



IR Spectrum B:

