

Playing with IR Tutor.

IR Tutor (IR = infrared) is an interactive software program developed at Columbia University in the early 1990s by Professor Turro and Professor Fine and produced by Charles Abrams, who was a student here at the time. IR Tutor will be the basis for learning how to interpret infrared spectra. Of the various forms of spectroscopy, IR spectroscopy allows us to "see" the functional groups in a molecule against the background of a hydrocarbon backbone. Absorption of IR light causes the excitation of vibrations of a molecule, not the excitation of the electrons of a molecule, which is the case when UV or visible light is absorbed.

Vibrations consist of the motion of two or more atoms relative to one another. The frequencies and energies of these vibrations depend on the kinds of bonds that connect the atoms together and the masses of the atoms. The following rules will serve as an important guideline: The frequency of a vibration will increase as the strength of the bond between the atoms increases and will decrease as the masses of the atoms involved in the vibration increase. Thus, the frequency increases with increasing bond strength and decreases with increasing mass. These rules come from the use of a simple harmonic oscillator for vibrating atoms, as is explained by IR Tutor and the reading which was sent to you earlier in the week.

Recall that functional groups provide atoms with characteristic spectroscopic properties. Each functional group will possess an absorption at a characteristic frequency. Thus, when inspecting an IR spectrum of an unknown, we look at certain frequencies to see if there is a signal for an absorption of light there. If there is one, we deduce the functional group is present in the molecule and if there is none, we deduce the functional group is absent.

The Strategy of Using IR Tutor

The basic idea is to first start to inspect the IR spectra of saturated hydrocarbons and to assign the signals to the vibrations of CH and CC atoms. These signals will be expected to occur in all compounds containing a functional group in addition to the saturated hydrocarbon "backbone". ***Any new signals that don't correspond to a standard must be assigned to the vibrations of a functional group.*** By going through the exercises below you will be able to figure out how to assign signals to the important functional groups such as C=C bonds, C=O bonds, etc.

The Structure of IR Tutor

IR tutor consists of three main modules:

- (1) Introduction.
- (2) Theory of IR spectroscopy.
- (3) Interpretation of IR spectra.

The third module, **Interpretation of IR spectra**, is the heart of the program. One can start there and play with the spectra after reading the following general information about the program. After playing with the Interpretation module, you can go back to the Introduction and Theory modules. There will be an interactive context with these modules after you've played with the Interpretation module a bit.

- (1) The module **Introduction** provides a brief review of the following submodules:

- (a) Definition of spectroscopy.
- (b) Nature of light.
- (c) Measurement of IR spectra.

(2) The **Theory of IR spectroscopy** module provides a brief review of the following submodules:

- (a) Classical model of a vibrating molecule
- (b) Quantum mechanical model of a vibrating molecule
- (c) Normal modes and group frequencies

(3) The **Interpretation of Spectra** module provides a brief review of the following submodules:

- (a) a set of spectra of the following molecules: n-hexane, 2,3-dimethylbutane, 1-hexene, 1-heptyne, 1-heptylcyanide, methyl benzene (toluene), 1-hexanol, 1-hexylamine, 1-heptaldehyde, 3-heptanone, ethyl acetate, butyric anhydride.
- (b) for each spectrum the vibration associated with each signal in the spectrum can be animated by simply clicking on the body of the peak.
- (c) under the control menu a summary of all of the key vibrations can be seen in one screen.
- (d) A set of comparison spectra are provided as a pdf file labeled **IRTutor_ComparisonSpectra.pdf**. You can use this file to compare spectra that you select in IR Tutor to the spectra of other functional groups.

A number of exercises are given below and will be dealt with in class on Monday. If you get a chance over the weekend, please download IR Tutor and play with it.

Exercise 1: Comparison of hexane and dimethylbutane.

- (1) Go to module 3, the interpretation of spectra.
- (2) Select hexane as a spectrum.
- (3) Starting at the left hand side of the spectrum, click on the signal somewhere in the middle of the band. An animation of the vibration responsible for the signal will appear. For the band around 3000 cm^{-1} there are several vibrations of similar frequency which are responsible for the signal.
- (4) Select "expand" and again click on the signals which are better separated
- (5) ***A pdf of all spectra (IRTutor_ComparisonSpectra.pdf) comparing them to hexane will be sent to you to assist in this exercise.***
- (6) Select dimethylbutane from the comparison spectra.
- (7) Notice the similarities and differences between the spectrum of hexane and dimethylbutane.
- (8) Make some conclusions concerning the two spectra based on the similarities and differences.

Exercise 2: Comparison of 1-hexene and hexane.

- (1) Go to module 3, the interpretation of spectra.
- (2) Select *hexene* as a spectrum.
- (3) Starting at the left hand side of the spectrum, click on the signal somewhere in the middle of the band. An animation of the vibration responsible for the signal will appear. For the band around 3000 cm^{-1} there are several vibrations of similar frequency which are responsible for the signal.
- (4) Select "expand" and again click on the signals which are better separated
- (5) ***A pdf of all spectra (IRTutor_ComparisonSpectra.pdf) comparing them to hexane will be sent to you to assist in this exercise.***
- (6) Select *hexene* from the comparison spectra.
- (7) Notice the similarities and differences between the spectrum of hexane and hexene.
- (8) Make some conclusions concerning the two spectra based on the similarities and differences.

Exercise 3: Comparison of hexane and 3-heptanone.

- (1) Go to module 3, the interpretation of spectra.
- (2) Select *hexane* as a spectrum.
- (3) ***A pdf of all spectra (IRTutor_ComparisonSpectra.pdf) comparing them to hexane will be sent to you to assist in this exercise. Select 3-heptanone from the comparison spectra.***
- (4) Notice the similarities and differences between the spectrum of hexane and 3-heptanone.
- (5) What are the major differences in the two spectra?
- (6) Make some conclusions concerning the two spectra based on the similarities and differences.

Additional Optional Exercises: Repeat the above strategies by comparing hexane to 1-hexanol (Exercise 4), 1-heptanoic acid (Exercise 5), 1-heptylcyanide (Exercise 6) and 1-heptyne (Exercise 7).