4.5 IR Data Table

Learning Objectives

- Understand where certain group frequencies are
- Be able to read and understand the data table for IR spectroscopy

As stated in the previous section, similar bonds will show up grouped near the same frequency because they tell us about the presence or absence of specific functional groups in a sample. From there, a data table of approximate frequencies for different types of bonds has been created to use to help IR spectrum analysis.

Table of Common IR Absorptions.

Approximate Frequency (cm^{-1})	Description	Bond Vibration	Notes
3500 - 3200	broad, round	O-H	much broader, lower frequency (3200-2500) if next to C=O
3400-3300	weak, triangular	N-H	stronger if next to C=O
3300	medium-strong	=C-H (sp C-H)	
3100-3000	weak-medium	=C-H (sp2 C-H)	can get bigger if lots of bonds present
3000-2900	weak-medium	-C-H (sp3 C-H)	can get bigger if lots of bonds present
2800 and 2700	medium	C-H in O=C-H	two peaks; "alligator jaws"
2250	medium	C≡N	
2250-2100	weak-medium	C≡C	stronger if near electronegative atoms
1800-1600	strong	C=O	lower frequency (1650-1550) if attached to O or N middle frequency if attached to C, H higher frequency (1800) if attached to Cl
1650-1450	weak-medium	C=C	lower frequency (1600-1450) if conjugated (i.e. C=C-C=C) often several if benzene present
1450	weak-medium	H-C-H bend	
1300 - 1000	medium-strong	C-O	higher frequency (1200-1300) if conjugated (i.e. O=C-O or C=C-O)
1250-1000	medium	C-N	
1000-650	strong	C=C-H bend	often several if benzene present

Note: strong, medium, weak refers to the length of the peak (in the y axis direction).

Note: spectra taken by ATR method (used at CSB/SJU) have weaker peaks between 4000-2500 cm^{-1} compared to reference spectra taken by transmittance methods (typical on SDBS and other sites).

Exercise 1

What wavenumber range would you predict the triple bond region to be?

Answer

2200 - 2500 cm^{-1}

Exercise 2

How could you determine the presence of an aldehyde and rule out a ketone?

Answer

The aldehyde would have peaks at 2700 and 2800 cm-1, whereas the ketone would lack these. The absorption is due to the the Csp^2-H bond.

Exercise 3

How can you tell the difference between and alcohol and a carboxylic acid?

Answer

Here the main point of difference is either the presence of a carbonyl (C=O) or its absence. The carboxylic acid contains a C=O, so you would expect a peak somewhere between 1800-1600 cm^{-1}, whereas an alcohol would not have a peak here.
