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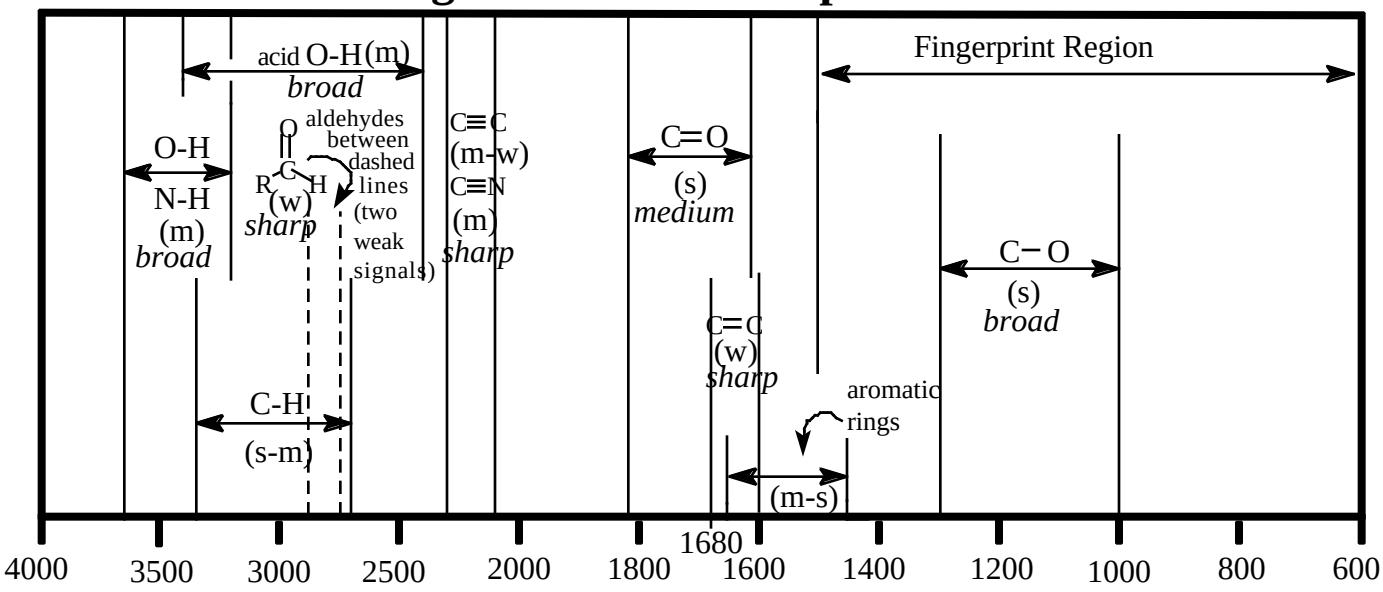
Regions of Infrared Spectrum



Wave Number (cm $^{-1}$)

Intensities	Width
s = strong	*broad*
m = medium	*medium*
w = weak	*sharp*

Before interpreting IR (or NMR) spectra, be sure to determine the degrees of unstaturation. This helps you decide if you have rings or multiple bonds in the unknown molecule. See page 450, section 11.6 in Vollhardt and Schore, 4th Edition, for a good explanation.

NOTES: 1. Do not be overly concerned with whether a signal you are inspectingconforms exactly to the intensities and widths listed here. The most important factor is matching the group's functional range in wave number.

2. The vertical axis in a normal spectrum indicates the strength of the signal, but the height of the placement of functional groups in this guide mean nothing. We are just finding a clear place to type.

2.8 HOW TO APPROACH THE ANALYSIS OF A SPECTRUM (OR, WHAT YOU CAN TELL AT A GLANCE)

In trying to analyze the spectrum of an unknown, you should concentrate your first efforts toward determining the presence (or absence) of a few major functional groups. The C=O, O–H, N–H, C–O, C=C, C≡C, C≡N, and NO_2 peaks are the most conspicuous and give immediate structural information if they are present. Do not try to make a detailed analysis of the CH absorptions near 3000 cm^{-1} (3.33 μ); almost all compounds have these absorptions. Do not worry about subtleties of the exact type of environment in which the functional group is found. Below is a major check list of the important gross features.

1. Is a carbonyl group present?
   The C=O group gives rise to a strong absorption in the region 1820–1660 cm^{-1} (5.5–6.1 μ). The peak is often the strongest in the spectrum and of medium width. You can't miss it.

2. If C=O is present, check the following types (if absent, go to 3).

ACIDS	is OH also present?
	– *broad* absorption near 3400–2400 cm^{-1} (usually overlaps C–H)
AMIDES	is NH also present?
	– medium absorption near 3500 cm^{-1} (2.85 μ) sometimes a double peak, with equivalent halves
ESTERS	is C–O also present?
	– strong intensity absorptions near 1300–1000 cm^{-1} (7.7–10 μ)
ANHYDRIDES	have *two* C=O absorptions near 1810 and 1760 cm^{-1} (5.5 and 5.7 μ)
ALDEHYDES	is aldehyde CH present?
	–two weak absorptions near 2850 and 2750 cm^{-1} (3.50 and 3.65 μ) on the right-hand side of CH absorptions
KETONES	The above 5 choices have been eliminated

3. If C=O is absent

ALCOHOLS, PHENOLS	Check for OH
	– *broad* absorption near 3600–3300 cm^{-1} (2.8–3.0 μ)
	– confirm this by finding C–O near 1300–1000 cm^{-1} (7.7–10 μ)
AMINES	Check for NH
	– medium absorptions(s) near 3500 cm^{-1} (2.85 μ)
ETHERS	Check for C–O (and absence of OH) near 1300–1000 cm^{-1} (7.7–10 μ)

4. Double Bonds and/or Aromatic Rings
   – C=C is a *weak* absorption near 1650 cm^{-1} (6.1 μ)
   – medium to strong absorptions in the region 1650–1450 cm^{-1} (6–7 μ) often imply an aromatic ring
   – confirm the above by consulting the CH region; aromatic and vinyl CH occurs to the left of 3000 cm^{-1} (3.33 μ) (aliphatic CH occurs to the right of this value)

5. Triple Bonds
   – C≡N is a medium, sharp absorption near 2250 cm^{-1} (4.5 μ)
   – C≡C is a weak but sharp absorption near 2150 cm^{-1} (4.65 μ)
   Check also for acetylenic CH near 3300 cm^{-1} (3.0 μ)

6. Nitro Groups
   – *two* strong absorptions at 1600–1500 cm^{-1} (6.25–6.67 μ) and 1390–1300 cm^{-1} (7.2–7.7 μ)

7. Hydrocarbons
   – none of the above are found
   – major absorptions are in CH region near 3000 cm^{-1} (3.33 μ)
   – very simple spectrum, only other absorptions near 1450 cm^{-1} (6.90 μ) and 1375 cm^{-1} (7.27 μ)

The beginning student should resist the idea of trying to assign or interpret *every* peak in the spectrum. You simply will not be able to do this. Concentrate first on learning these *major* peaks.