CHM 422 Organic Synthesis, Dr. Laurie S. Starkey

Interpretation of Infrared Spectra: a Basic Approach

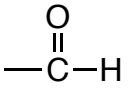
"Read" the spectrum from left to right and pick out any of the following obvious bands.
Next, look to the weaker bands for additional evidence of the FG's you suspect are present.

Obvious bands (cm^{-1})	**Functional Group**	**Notes/Add'l evidence**
3500–3200 (m)	O–H N–H	broad signal (water?!)
3200–3000 (m-s)	C–H, sp^2 (aromatic, alkene)	subsitution patterns <1000
3000-2800 (s)	C–H, sp^3 (alkane)	C–H bend at 1460, 1380
2250–2000 (m-w)	C≡N C≡C	often weak
1800–1600 (s)	C=O	see table, lowered by conjugation

(s) = strong, (m) = medium, (w) = weak, (v) = variable

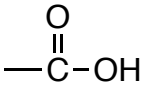
Other peaks to look for:

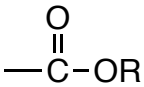
≡C–H sp C–H stretch is sharp peak around 3300 (s)


aldehyde C–H stretch appears as two sharp peaks 2900–2800 and 2800–2700 (w)

C=C stretches occur 1680–1630 with variable intensity (v) and will disappear if symmetrical.

C–O stretches occur 1150–1050 and are typically sharp (s)


Carboxylic acids should be obvious because the H-bonded dimer has a HUGE O–H stretch (3400–2400) that overlaps with the C–H stretch bands. Acids will also have a C=O stretch (1725–1700) and a C–O stretch (1320–1210).


Since esters have two C–O bonds, they typically have two C–O stretches. Together with the C=O stretch, it's known as the "rule of 3" (~1700, 1200, 1100).

alkene C–H bend	1000–700	} gives excellent information on
benzene C–H bend	850–700 (+ overtone 2000–1700)	} substitution patterns (o,m,p, etc)

C=N is not a common FG and C–N stretches are typically not useful.

DO NOT try to interpret every little peak in the spectrum but DO recognize which ones are significant and are giving you clues to the sample's structure. It takes practice!