Spectroscopy

Infrared (IR) spectroscopy measures bond vibration frequencies in a molecule and is used to determine the functional group.

Mass spectrometry (MS) fragments the molecule and measures mass. MS can give the molecular weight of the compound and functional groups.

Nuclear magnetic resonance (NMR) spectroscopy analyzes environment the Hs in a compound. This gives clues as to the alkyl and other functional groups.

Ultraviolet (UV) spectroscopy uses electronic transitions to determine bonding patterns.

IR Stretching Regions

Fingerprint Region – 600 – 1400 cm^{-1}

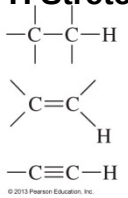
C–C Stretching

C-C	1200 cm^{-1}
C=C	1660 cm^{-1}
C≡C	<2200 cm^{-1}

Conjugation lowers the frequency:

isolated C=C	1640–1680 cm–1
conjugated C=C	1620–1640 cm–1
aromatic C=C	approx. 1600 cm–1

C-H Stretching



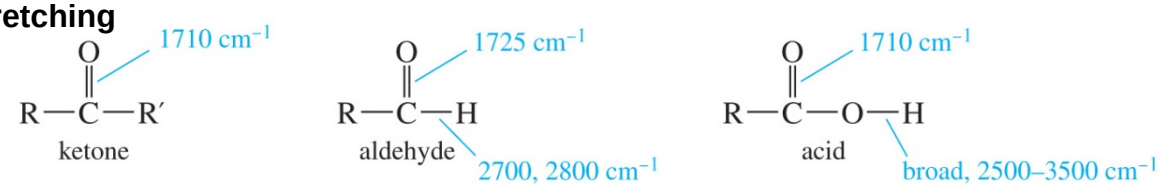
—C—C—H	sp^3 hybridized, one-fourth *s* character	2800–3000 cm^{-1}
C=C (H)	sp^2 hybridized, one-third *s* character	3000–3100 cm^{-1}
—C≡C—H	*sp* hybridized, one-half *s* character	3300 cm^{-1} (sharp)

O—H and N—H Stretching

Both of these occur around 3300 cm^{-1}, but they look different:

- Alcohol O—H is broad with rounded tip.
- Secondary amine (R_2NH) is broad with one sharp spike.
- Primary amine (RNH_2) is broad with two sharp spikes.

C-O Stretching



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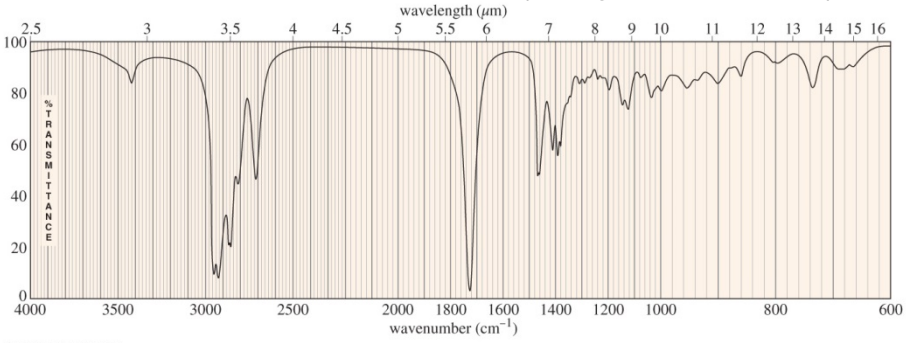
C-N Stretching

C—N	1200 cm^{-1}	usually strong
C=N	1660 cm^{-1}	
C≡N	>2200 cm^{1}	
C≡C	<2200 cm^{-1} (usually moderate or weak)	



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Outside the fingerprint region, a strong peak about 1720 cm^{-1}, and an unusual C–H stretching region. The C–H region has two additional peaks around 2720 and 2820 cm^{-1}. The strong peak at 1725 cm^{-1} must be a C=O, and the peaks at 2720 and 2820 cm^{-1} suggest an aldehyde.

The weak peak around 3400 cm^{-1} might be mistaken for an alcohol O–H. From experience, we know alcohols give much broader O–H absorptions. May be from an impurity of water or hydrate of the aldehyde

You have an unknown with an absorption at 1680 cm^{-1},it might be an amide, an isolated double bond, a conjugated ketone, a conjugated aldehyde or a conjugated carboxylic acid? Describe what other characteristics to look for to figure out which one it might be.

Amide: (1680 is strong.) Look for N-H absorptions with spikes around 3300 cm^{-1}.

Isolated double bond: (1680 is weak or moderate.) Look for =C-H absorptions just above 3000 cm^{-1}.

Conjugated ketone: (1680 peak is strong). There must be a double bond nearby, conjugated with the C=O, to lower the C=O frequency to 1680 cm^{-1}. Look for C=C of the nearby double bond (1620-1640) and its =C-H above 3000.

Conjugated aldehyde: (1680 peak is strong). Look for the aldehyde C-H stretch about 2700-2800 cm^{-1}. Also look for the C=C and C-H of the nearby double bond (1620 to 1640 and just above 3000)

Conjugated carboxylic acid: (1680 peak is strong). Look for the characteristic acid O-H stretch centered on top of the C-H stretch around 3000 cm^{-1}. Also look for the C=C and C-H of the nearby double bond (1620 to 1640 and just above 3000)