

Alkyl, alkenyl and alkynyl groups

C-H stretching frequencies:

$sp^3$	-C-H	2800-2960 $cm^{-1}$	C-C bending	1420-1480
$sp^2$	=C-H	3000-3100	C=C stretch	1620-1680
$sp$	$\equiv$ C-H	3300	$C\equiv C$	2100-2260

C-C stretching frequencies:

C-C	1200	without functional groups, very little dipole, weak bands		
C=C	1650	C=C isolated	1680	bond order = 1
		C=C conjugated	1625	bond order = 1+
		C=C aromatic	1600	bond order = 1.5
$C\equiv C$	2200	terminal alkynes show C-H (3300) and triple bond (2200) internal triple bonds have no C-H and triple bond is weak		
C-C	bending	1420-1480		

Bands below 3000 suggest alkanes.

Bands just above 3000 suggest alkene =C-H and one should look for C=C stretch around 1660.

Bands at 3000 suggest alkyne  $\equiv$ C-H and one should look for C C stretch at 2200

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Alcohols 3300 O-H stretch often very broad due to hydrogen bonding

1000-1200 C-O stretch- not reliable since other groups absorb here also

Amines 3300 N-H stretch weaker broad peak with "spikes"

(1 amine  $R_2NH$ ) one spike; (2 amine  $RNH_2$ ) two spikes

(3  $R_3N$ ) amines do not have N-H band

Hydrogen bonding causes the broadening of O-H and N-H bands.

Dilute samples have sharp peaks.

Other functional groups with O-H and N-H bands:

Carboxylic acids have O-H stretch at 3000.

The strong dimer hydrogen bonding lowers the frequency of O-H band and often overlaps with the C-H region.

Amides have N-H stretching bands similar to amines (of course the C=O is present to distinguish amides from amines)

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Carbonyl groups      C=O stretch      1630-1780 variable

C=O bands are higher frequency than C=C bands because the C=O bond is stronger.

Aldehydes, ketones and carboxylic acids all have the C=O band approximately the same frequency  $\sim 1710 \text{ cm}^{-1}$

Lower frequency:      Amides  $\sim 1680 \text{ cm}^{-1}$  or less.

Higher frequency:      Esters  $\sim 1730-1750 \text{ cm}^{-1}$

Acid chlorides and anhydrides  $\sim 1820 - 1750 \text{ cm}^{-1}$

Cyclic esters and ketones  $\sim 1780 \text{ cm}^{-1}$

Diagnostic peaks that accompany carbonyl groups:

aldehydes C-H stretch 2700-2900 (two bands, medium)

esters C-O stretch (ether oxygen) 1300

acids O-H stretch 3200-300 (broad) often overlaps with C-H bands