Ch 12

Note Title 10/11/2005

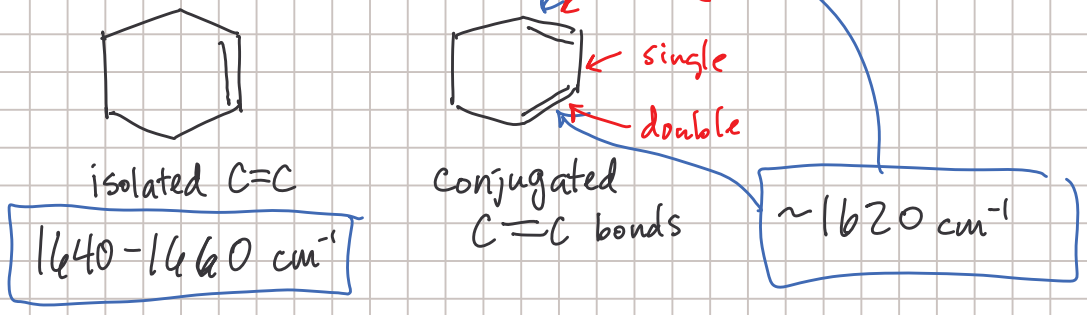
C–C bonds

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

alkenes C=C containing

isolated : on their own

conjugated : alternating double/single bonds



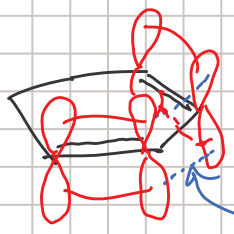
isolated C=C

1640-1660 cm^{-1}

conjugated C=C bonds

~1620 cm^{-1}

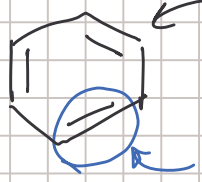
conjugated isolated



some overlap between center 2 p orbitals

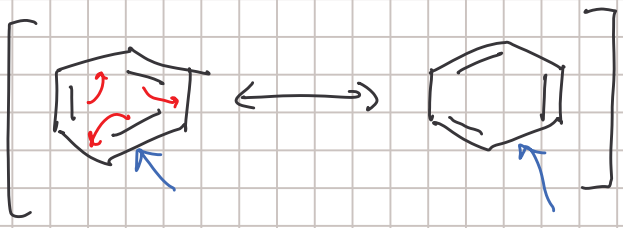
each π bond missing a small amt of e^- density b/c of extra overlap

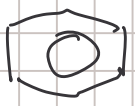
→ weakened bonds → lower freq.



← aromatic (C=C conjugated all around ring)

benzene





So in between each C–C there's essentially only ½ of a pi bond

C=C	isolated	1640–1660 cm^{-1}
	conjugated	1620 cm^{-1}
	aromatic	1600 cm^{-1}

alkynes Contains C≡C triple bond

any hydrocarbon group → R–C≡C–H terminal alkyne (C≡C 2100–2200 cm^{-1})

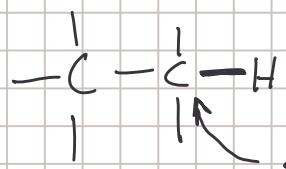
R–C≡C–R′ internal alkyne (weak or non-existent)

$CH_3-C\equiv C-CH_3$ no C≡C observed

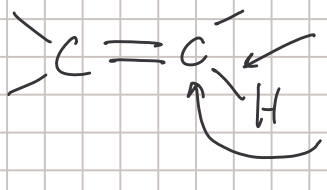
$CH_3-C\equiv C-CH_2CH_3$ very weak C≡C (2100–2200 cm^{-1})

$CH_3CH_2CH_2-C\equiv C-H$ strong C≡C (2100–2200 cm^{-1})

C–H bonds

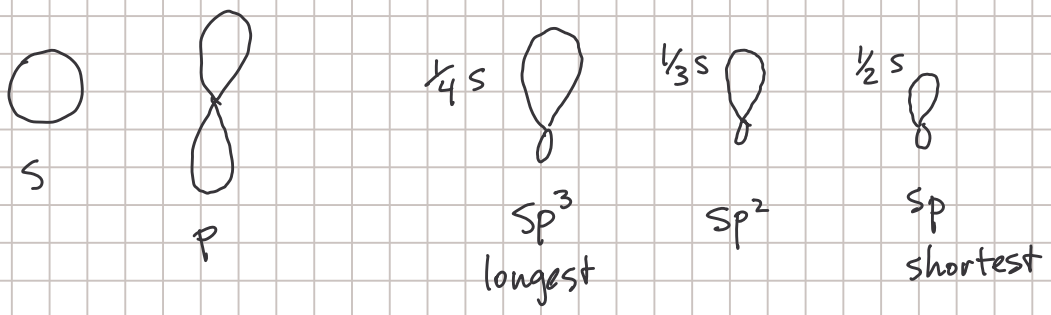


sp^3 hyb. C–H 2800 - 3000 cm^{-1}



"more s character" = shorter = stronger bond

sp^2 C–H 3000 - 3100 cm^{-1}

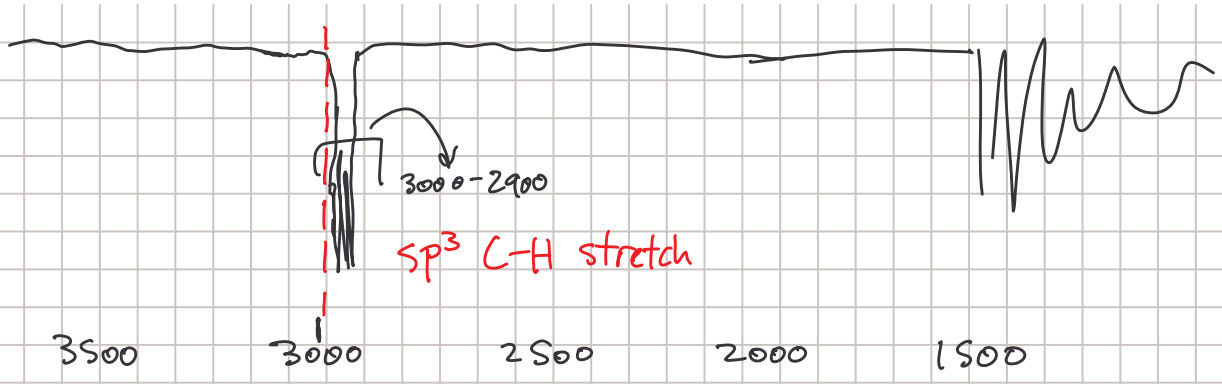


–C≡C–H sp C–H ~3300 cm^{-1}

hydrocarbons

C≡C	terminal	2100-2200
	internal	" but weaker
C=C	isolated	1640-1660 ←
	conjugated	~1620
	aromatic	~1600
C–H	sp^3	2800 - 3000
	sp^2	3000 - 3100
	sp	3300

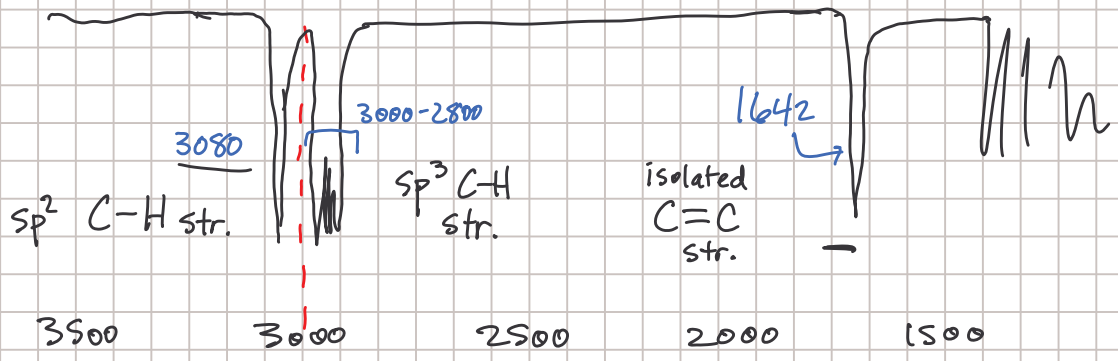
all above are "stretch" frequencies



must be an alkane

<1600 can usually be ignored

"fingerprint region"

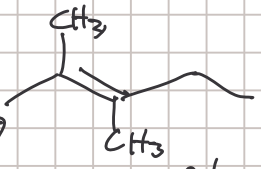


this is an alkene b/c it has C=C

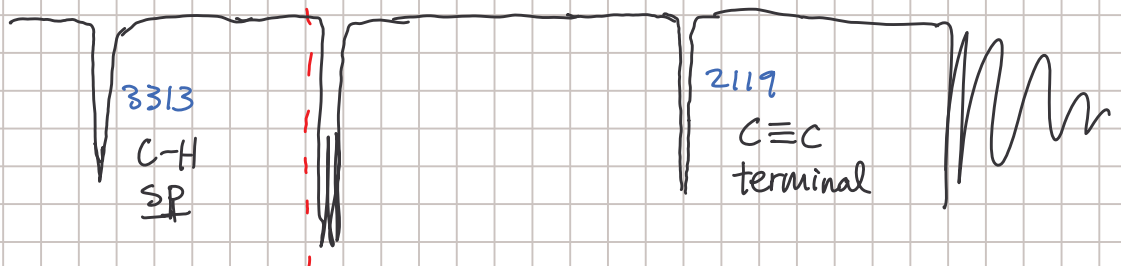
is it terminal or internal?

most likely terminal - strong C=C

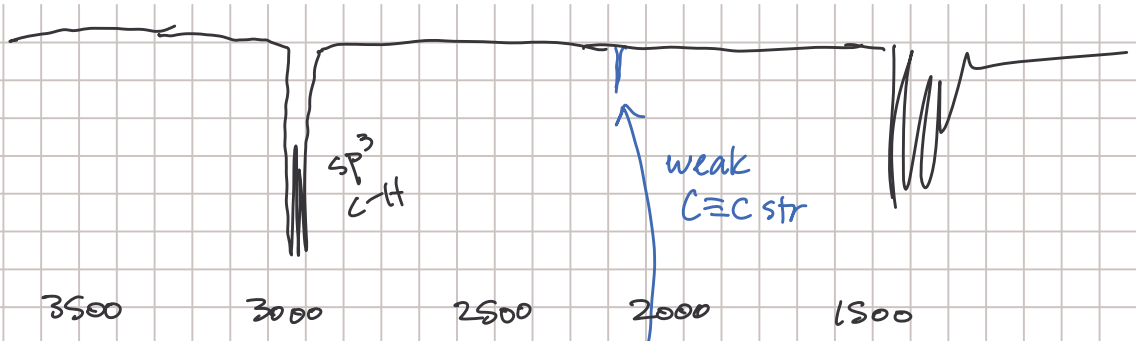
strong sp² CH



weak C=C and no sp² C-H must be internal!



must be terminal alkyne b/c strong C≡C & sp C-H



$CH_3CH_2C{\equiv}CCH_2CH_3$ very similar to alkane spectrum

symmetrical C≡C = invisible

$CH_3CH_2CH_2C{\equiv}CCH_3$

Alcohols & amines

Alcohol : R–O–H

Amine : $R-NH_2$ (1° primary) or $R-\underset{H}{N}-R'$ (2° secondary)

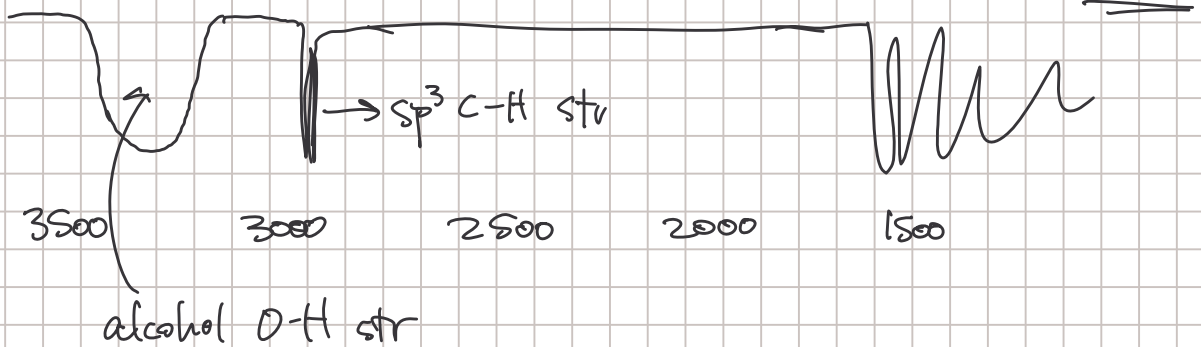
for $-\overset{\delta^-}{O}-\overset{\delta^+}{H}$ and $-\overset{\delta^-}{N}-\overset{\delta^+}{H}$ the H can hydrogen-bond

many different states of these H's in a sample (may be strongly H-bonded, or may be totally free or anywhere in between)

O-H and N-H IR stretches are

BROAD peaks

R-O-H alcohol O-H stretch = centered 3300 cm^{-1} broad



$CH_3CH_2CH_2OH$ for instance