INFRA-RED SPECTROSCOPY

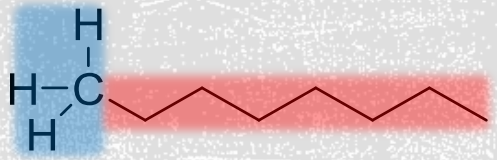
Characteristic Group Vibrations of Organic Molecules

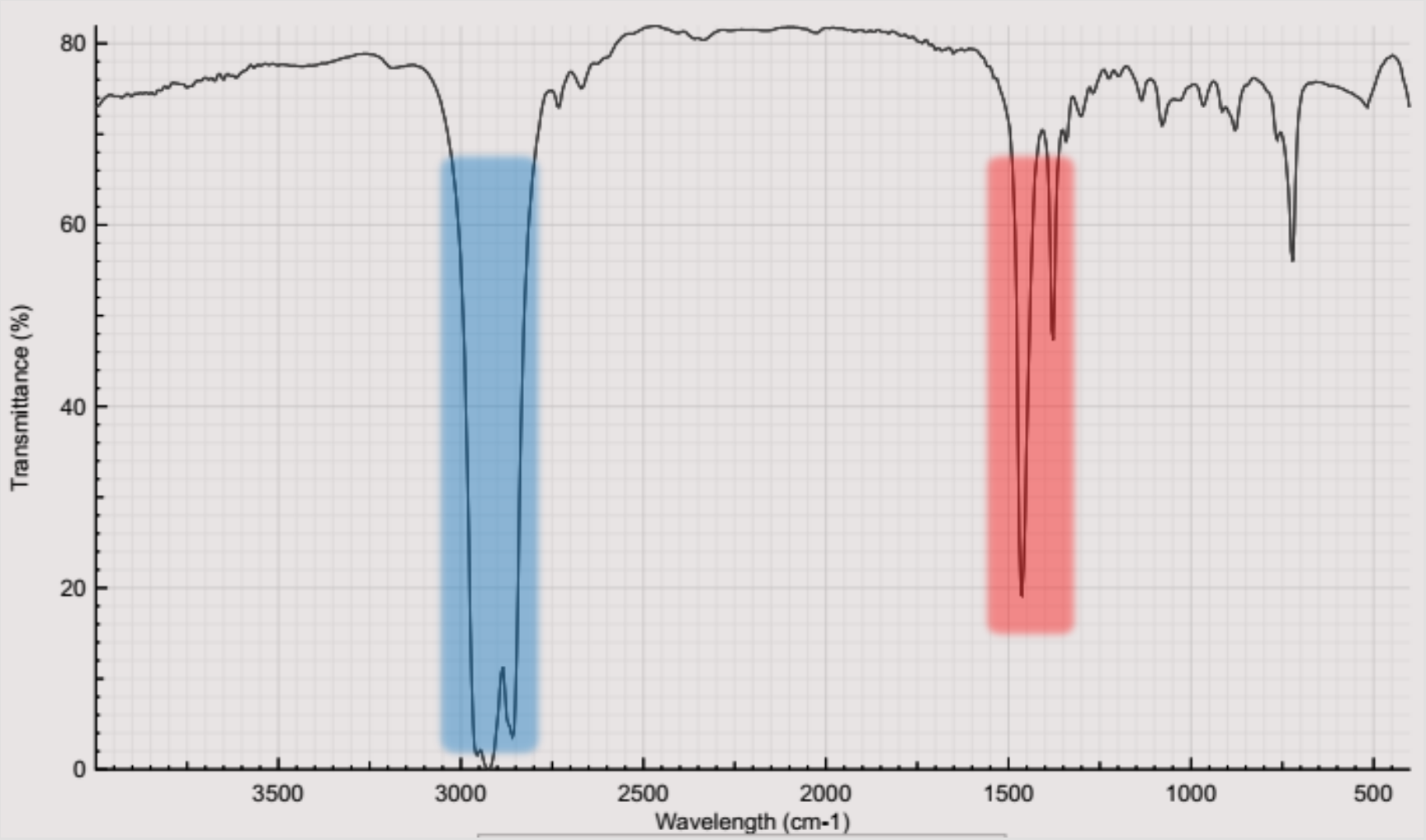
5

Part II

2021-2022

OCTANE





Alkanes – combination of ***C-C*** and ***C-H*** bonds

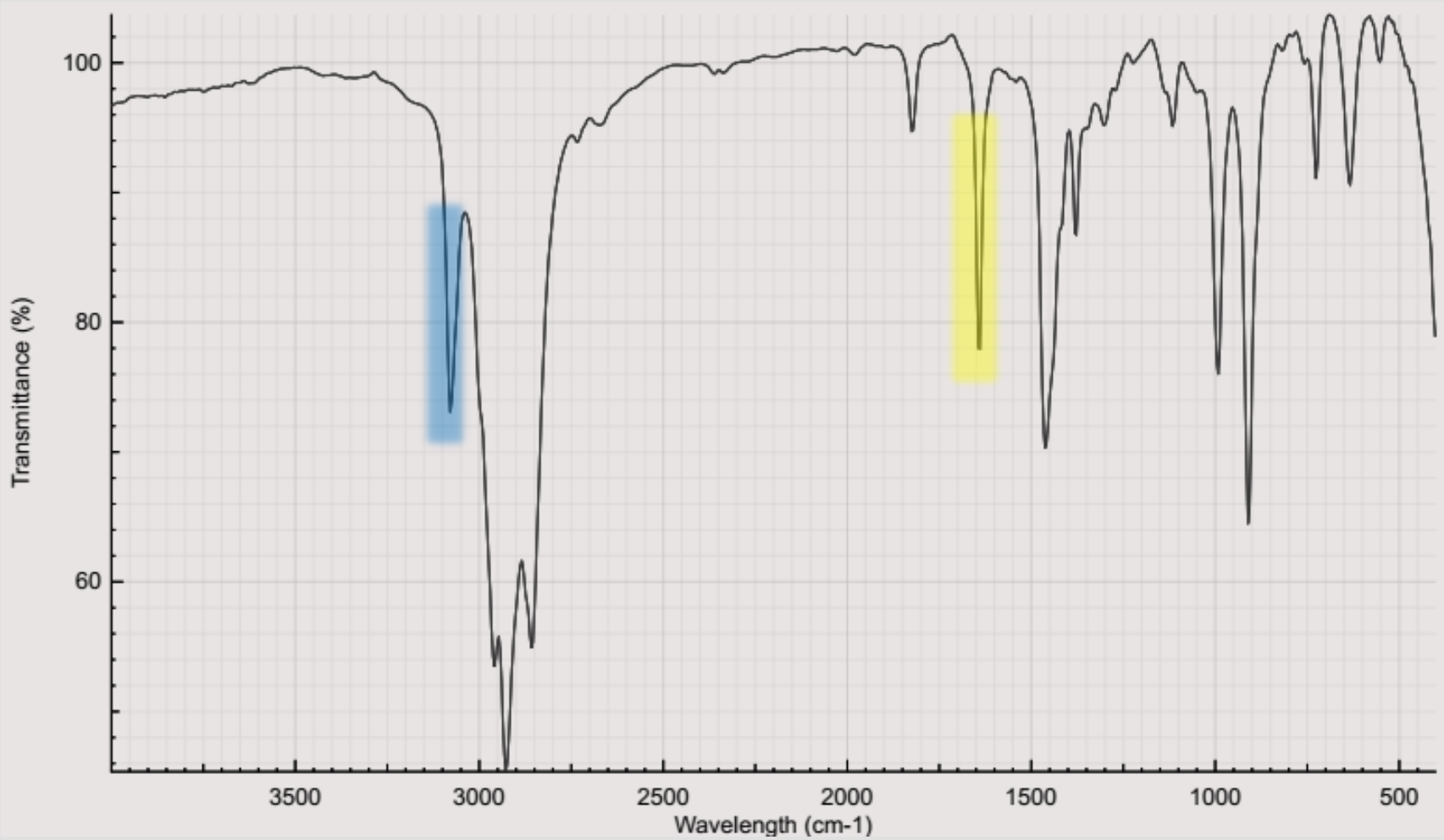
C-C stretches and bends 1360-1470 cm^{-1}

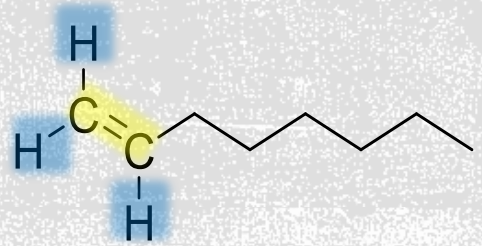
CH_2-CH_2 bond 1450-1470 cm^{-1}

CH_2-CH_3 bond 1360-1390 cm^{-1}

sp^3 ***C-H*** between 2800-3000 cm^{-1}

1-OCTENE





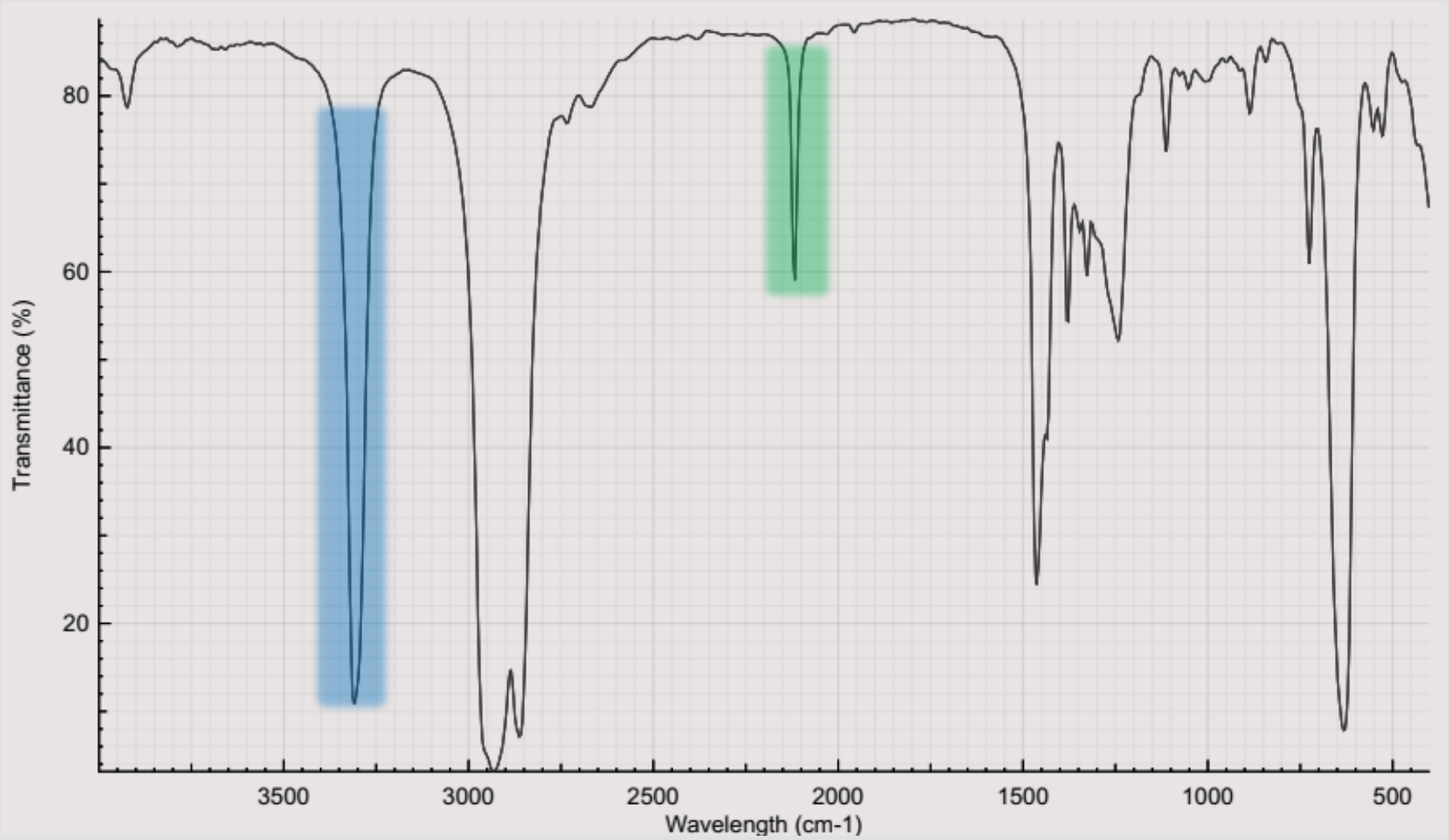
Alkenes – addition of the C=C and vinyl C-H bonds

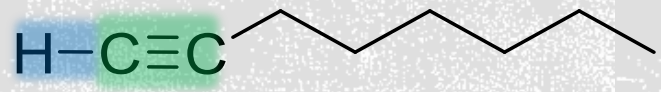
C=C stretch at 1620-1680 cm-1 weaker as substitution increases

vinyl **C-H** stretch occurs at 3000-3100 cm-1

The difference between alkane, alkene or alkyne **C-H** is important! If the band is slightly above 3000 it is vinyl sp2 C-H or alkynyl sp C-H if it is below it is alkyl sp3 C-H

1-OCTYNE





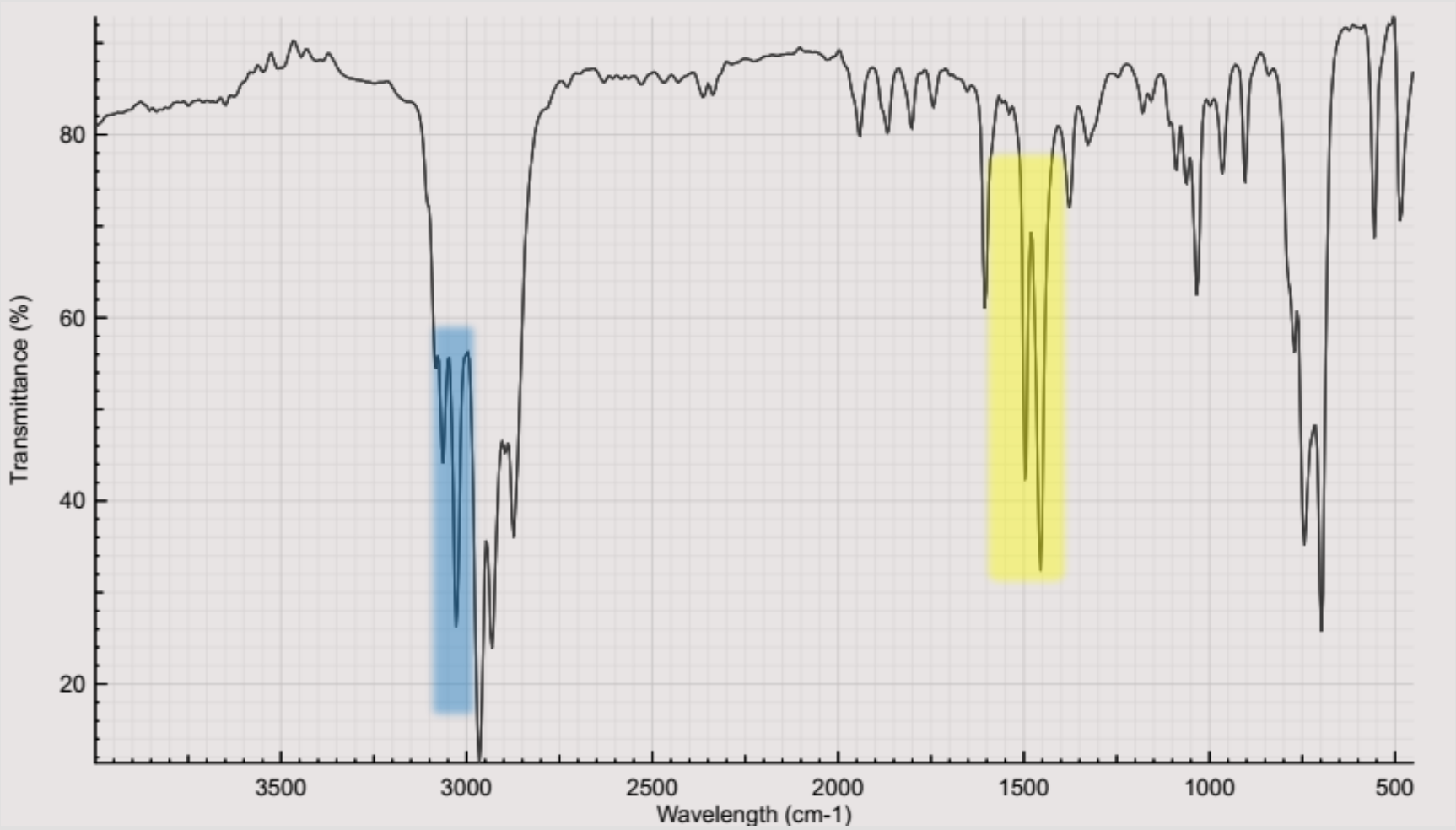
Alkynes – addition of the C=C and vinyl C-H bonds

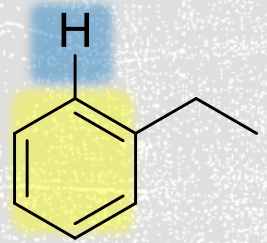
C≡C stretch 2100-2260 cm-1; strength depends on asymmetry of bond, strongest for terminal alkynes, weakest for symmetrical internal alkynes

C-H for terminal alkynes occurs at 3200-3300 cm-1

Internal alkynes (R-C≡C-R) would not have this band!

ETHYL BENZENE



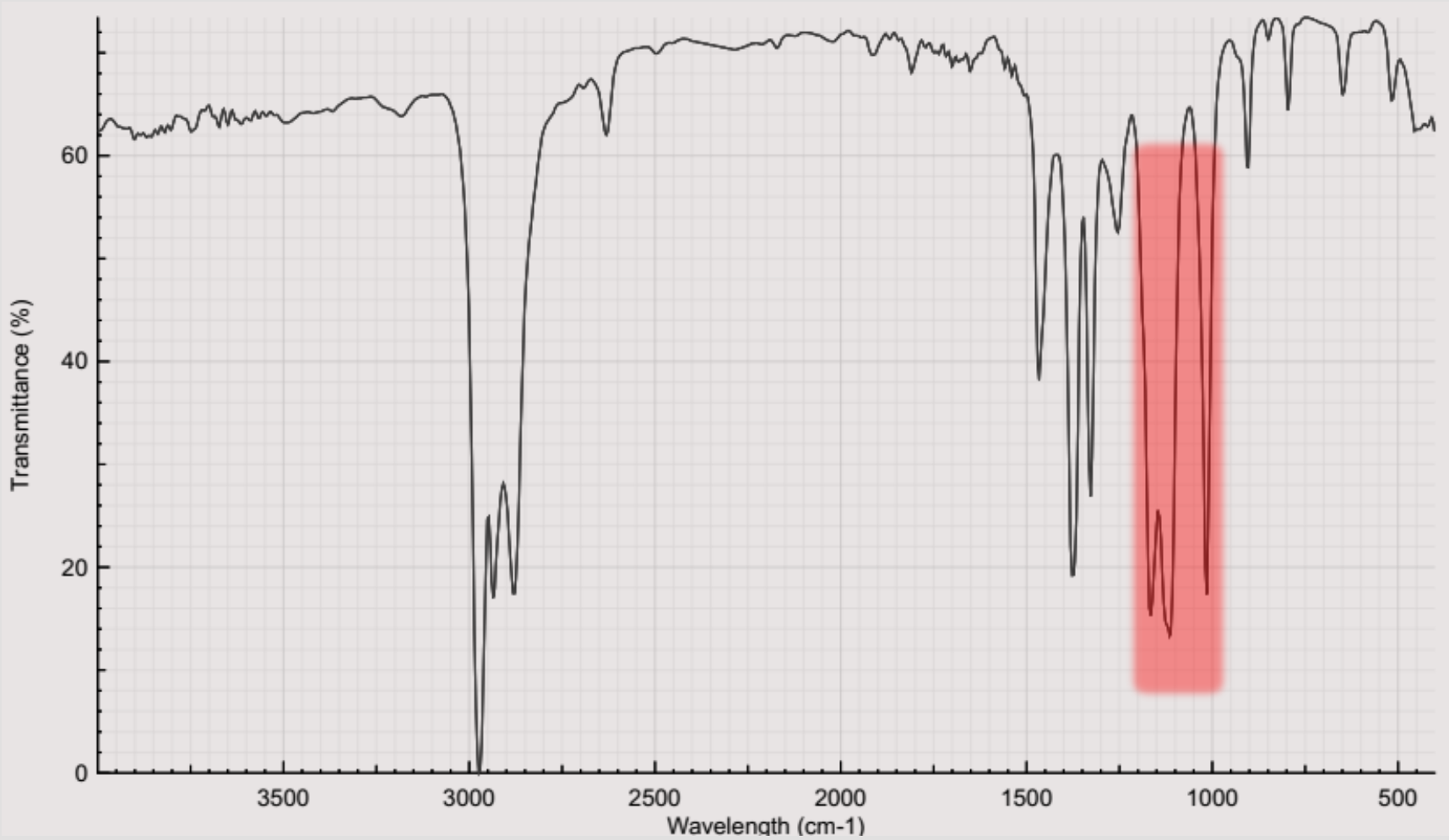


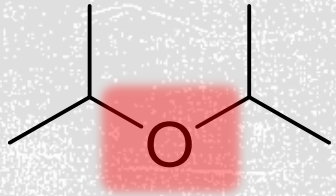
Aromatics : Due to the delocalization of e- in the ring, C-C bond order is 1.5, the stretching frequency for these bonds is slightly lower in energy than normal C=C

These show up as a pair of sharp bands, 1500 & 1600 cm^{-1}, (lower frequency band is stronger)

C-H bonds off the ring show up similar to vinyl C-H at 3000-3100 cm^{-1}

DIISOPROPYL ETHER



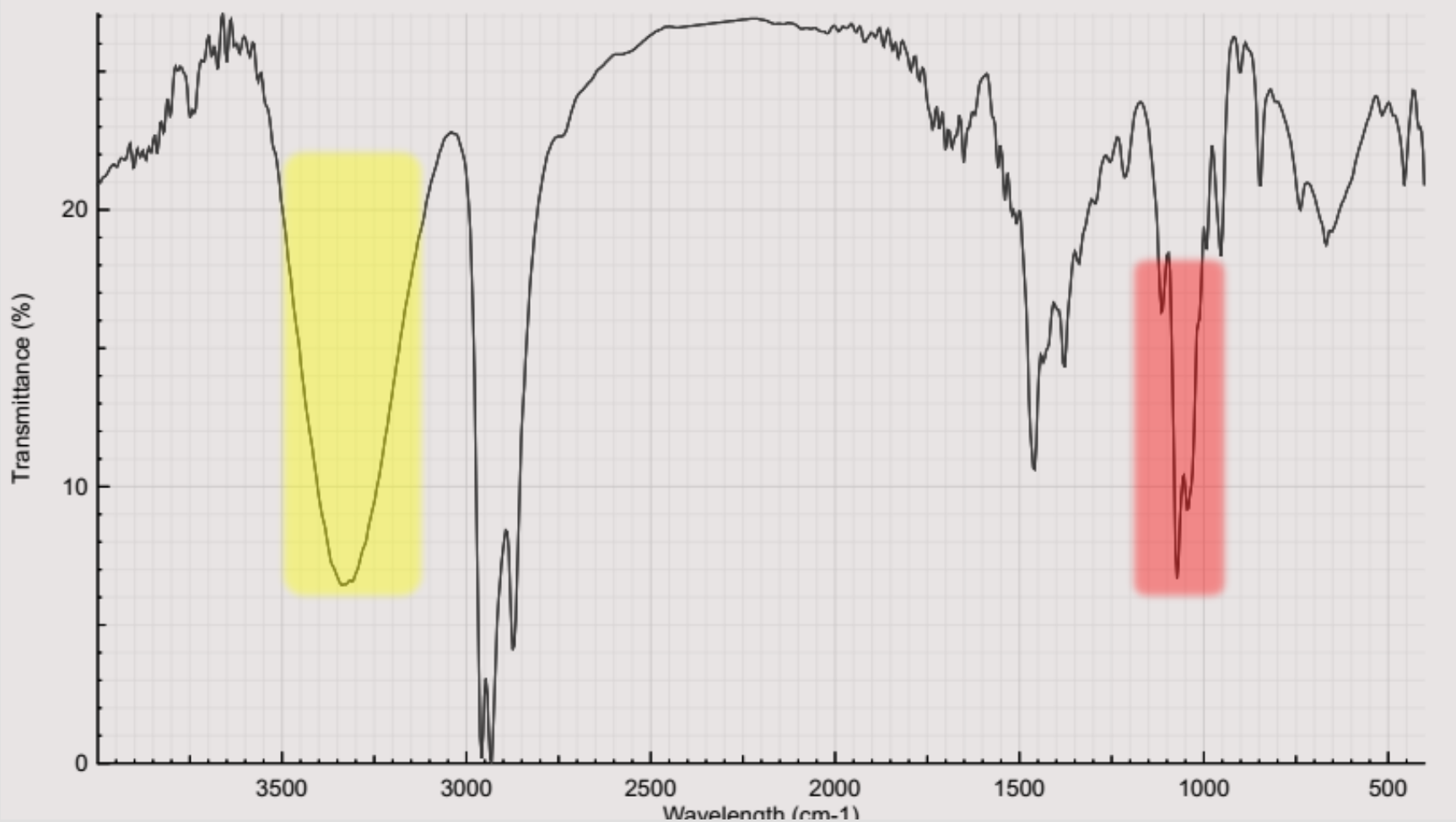


Ethers – addition of the C-O-C asymmetric band and vinyl C-H bonds

Show a strong band for the antisymmetric ***C-O-C*** stretch at 1050-1150 cm-1

Otherwise, dominated by the hydrocarbon component of the rest of the molecule

1-BUTANOL



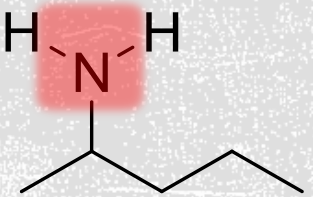
Alcohols: Strong, broad **O-H** stretch from 3200-3400 cm^{-1}

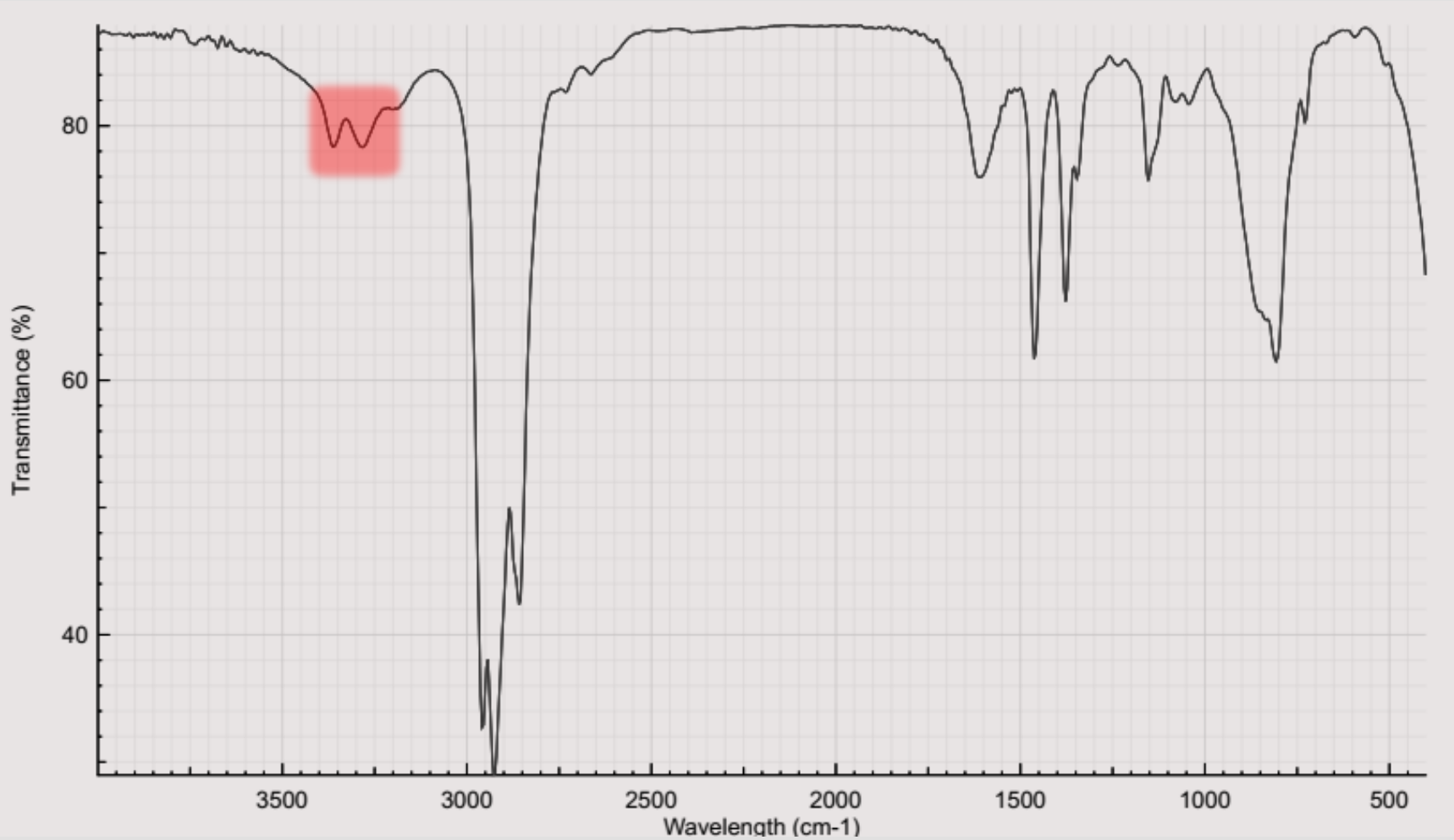
Like ethers, **C-O** stretch from 1050-1260 cm^{-1}

Band position changes depending on the alcohols substitution: 1° 1075-1000; 2° 1075-1150; 3° 1100-1200; phenol 1180-1260

The shape is due to the presence of hydrogen bonding

2-AMINOPENTANE





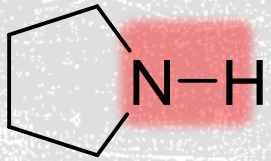
Amines - Primary

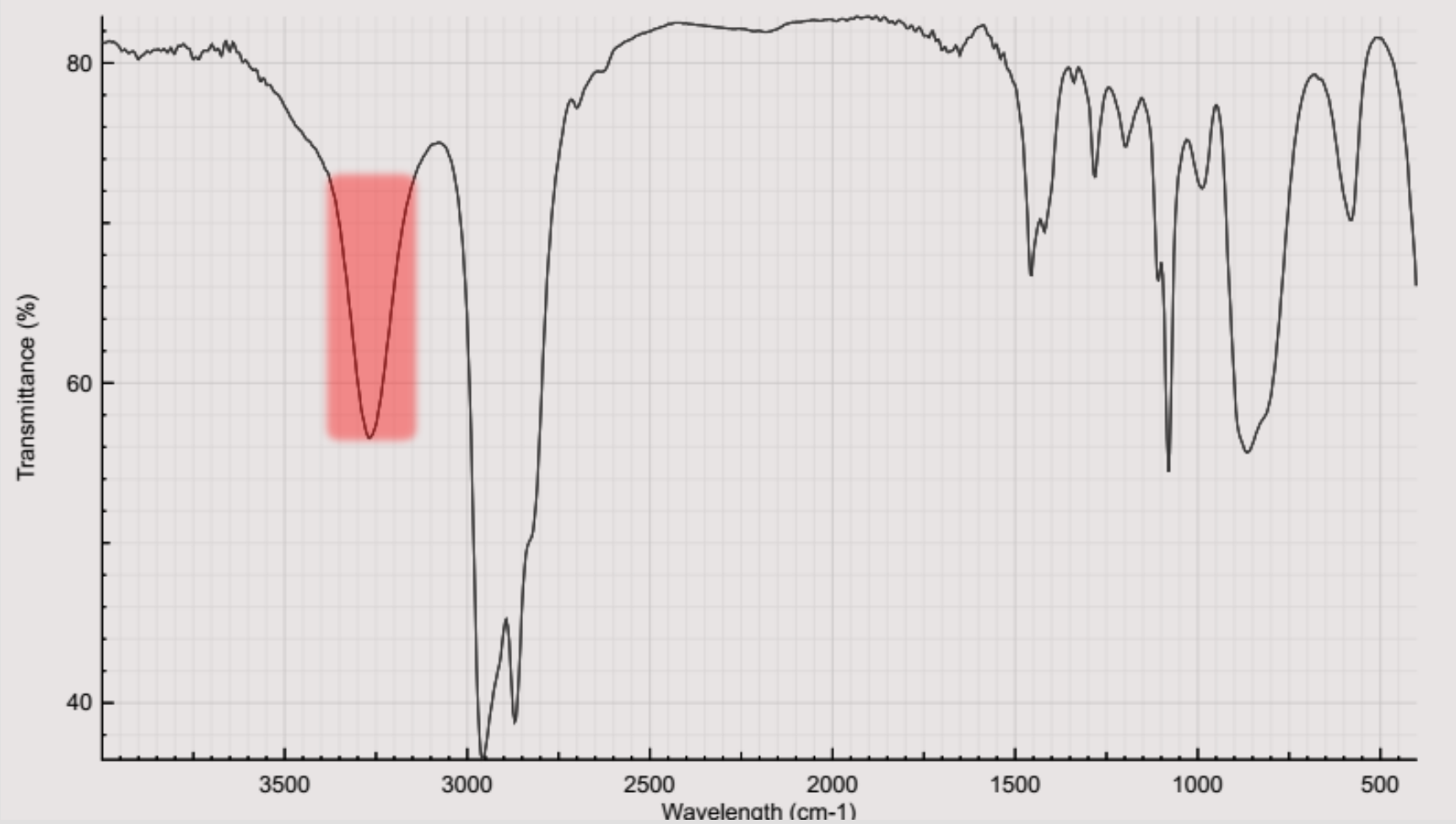
Shows the –N-H stretch for NH_2 as a doublet between 3200-3500 cm^{-1} (symmetric and anti-symmetric modes)

-NH_2 has deformation band from 1590-1650 cm^{-1}

Additionally there is a "wag" band at 780-820 cm^{-1} that is not diagnostic

PYRROLIDINE



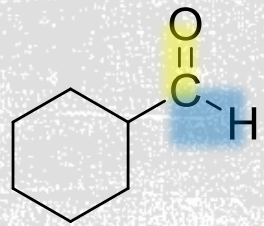


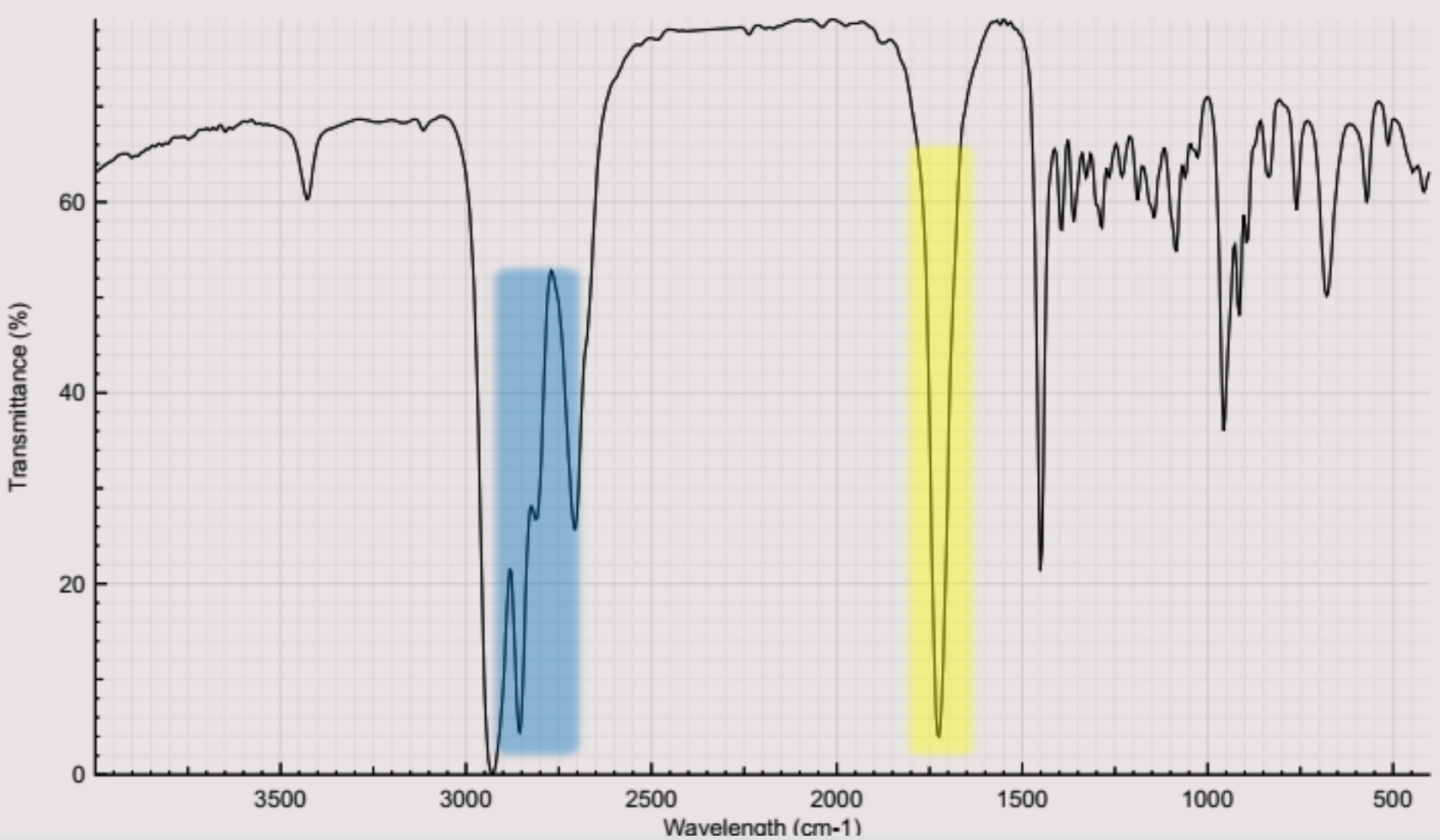
Amines – Secondary

N-H band for R_2N-H occurs at 3200-3500 cm^{-1} as a single sharp peak weaker than –**O-H**

Tertiary amines (R_3N) have no N-H bond and will not have a band in this region

Cyclohexyl carboxaldehyde





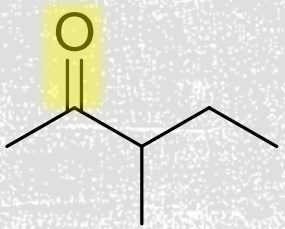
Aldehydes

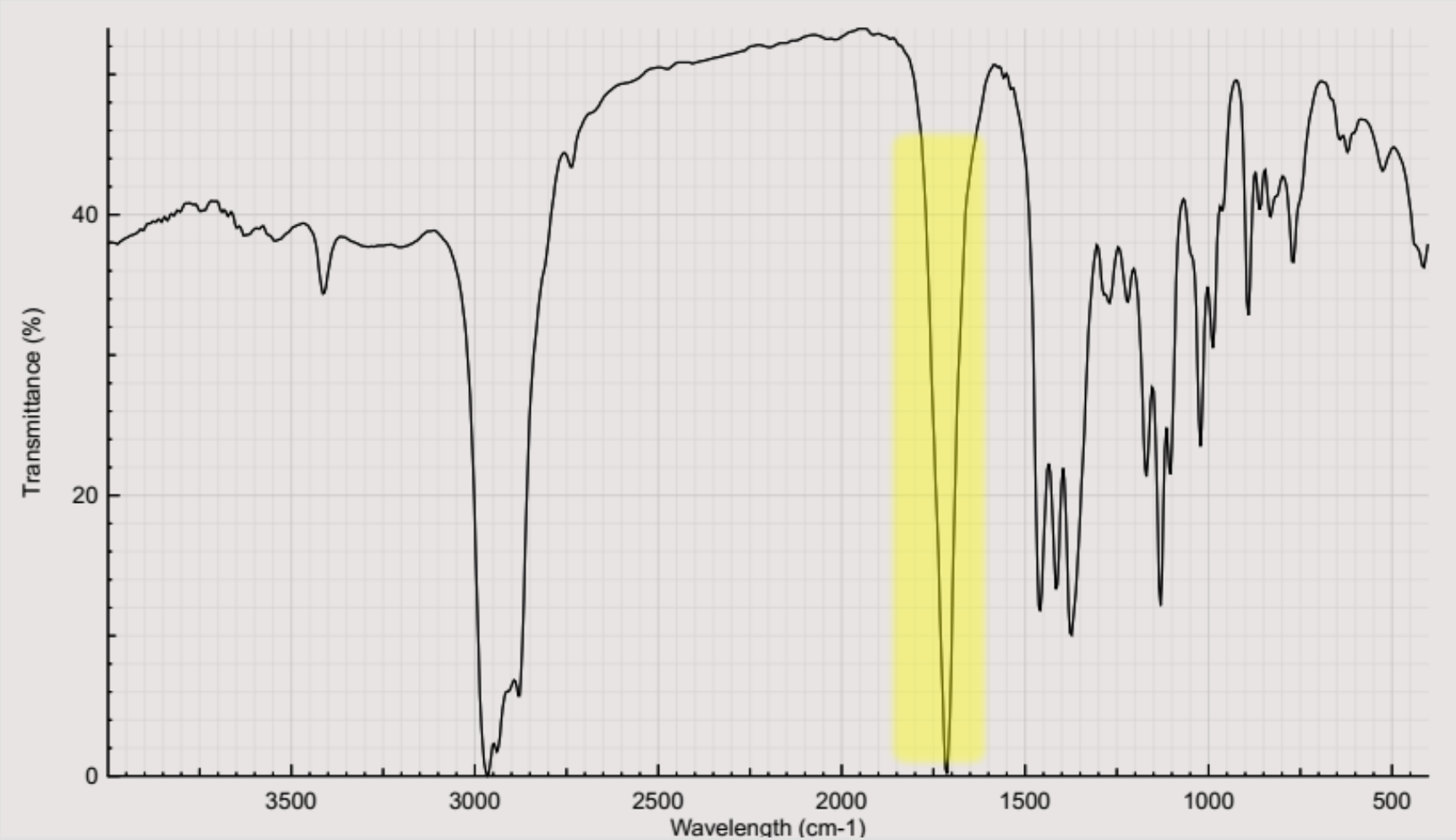
C=O (carbonyl) stretch from 1720-1740 cm-1

Band is sensitive to conjugation, as are all carbonyls (upcoming slide)

A highly unique sp2 C-H stretch appears as a doublet, 2720 & 2820 cm^{-1} called a "Fermi doublet"

3-METHYL-2-PENTANONE



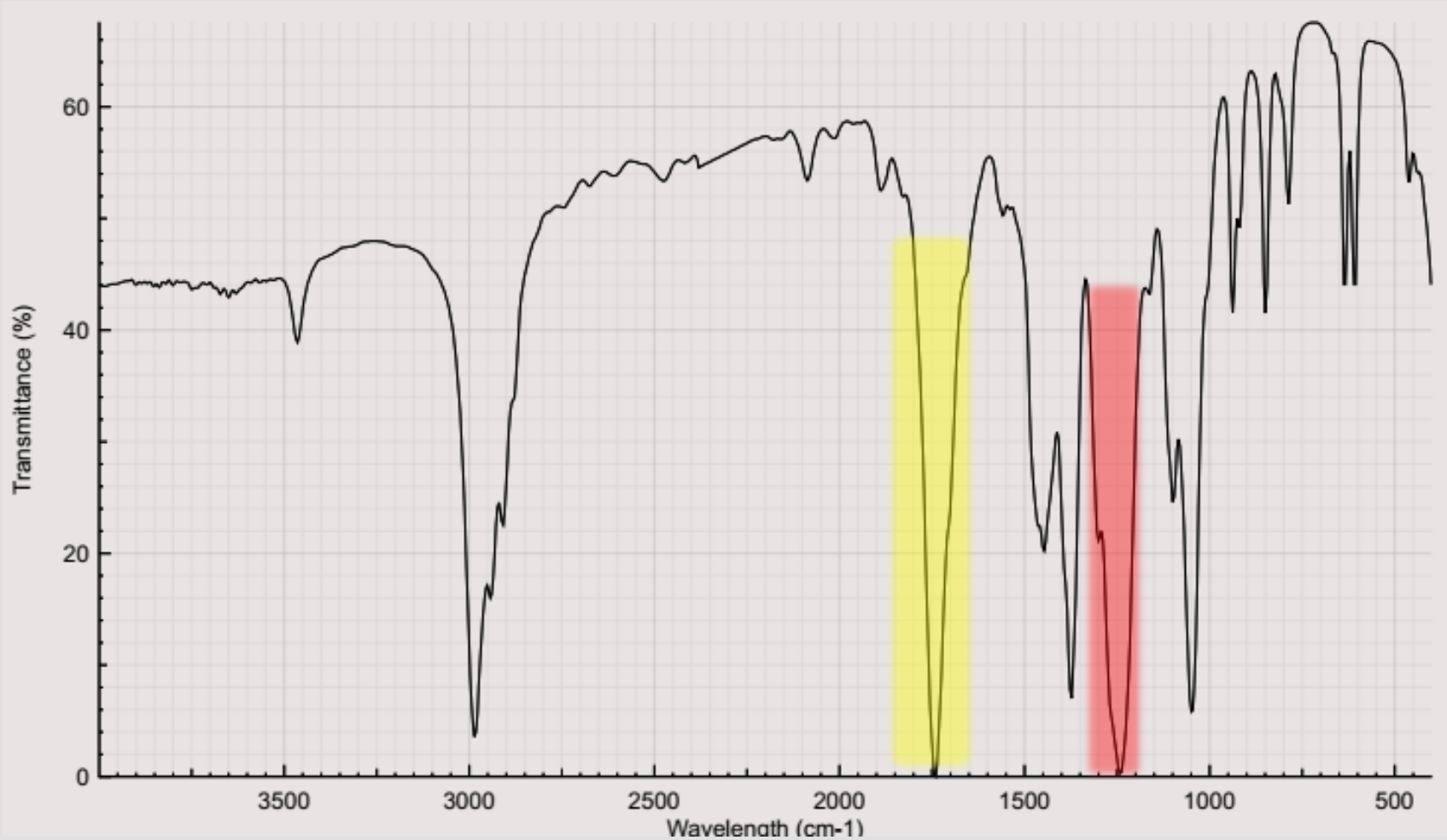


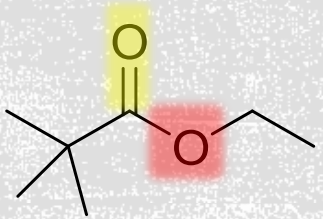
Ketones:

Simplest of the carbonyl compounds as far as IR spectrum – carbonyl only

C=O stretch occurs at 1705-1725 cm^{-1}

Ethyl Pivalate



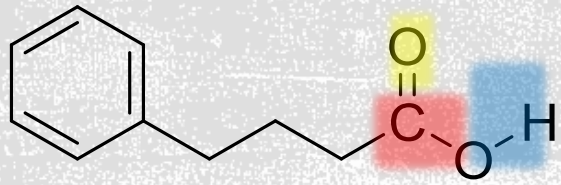


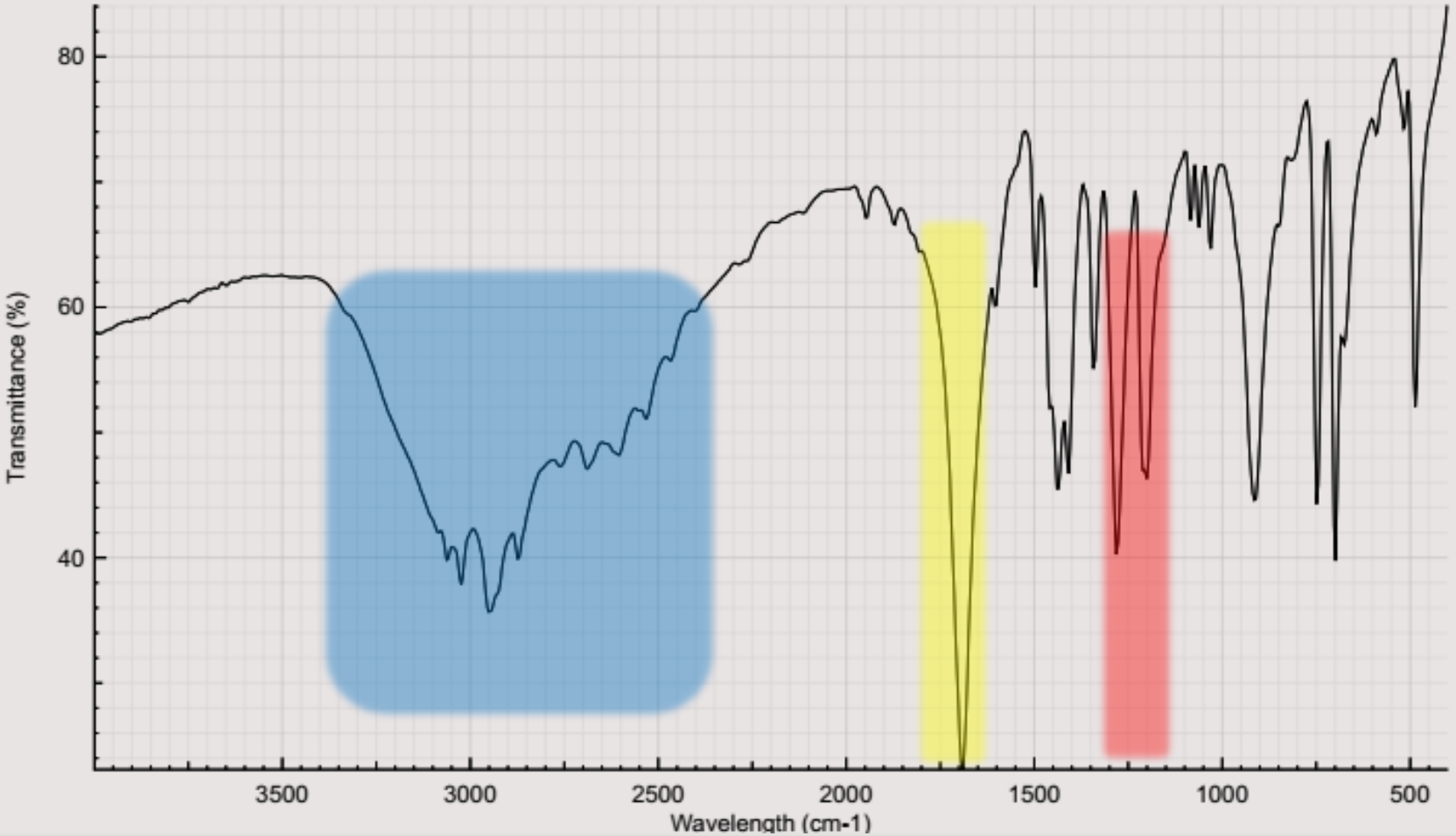
Esters

C=O stretch at 1735-1750 cm^{-1}

Strong band for ***C-O*** at a higher frequency than ethers or alcohols at 1150-1250 cm^{-1}

4-PHENYLBUTYRIC ACID





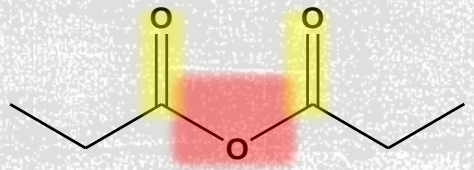
Carboxylic Acids:

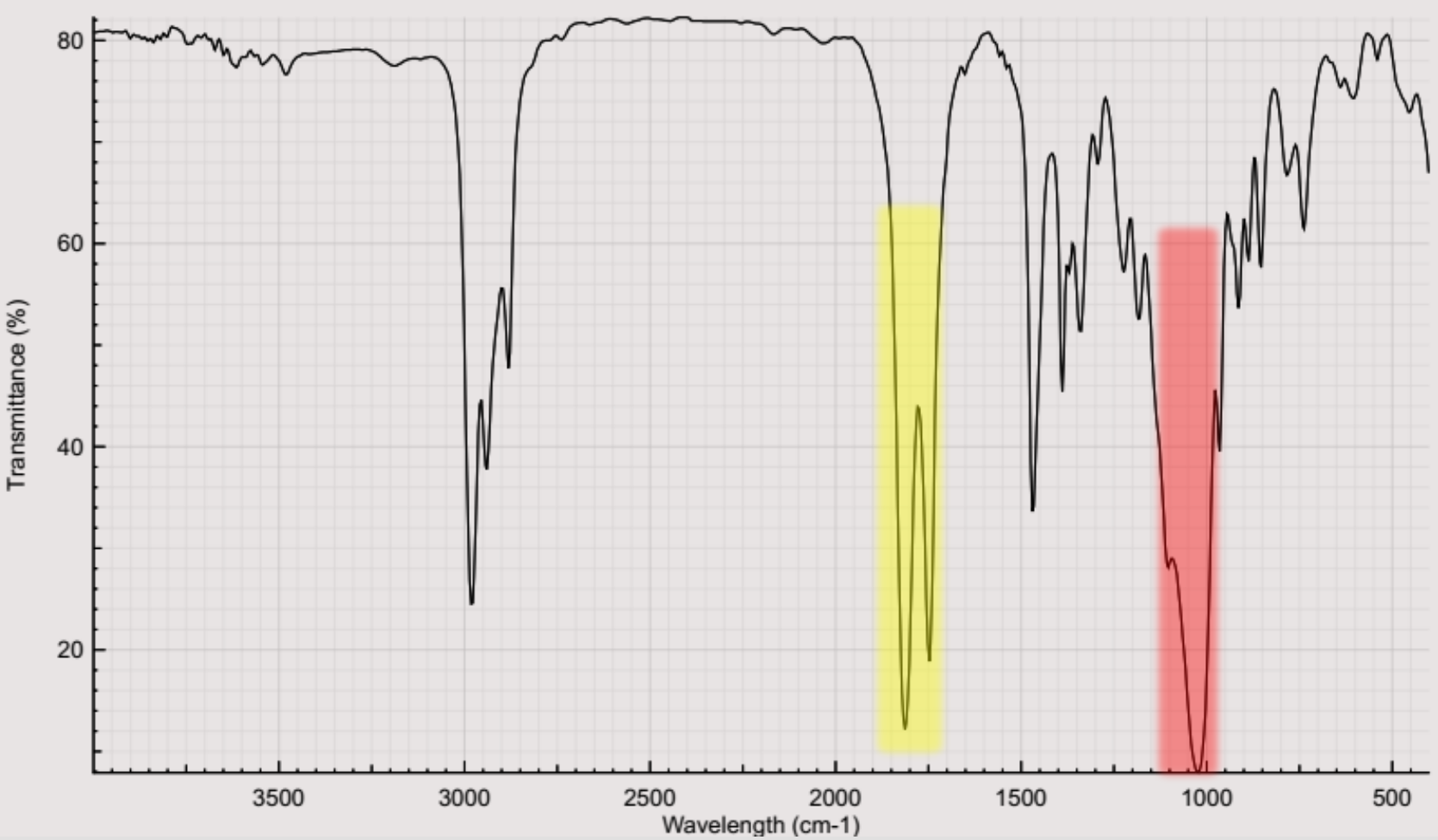
Give the messiest of IR spectra

C*=*O band occurs between 1700-1725 cm^{-1}

The highly dissociated ***O*-*H*** bond has a broad band from 2400-3500 cm^{-1} covering up to half the IR spectrum in some cases

Propionic anhydride





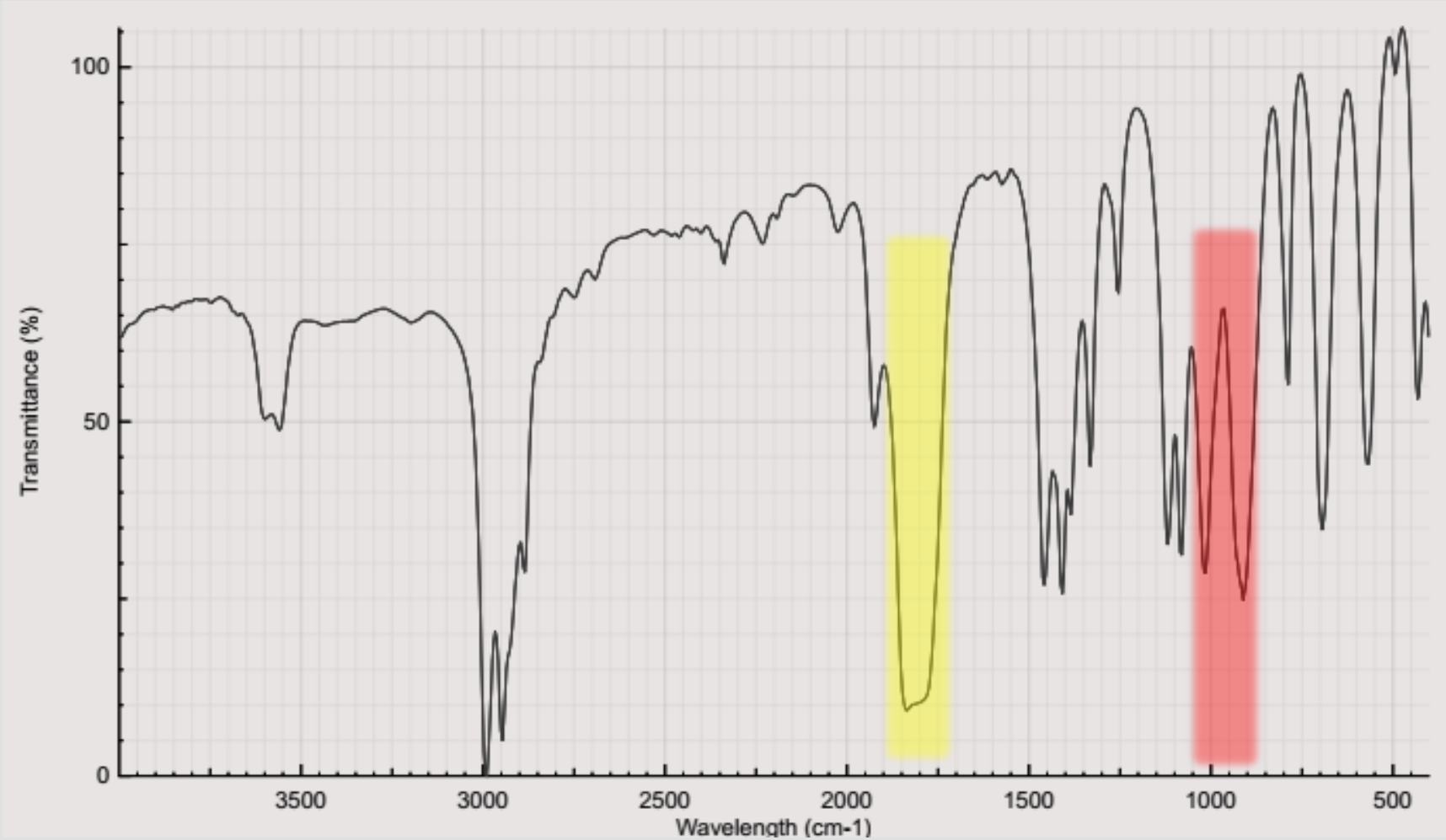
Acid anhydrides

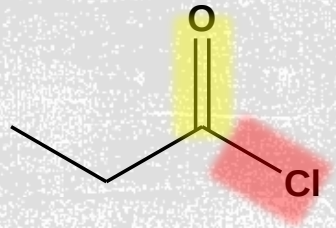
Coupling of the anhydride though the ether oxygen splits the carbonyl band into two with a separation of 70 cm^{-1}

Bands are at 1740-1770 cm^{-1} and 1810-1840 cm^{-1}

Mixed mode ***C-O*** stretch at 1000-1100 cm^{-1}

Propionyl Chloride



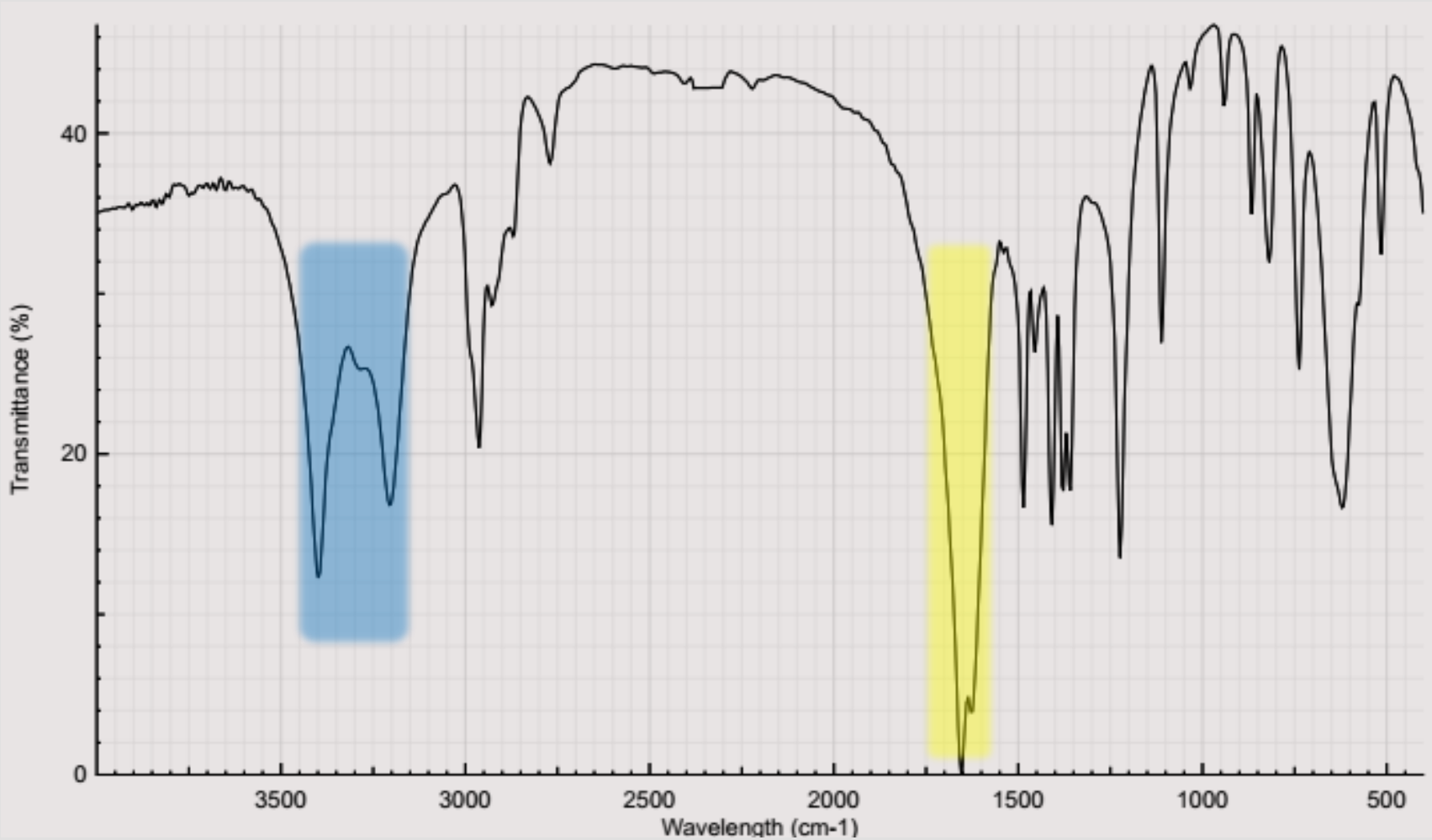


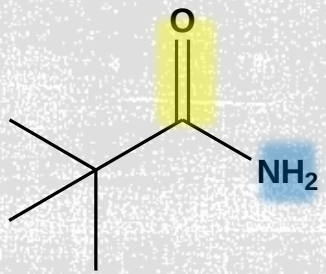
Acid halides

C=O band at 1770-1820 cm^{-1}

Bonds to halogens, due to their size (see Hooke's Law derivation) occur at low frequencies, only **Cl** is light enough to have a band on IR, **C-Cl** is at 600-800 cm^{-1}

PIVALAMIDE





Amides

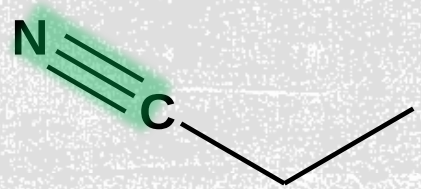
Display features of amines and carbonyl compounds

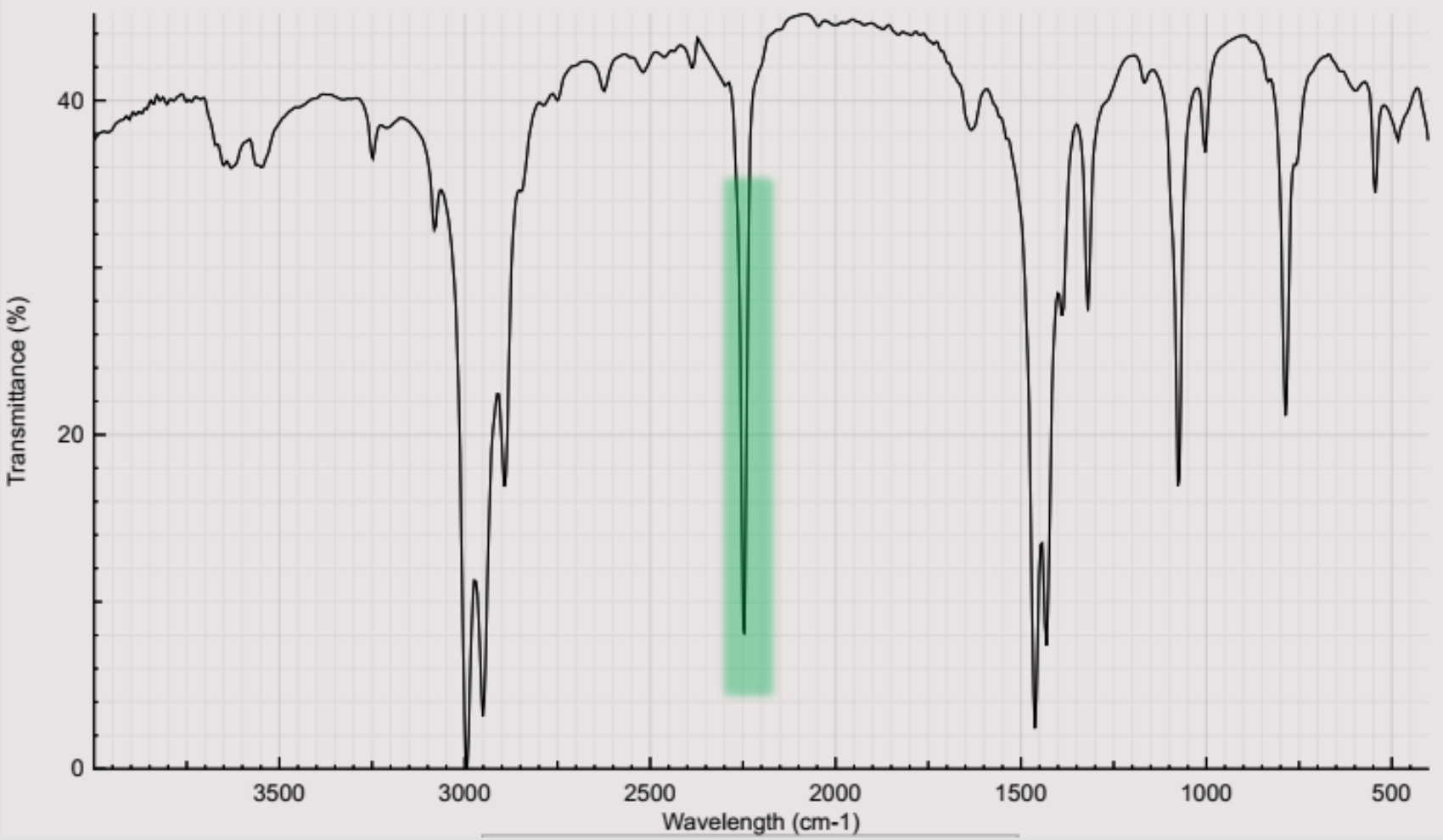
C=O stretch at 1640-1680 cm^{-1}

If the amide is primary ($-NH_2$) the N-H stretch occurs from 3200-3500 cm^{-1} as a doublet

If the amide is secondary (-NHR) the N-H stretch occurs at 3200-3500 cm^{-1} as a sharp singlet

PROPIONITRILE





Nitriles (the cyano- or **-C≡N** group)

Principle group is the carbon nitrogen triple bond at 2100-2280 cm^{-1}

This peak is usually much more intense than that of the alkyne due to the electronegativity difference between carbon and nitrogen