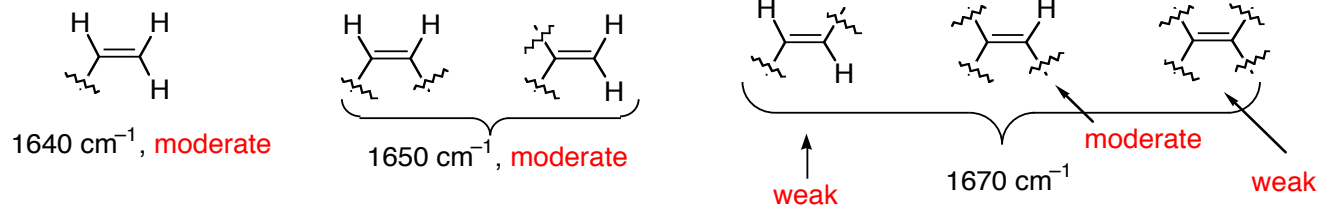




## Unconjugated Alkenes

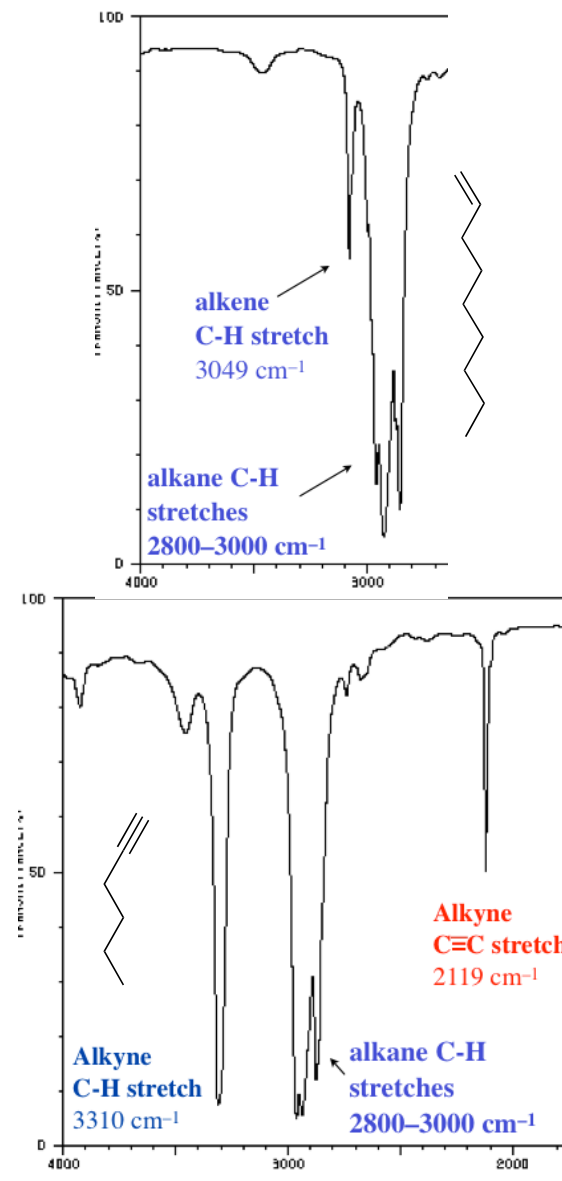
- **C=C-H**:  
- stretch:  $\geq 3000\text{ cm}^{-1}$

- linear alkenes:  
- C=C stretch: moderate to weak absorption at  $1667\text{--}1640\text{ cm}^{-1}$

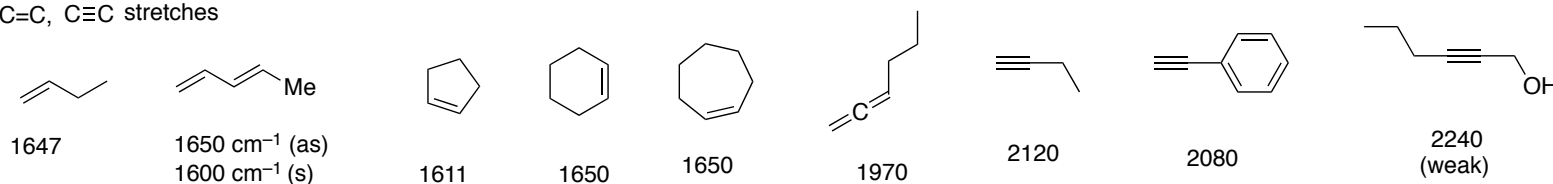


## Alkynes

- **C≡C** stretch: weak absorption at  $2260\text{--}2100\text{ cm}^{-1}$ 
  - not observed for symmetrical alkynes (v. weak for 'pseudo' symmetric alkynes)
  - terminal alkynes ( $\text{R-C}\equiv\text{C-H}$ ) absorptions are stronger than internal ( $\text{R-C}\equiv\text{C-R}$ ) absorptions
- **C≡C-H** stretch:
  - $3333\text{--}3267\text{ cm}^{-1}$
  - strong, narrow (as compared to OH or NH)



examples of  
C=C, C≡C stretches



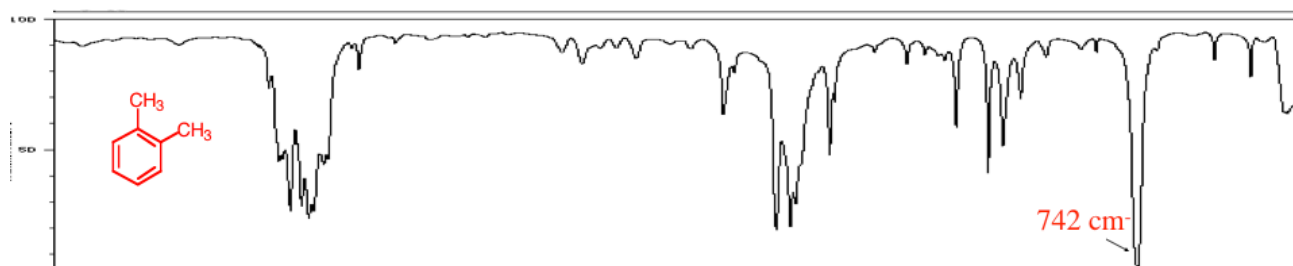
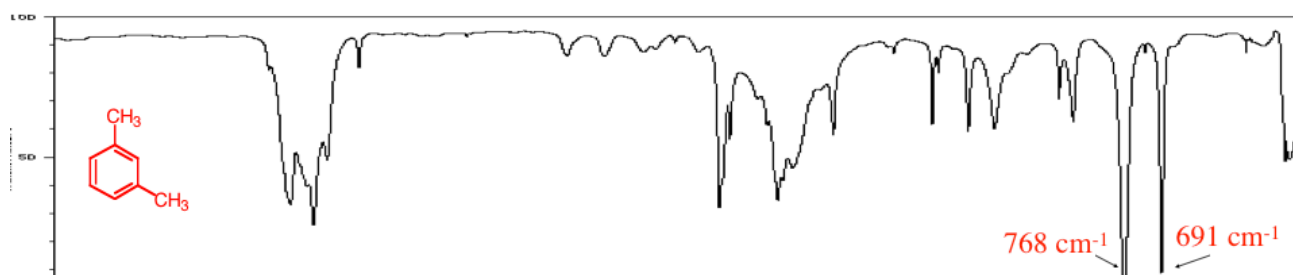
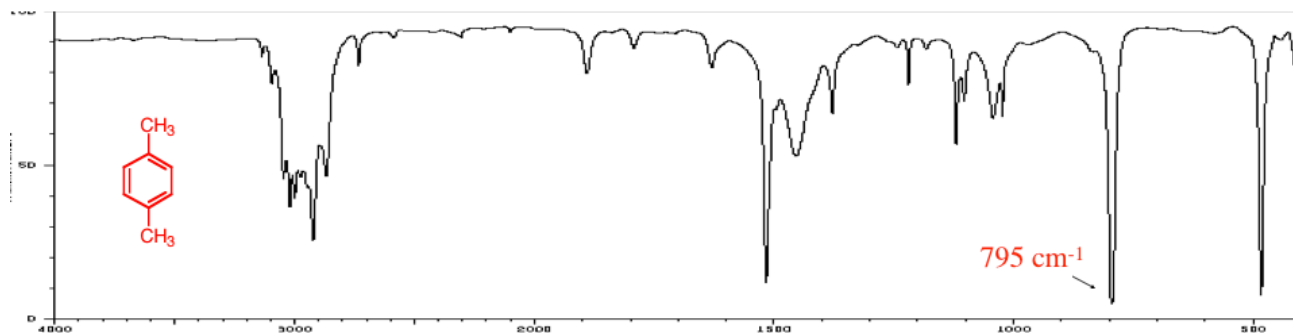
## Mononuclear Aromatic Hydrocarbons (benzene)

- Out of plane bending of aromatic C-H bonds: most informative
  - 900–675  $\text{cm}^{-1}$
  - intense bands, strongly **coupled to adjacent hydrogens** on the ring
  - position and number of bands gives information about the substitution pattern (particularly useful for alkyl substituted aromatics. Substitution of polar groups can give rise to exceptions)

- C=C-H stretch: 3100–3000  $\text{cm}^{-1}$
- C=C stretch: 1600-1585; 1500-1400  $\text{cm}^{-1}$
- C=C out of plane ring bending: 600-420  $\text{cm}^{-1}$

### disubstituted benzenes

Out of plane bending of aromatic C-H bonds used to distinguish para, meta, ortho isomers



## Alcohols

**CH stretch** typically occurs as a broad peak centered @  $3300\text{ cm}^{-1}$  (spanning  $3550\text{-}3200\text{ cm}^{-1}$ ).

This peak is broad due to H-bonding

In rare cases where H-bonding is not present, the peak is sharp and at higher frequency

### C–O stretching Vibrations

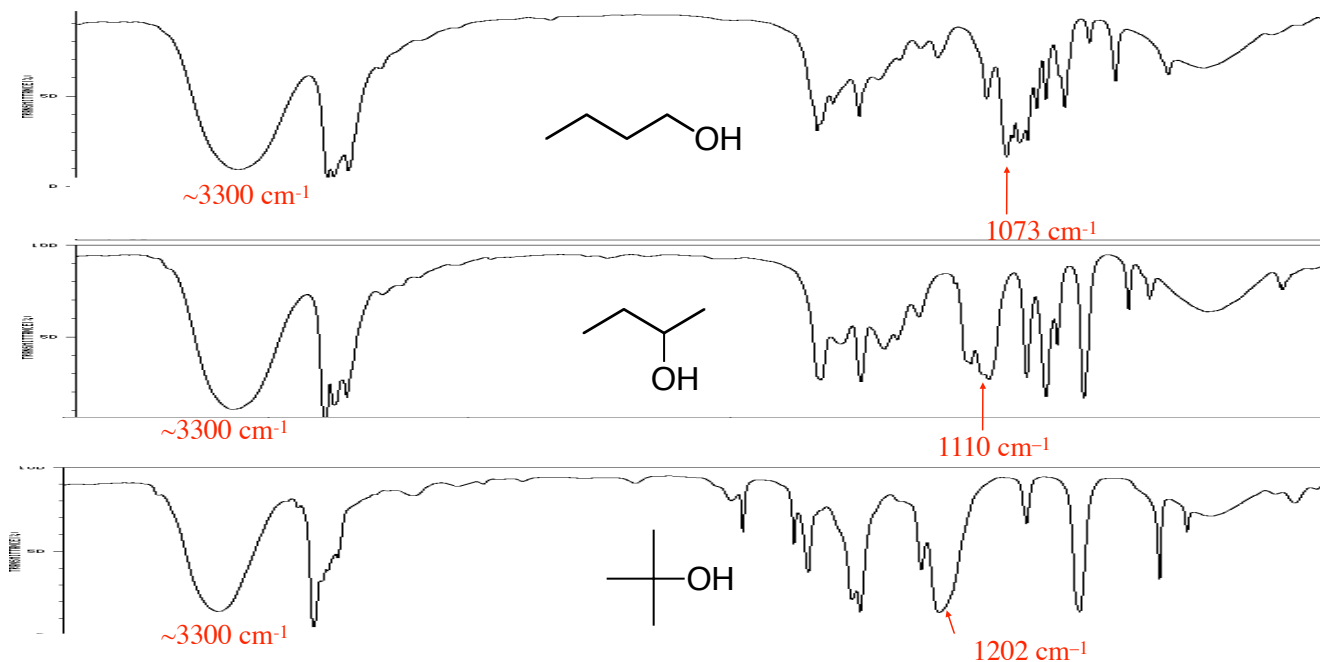
• Alcohols ( $1260\text{-}1000\text{ cm}^{-1}$ )

• Phenols ( $1800\text{-}1260\text{ cm}^{-1}$ )

primary alcohol:  $1050\text{-}1085\text{ cm}^{-1}$

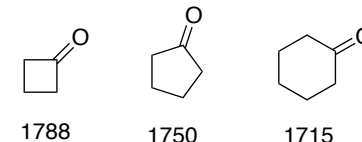
secondary alcohol:  $1085\text{-}1125\text{ cm}^{-1}$

tertiary alcohol:  $1125\text{-}1200\text{ cm}^{-1}$



## Ketones C=O stretch (see tables)

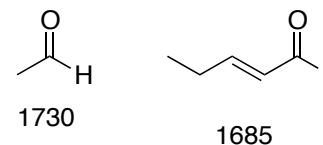
- **aliphatic**: 'normal' position of a neat aliphatic ketone is  $1715\text{ cm}^{-1}$
- **conjugation**: shifts position to lower frequency  
alkene or phenyl group causes absorption in the  $1685\text{-}1666\text{ cm}^{-1}$  region. For  $\alpha,\beta$ -unsaturated carbonyls, 2 absorptions may be observed
- **cyclic ketones** The bond angle influences the absorption frequency of the C=O



## Aldehydes

### C=O stretch (see tables)

- Aliphatic aldehydes: C=O stretch at  $1740\text{-}1720\text{ cm}^{-1}$
- Electron withdrawing groups shift to higher frequency
- Conjugative groups shift to lower frequency ( $1710\text{-}1685\text{ cm}^{-1}$ )



### C-H stretch

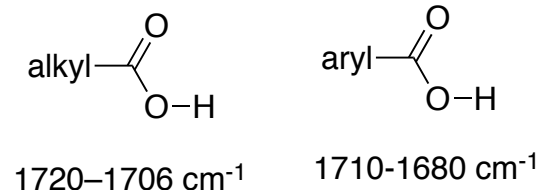
$2830\text{-}2695\text{ cm}^{-1}$  Often, two bands are observed

## Carboxylic Acids

**OH stretch** in the  $3300\text{-}2500\text{ cm}^{-1}$  region centered near  $3000\text{ cm}^{-1}$

### C=O stretch

- $1720\text{-}1705$  for aliphatic acids
- $1710\text{-}1680$  for conjugated acids

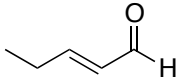


# C=O stretch tables

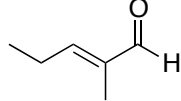
aldehydes, C=O



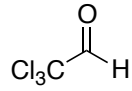
1730



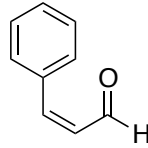
1685



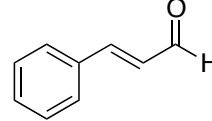
1690



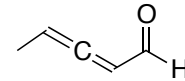
1768  $\text{cm}^{-1}$



1684



1674

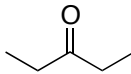


1688 (C=O)  
1932 (C=C)

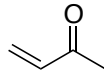
ketones, C=O



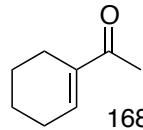
1715



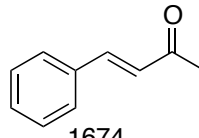
1720



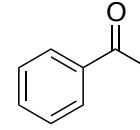
1684



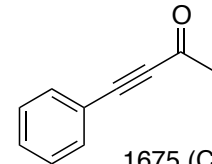
1685



1674



1685



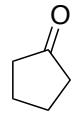
1675 (C=C)  
2203 (C=O)



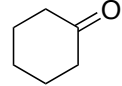
1813



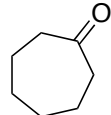
1788



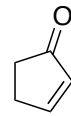
1750



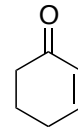
1715



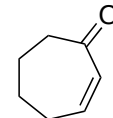
1706



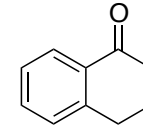
1715



1680



1665



1687

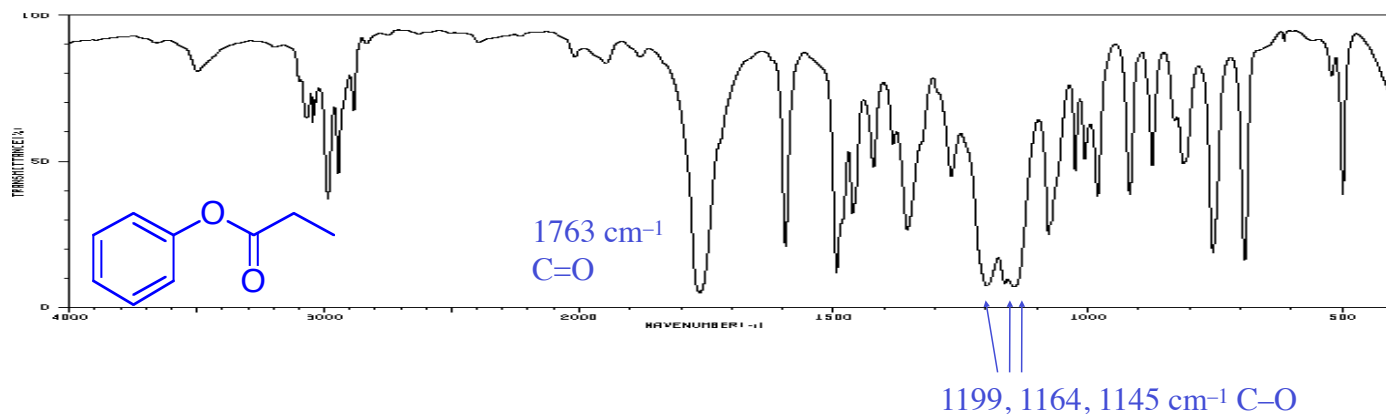
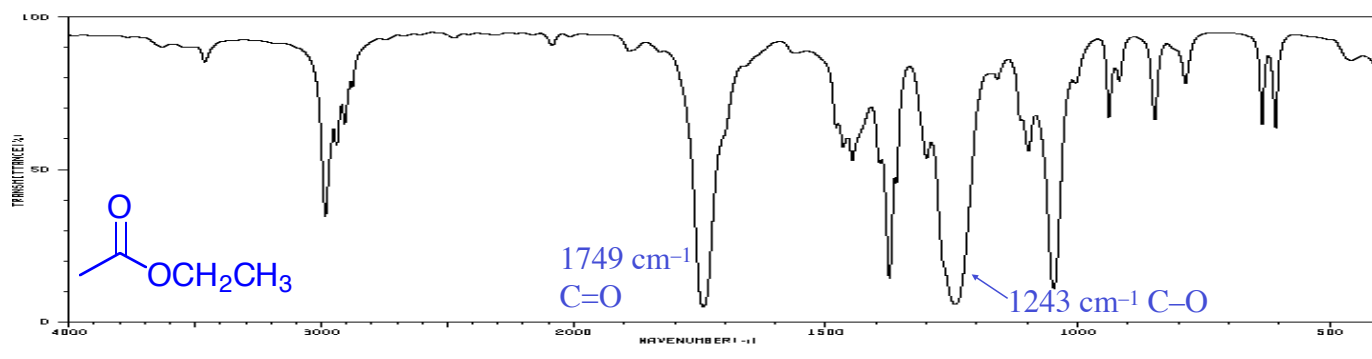
# Esters

## C=O stretch

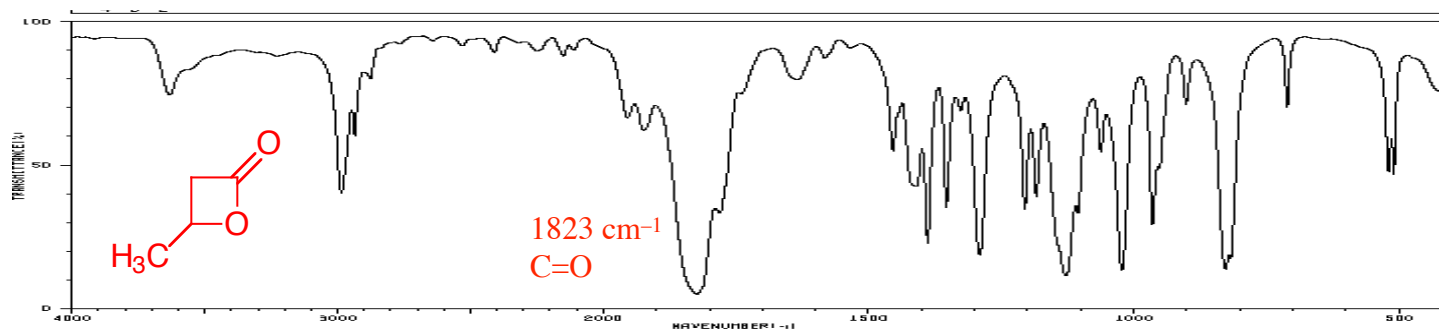
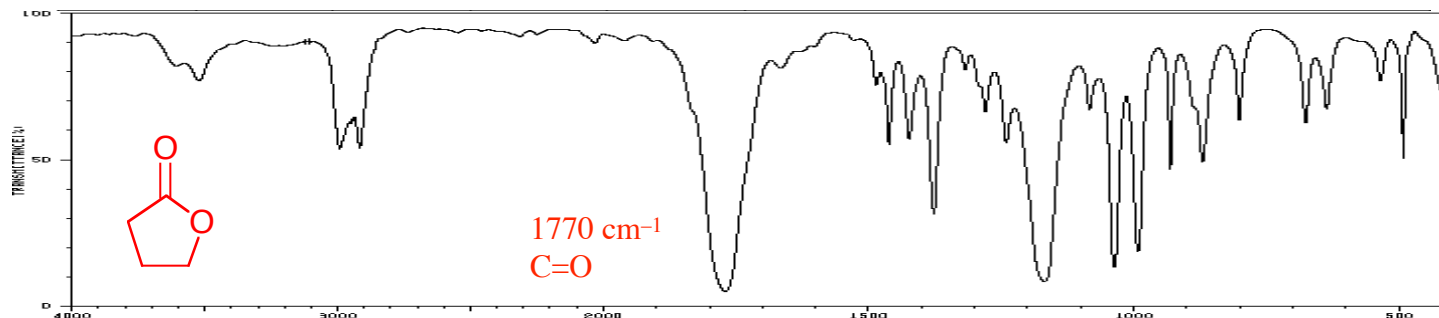
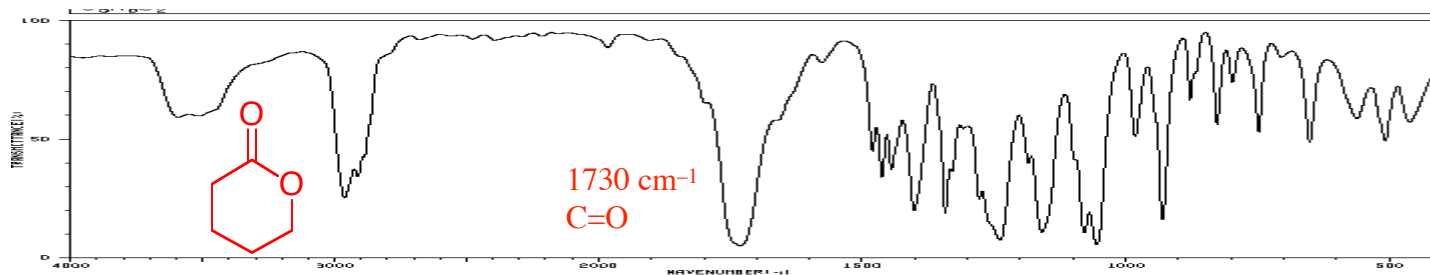
- saturated aliphatic esters: C=O: 1750–1735  $\text{cm}^{-1}$
- formates,  $\alpha,\beta$ -unsaturated, and benzoate esters: 1730–1715  $\text{cm}^{-1}$
- phenyl or vinyl esters: 1770–1780  $\text{cm}^{-1}$

## C–O stretches (strong absorptions; asymmetrical coupled vibrations)

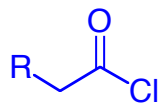
- saturated aliphatic esters (except acetates): C–O: 1210–1163  $\text{cm}^{-1}$
- acetates: 1240  $\text{cm}^{-1}$
- $\alpha,\beta$ -unsaturated esters: 1300–1160  $\text{cm}^{-1}$
- benzoate esters: 1310–1250  $\text{cm}^{-1}$



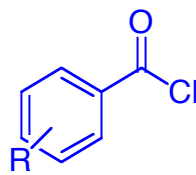
# Lactones: effect of Ring sizes



## Acid Halides



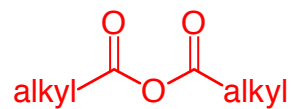
1815–1785  $\text{cm}^{-1}$



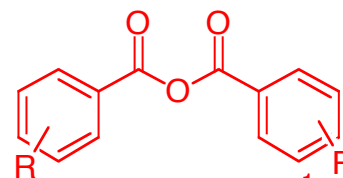
1800–1770  $\text{cm}^{-1}$

## Anhydrides

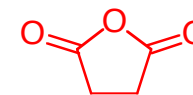
- Two carbonyl stretches (symmetrical and asymmetrical)



1818; 1750  $\text{cm}^{-1}$



1775; 1720  $\text{cm}^{-1}$

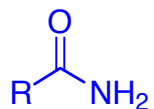


1865; 1782  $\text{cm}^{-1}$



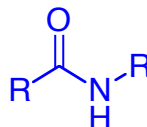
# amides

**NH stretch(es):** Primary amides produce two N-H stretch absorptions, secondary amides only one, and tertiary none.



Two bands

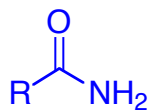
3520 (as), 3400 (s)  $\text{cm}^{-1}$



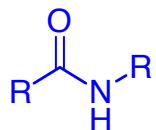
one bands

3500–3400  $\text{cm}^{-1}$

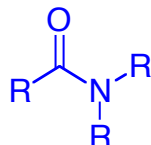
**C=O stretching (Amide I band):**



1690  $\text{cm}^{-1}$  (dilute)

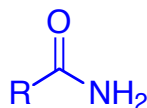


1680-1700  $\text{cm}^{-1}$  (dilute)

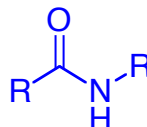


1680-1630  $\text{cm}^{-1}$

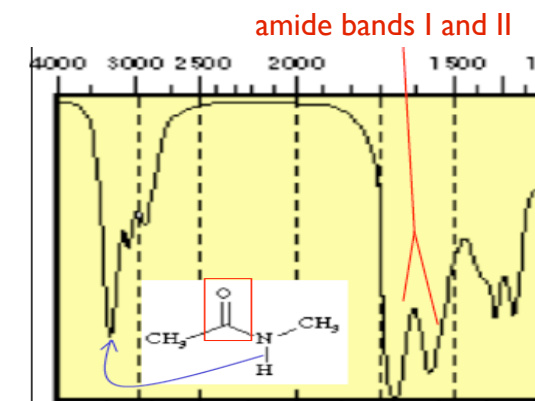
**NH Bending (Amide II band):**



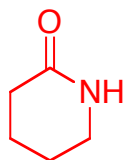
1620-1590  $\text{cm}^{-1}$



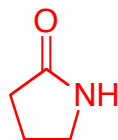
1550-1510  $\text{cm}^{-1}$



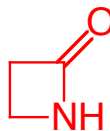
# Lactams



1650  $\text{cm}^{-1}$



1750-1700  $\text{cm}^{-1}$



1760-1730  $\text{cm}^{-1}$

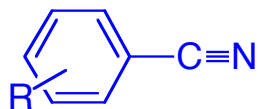
- NH stretching

- **primary** amines ( $\text{RNH}_2$ ) display two bands, near 3500 and 3400  $\text{cm}^{-1}$ . These represent 'free' asymmetrical and symmetrical stretches.
- **secondary** amines ( $\text{R}_2\text{NH}$ ) display one band near 3350-3310  $\text{cm}^{-1}$ .
- weaker and sharper than OH

## Nitriles



2260-2240  $\text{cm}^{-1}$



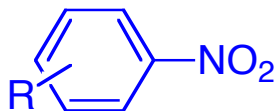
2240-2222  $\text{cm}^{-1}$

## Nitro compounds

- 2 bands from the asymmetrical and symmetrical stretching of the N=O bond



1550  $\text{cm}^{-1}$  and 1372  $\text{cm}^{-1}$



1550-1500  $\text{cm}^{-1}$  and 1360-1290  $\text{cm}^{-1}$