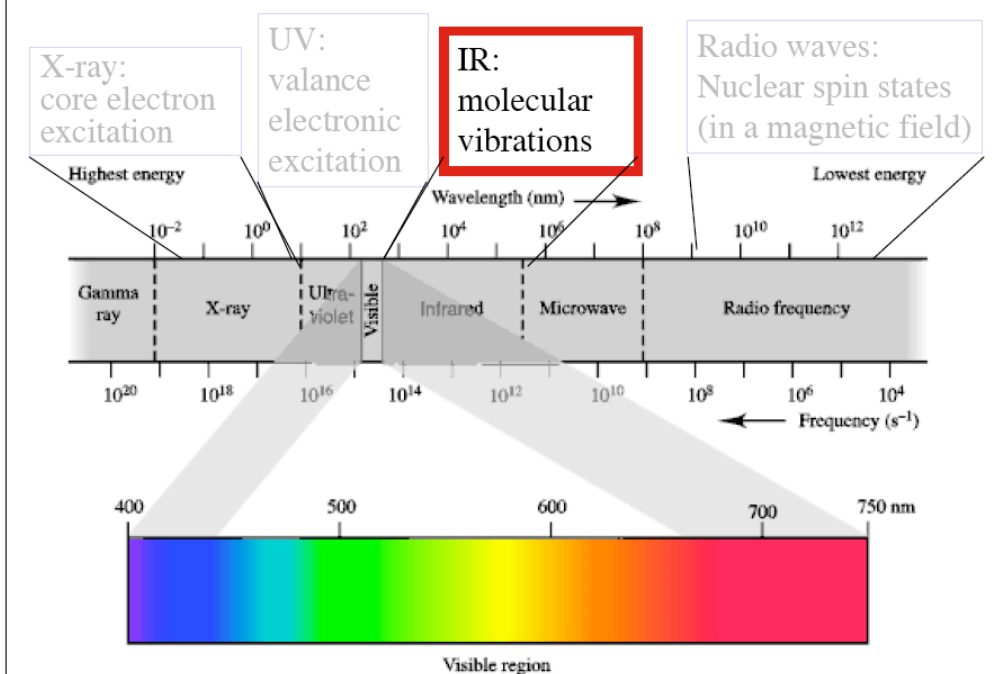


GOOD VIBRATIONS WITH IR SPECTROSCOPY:

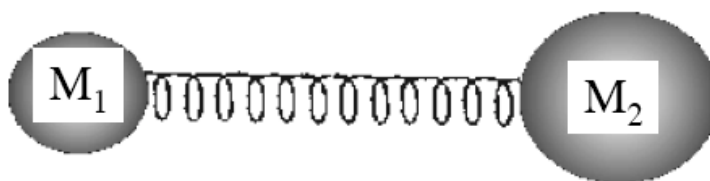


<http://ep.llnl.gov/msds/orgchem/spectroscopy.html#IR:>

<http://orgchem.colorado.edu/hndbksupport/irtutor/IRtheory.pdf>

IR tutor <http://members.aol.com/charlieabr/downloads.html>

<http://www.cem.msu.edu/~parrill/AIRS/>



$$\bar{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k(m+M)}{m \cdot M}}$$

$$\bar{\nu} = \nu/c = 1/\lambda$$

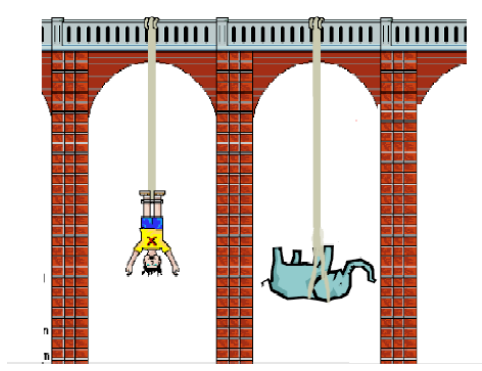
wavenumbers ← frequency ← wavelength

$\bar{\nu}$ units: cm^{-1}

- for excitation to occur, there must be an exact match between the frequency of the applied radiation and the frequency of the vibration
- in different compounds, the same type of functional group absorb in the same region of the IR

Factors that determine $\bar{\nu}$

1. Mass: larger mass = lower frequency (longer wavelength)



Factors that determine $\bar{\nu}$

2. Bond strength (k)

Stronger bonds (tighter springs) vibrate with higher frequency

3. Type of vibration

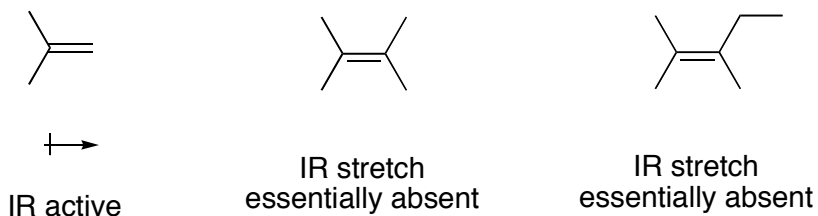
Stretching (along the line of the chemical bond)

ν_s

Bending (out of line with the chemical bond)

For the same bond, stretch is higher energy (i.e. higher frequency)

To see molecules in IR, transition must result in a dipole change

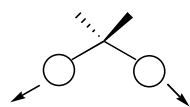


Coupled interactions occur when

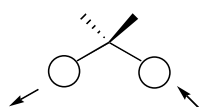
- 1) vibrations of bonds related by symmetry
- 2) common atoms between groups
- 3) independent groups absorb at same frequency

Commonly observed for CH₂ groups

Stretches

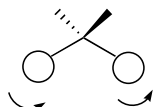


symmetrical

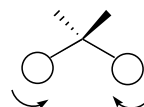


unsymmetrical

Bends in plane



rock
(symmetrical)



scissor
(unsymmetrical)

Table 11.2 Structural Units and Absorption Frequencies

BOND		TYPE OF COMPOUND	FREQUENCY (CM ⁻¹)
	(stretch)	Alkane	2800-3000
	(stretch)	Alkenes, aromatics	3000-3100
	(stretch)	Alkynes	3300
	(stretch)	Alcohols, phenols	3600-3650 (free) 3200-3500 (H-bonded) (broad)
	(stretch)	Carboxylic acids	2500-3300
	(stretch)	Amines	3300-3500 (doublet for NH ₂)
	(stretch)	Aldehyde	2720 and 2820
	(stretch)	Alkenes	1600-1680
	(stretch)	Aromatic	1500 and 1600
	(stretch)	Alkynes	2100-2270
	(stretch)	Aldehydes, ketones	1680-1740
	(stretch)	Nitriles	2220-2260
	(stretch)	Amines	1180-1360
	(bending)	Alkane	1375 (methyl)
	(bending)	Alkane	1460 (methyl and methylene)
	(bending)	Alkane	1370 and 1385 (isopropyl split)
	(bending)	R-CH=CH ₂	1000-960 and 940-900
	(bending)	R ₂ C=CH ₂	915-870
	(bending)	cis RCH=CHR	790-650
	(bending)	trans RCH=CHR	990-940
	(out-of-plane bending)	mono subst. benzene	770-730 and 710-690
	(out-of-plane bending)	o-subst. benzene	770-735
	(out-of-plane bending)	m-subst. benzene	810-750 and 710-690
	(out-of-plane bending)	p-subst. benzene	860-800
	(stretch)	Primary alcohol	1050-1085
	(stretch)	Secondary alcohol	1085-1125
	(stretch)	Tertiary alcohol	1125-1200
	(stretch)	Phenol	1180-1260

N-Alkanes

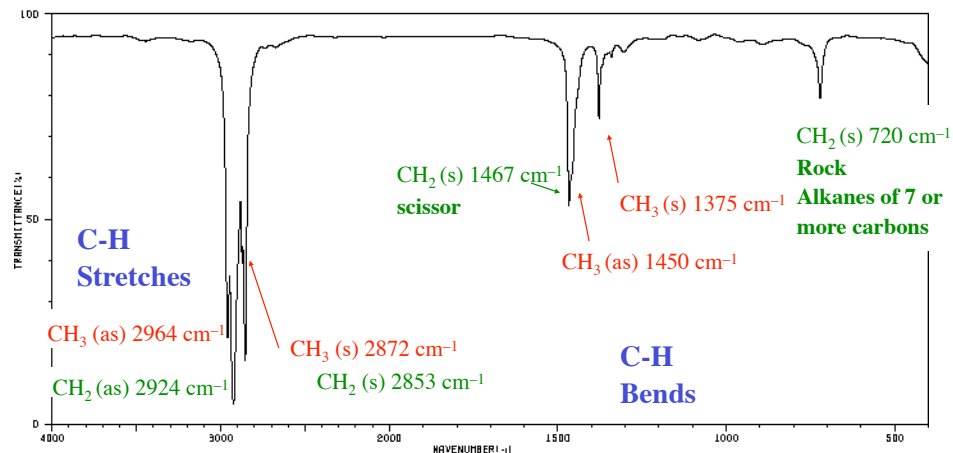
- interpreted in terms of 4 vibrations:
 - stretching and bending of C–H and C–C bonds
 - C–C bends: ca. 500 cm^{-1} (out of spectral window)
 - C–C stretches: $1200\text{--}800\text{ cm}^{-1}$, weak bands
not of value for interpretation (fingerprint)

more characteristic

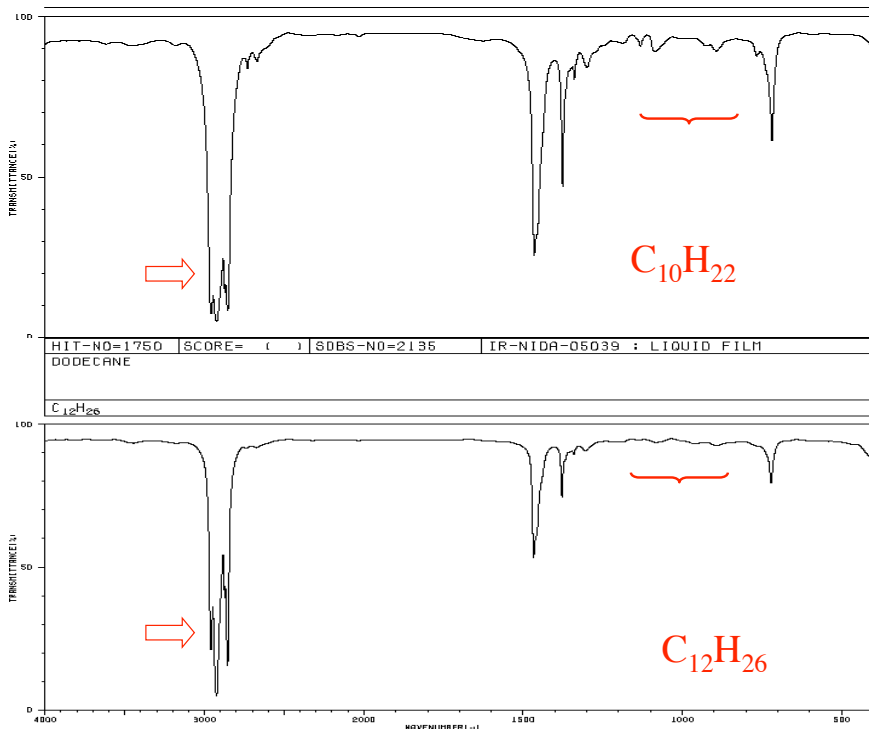
- C–H stretches: occurs from $3000\text{--}2840\text{ cm}^{-1}$
 - CH₃: 2962 cm^{-1} , asymmetrical stretch
 2872 cm^{-1} , symmetrical stretch
 - CH₂: 2926 cm^{-1} , asymmetrical stretch
 2853 cm^{-1} , symmetrical stretch

Note precision!

n-alkanes



Fingerprinting

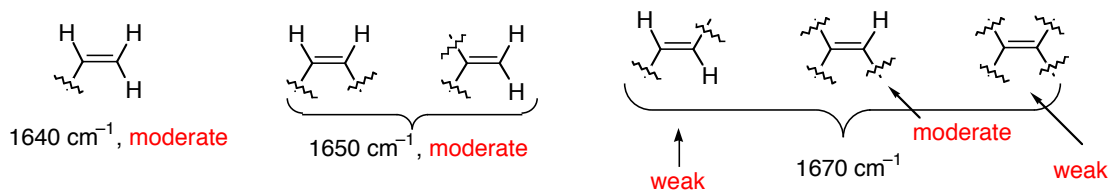


Similar
But Not
Identical

Unconjugated Alkenes

- linear alkenes:

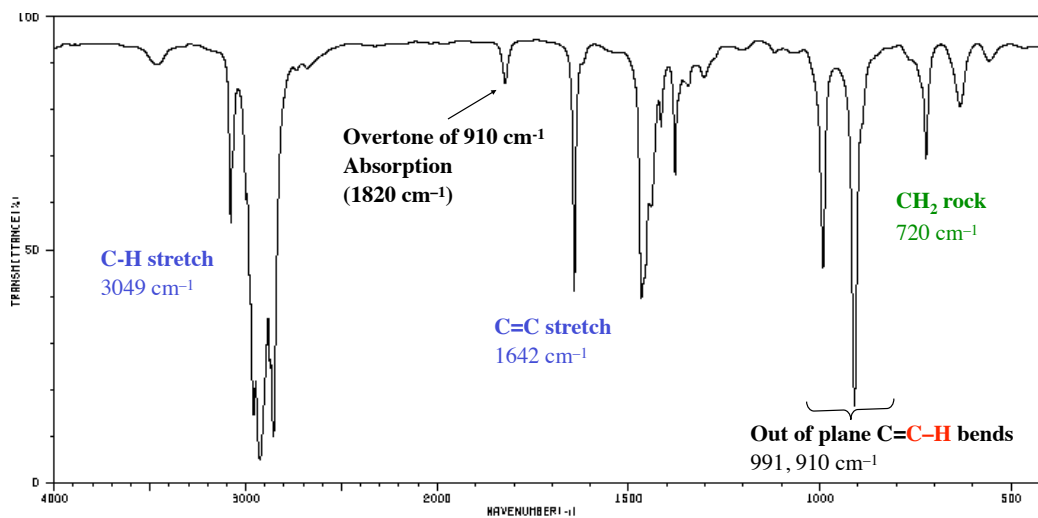
- C=C stretch: moderate to weak absorption at 1667-1640 cm⁻¹



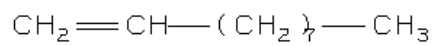
- C=C-H:

- stretch: ≥ 3000 cm⁻¹

Unconjugated Alkenes



1-decene



IR tutor

<http://members.aol.com/charlieabr/downloads.html>

- cyclic alkenes:

- C=C stretch: sensitive to ring strain



1650 cm^{-1}



1566 cm^{-1}



1641 cm^{-1}



1640 cm^{-1}



1650 cm^{-1}



1781 cm^{-1}

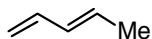
- cumulated alkenes:

- C=C=C stretch (asymmetric): 2000–1900 cm^{-1}

- conjugated alkenes:

- the alkene bond stretching vibrations in alkenes w/o a center of symmetry give rise to two C=C stretches

- for symmetrical molecules, e.g. butadiene, only the asymmetric stretch is observed

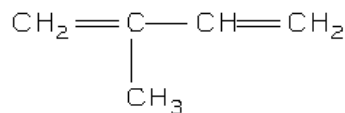
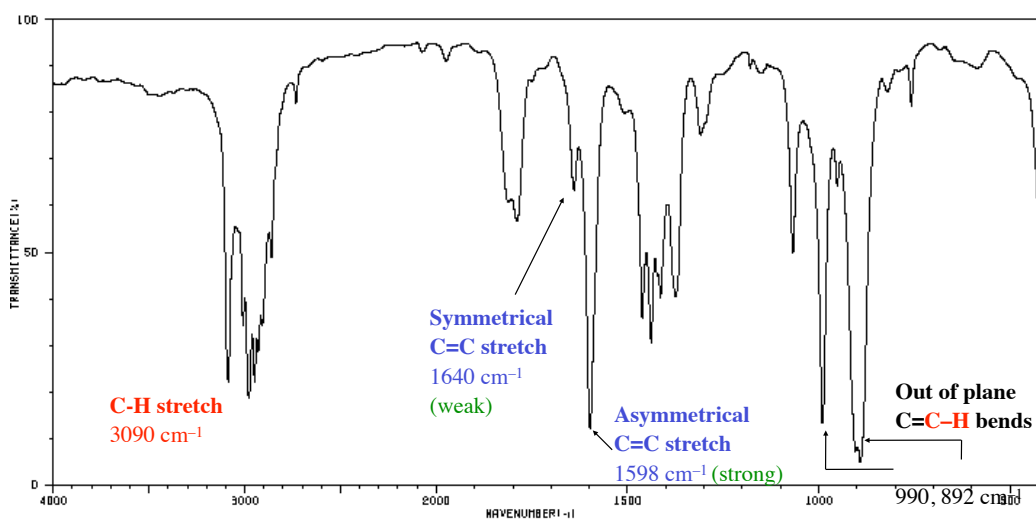


1650 cm^{-1} (as)
1600 cm^{-1} (s)



1600 cm^{-1} (as)

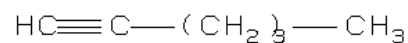
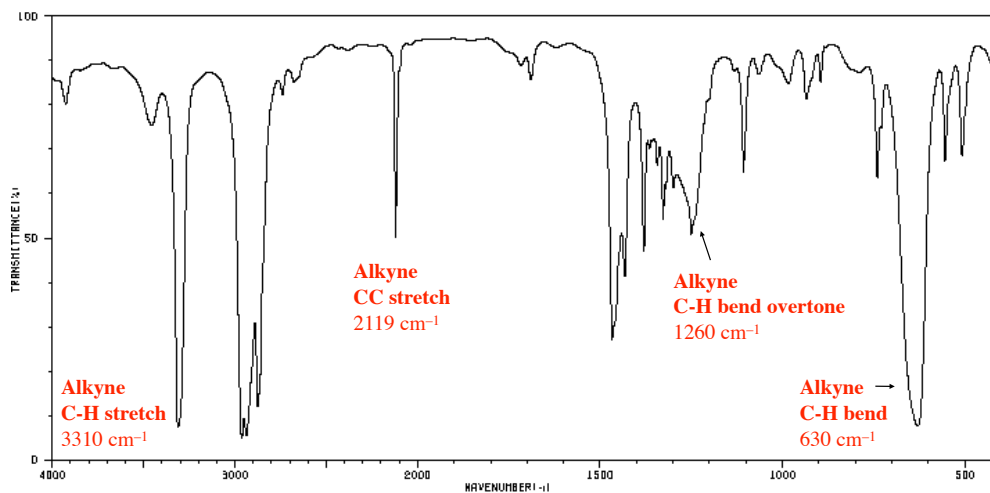
Conjugated Double Bonds



Alkynes

- $\text{—C}\equiv\text{C—}$ 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
- $\text{C}\equiv\text{C-H}$ stretch:
 - $3333\text{--}3267\text{ cm}^{-1}$
 - strong, narrow (as compared to OH or NH)
- $\text{C}\equiv\text{C-H}$ bend:
 - $700\text{--}610\text{ cm}^{-1}$: broad, strong absorption
 - $1400\text{--}1220\text{ cm}^{-1}$, overtone of above

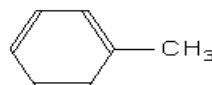
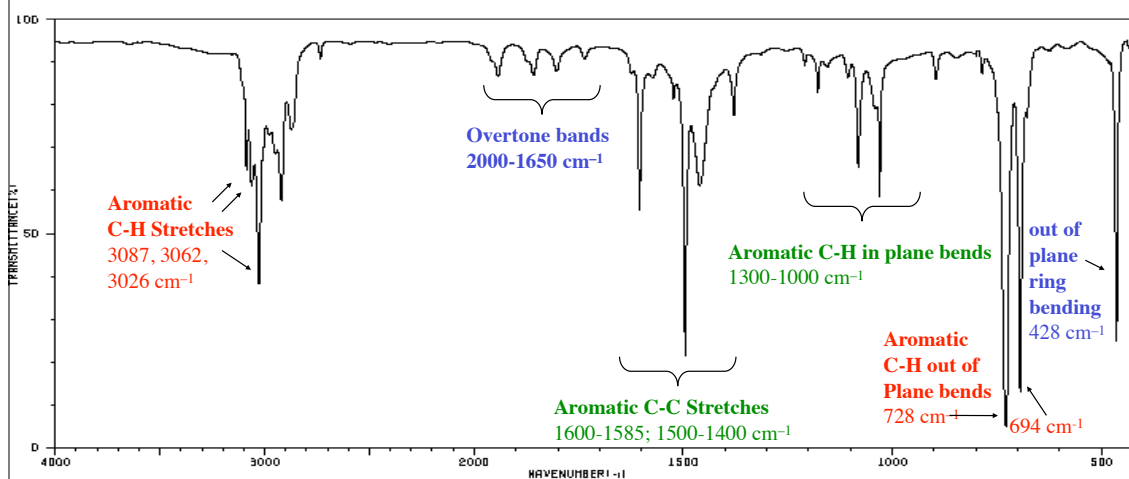
Terminal Alkynes

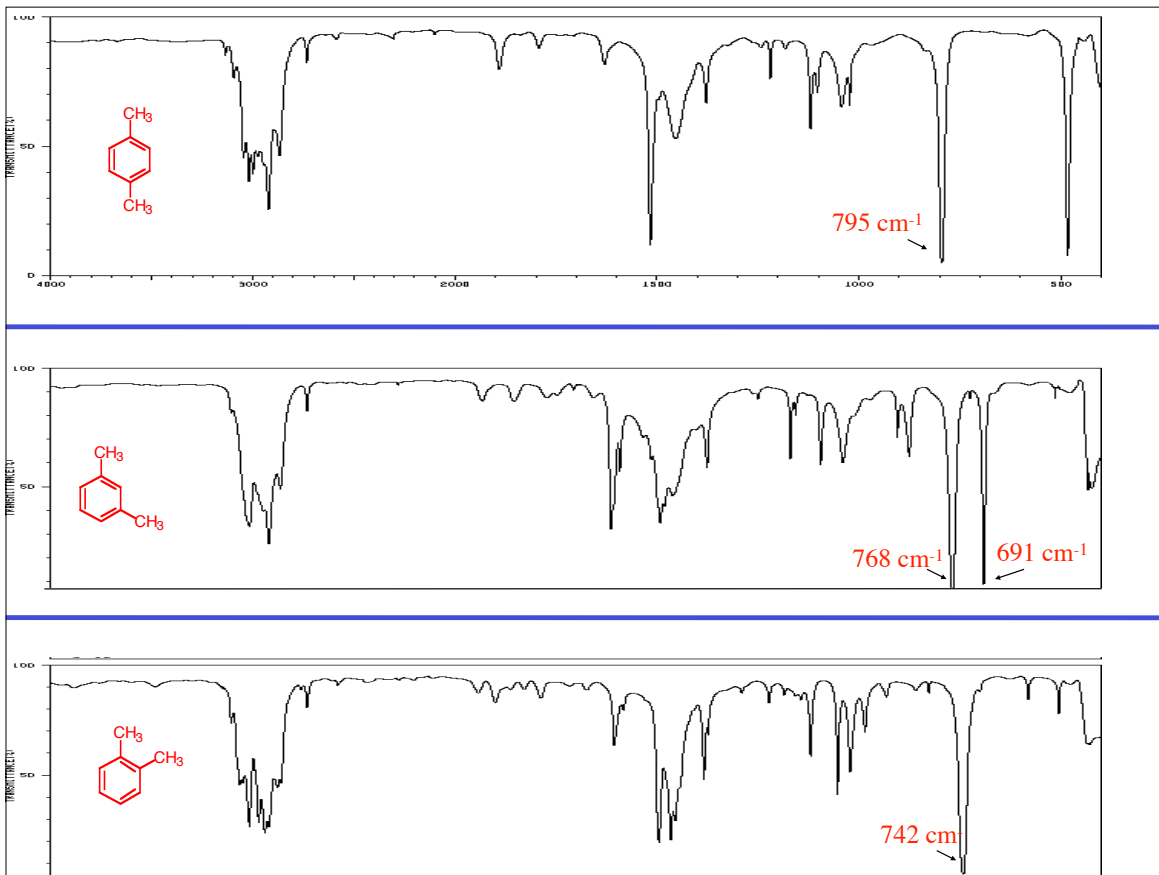


Mononuclear Aromatic Hydrocarbons (benzene)

- Out of plane bending of aromatic C-H bonds: most informative
 - 900–675 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 stretch: 3100–3000 cm^{-1}
- C=C stretch: 1600-1585; 1500-1400 cm^{-1}
- C=C out of plane ring bending: 600-420 cm^{-1}

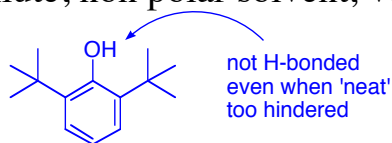
Mononuclear Aromatics



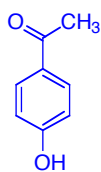


Alcohols and Phenols

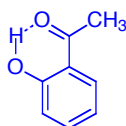
- Strongly dependent on hydrogen-bonding
 - non-hydrogen bonded OH groups absorb strongly in the 3700-3584 cm^{-1} range.
 - vapor phase; dilute, non polar solvent; very hindered



- Intermolecular hydrogen bonding occurs as conc. increases;
 - accompanied by a shift to lower freq. (3550-3200 cm^{-1}), at the expense of the free OH band
 - Pronounced for intramolecular H-bonding



3600 cm^{-1} in dilute CCl_4
3100 cm^{-1} neat



3077 cm^{-1} in dilute CCl_4
regardless of concentration

C–O stretching Vibrations

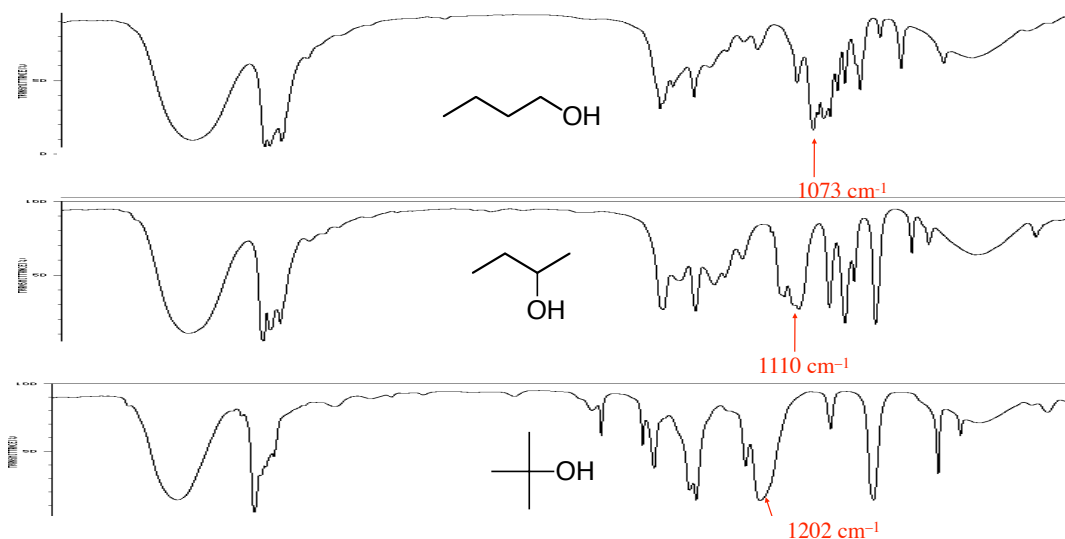
• Alcohols (1260-1000 cm^{-1})

• Phenols (1800-1260 cm^{-1})

primary alcohol: 1050-1085 cm^{-1}

secondary alcohol: 1085-1125 cm^{-1}

tertiary alcohol: 1125-1200 cm^{-1}



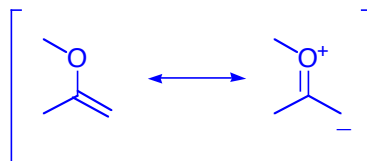
Ethers

- C–O–C stretching bands are most characteristic bands
 - strong because of strong dipole moment

aliphatic ethers: strong band due to asymmetrical stretching, 1150-1085 cm^{-1} (usually 1125 cm^{-1})
weak band due to symmetrical stretching (lower freq)

Alkyl aryl ethers: asymmetrical stretch at 1275-1200 cm^{-1}
symmetrical stretch at 1075-1020 cm^{-1}

Vinyl alkyl ethers: asymmetrical stretch at 1225-1200 cm^{-1}
symmetrical stretch at 1075-1020 cm^{-1}



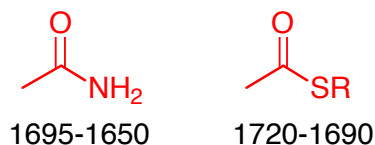
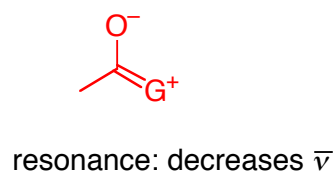
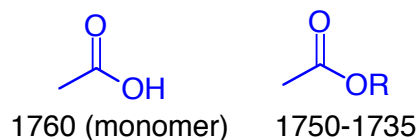
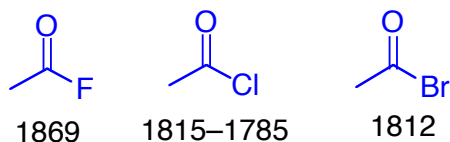
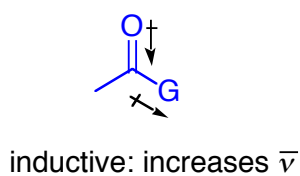
Carbonyls

C=O stretch— easily recognized, intense band

- Ketones, aldehydes, acids, esters, lactones, acid halides, anhydrides, amides and lactams all show C=O stretching in the region 1870-1540 cm^{-1} .
- Position is determined by (1) physical state (2) electronic and mass of neighboring groups (3) conjugation (4) hydrogen bonding (5) ring strain

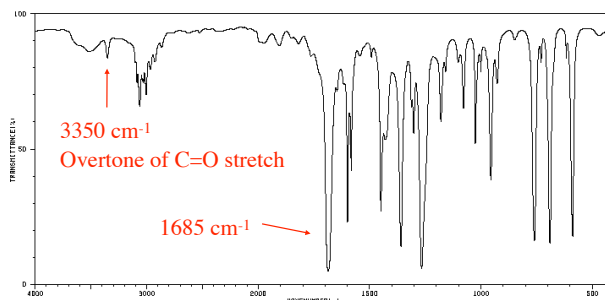
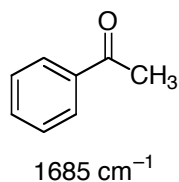
Ketones

- **aliphatic**: 'normal' position of a neat aliphatic ketone is 1715 cm^{-1}
- **competing effects**

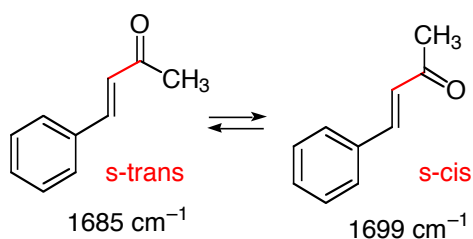


Ketones

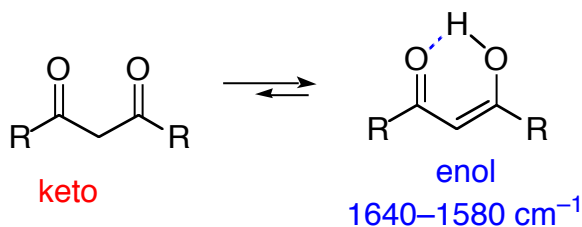
- **conjugation**: shifts position to lower frequency
alkene or phenyl group causes absorption in the 1685-1666 cm^{-1} region. For α,β -unsaturated carbonyls, 2 absorptions may be observed



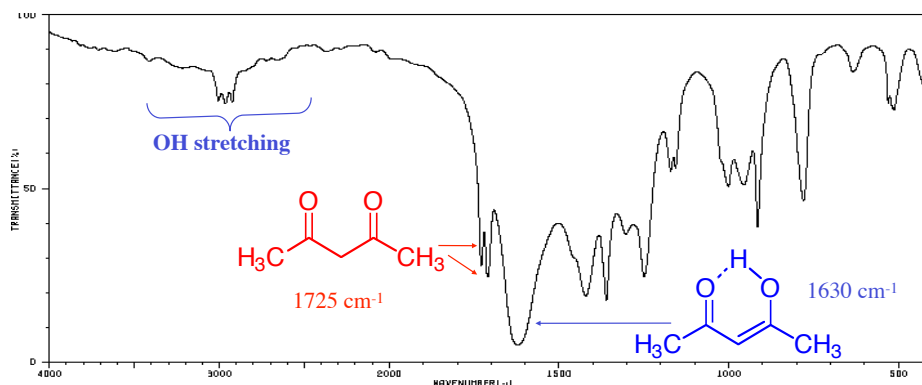
- For α,β -unsaturated carbonyls, 2 absorptions may be observed



1,3-Diketones

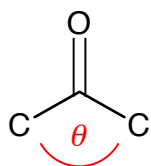


hydrogen bonding
broadens and shifts
the carbonyl absorption
to shorter $\bar{\nu}$

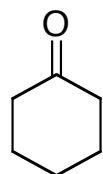


Cyclic Ketones

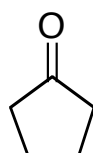
The bond angle influences the absorption frequency of the C=O



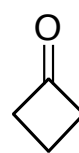
In strained rings, interaction with the adjacent C-C bonds increases the frequency of C=O stretching



1715 cm⁻¹



1751 cm⁻¹

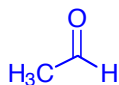


1775 cm⁻¹

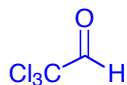
Aldehydes

C=O stretch

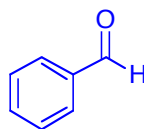
- Aliphatic aldehydes: C=O stretch at 1740-1720 cm⁻¹
- Electron withdrawing groups shift to higher frequency
- Conjugative groups shift to lower frequency (1710-1685 cm⁻¹)



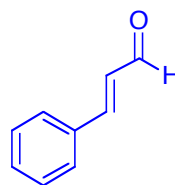
1730 cm⁻¹



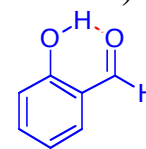
1768 cm⁻¹



1703 cm⁻¹



1678 cm⁻¹



1666 cm⁻¹

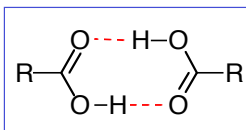
C-H stretch

2830–2695 cm⁻¹ Often, two bands are observed (the other is a result of an overtone of the C-H bend of the aldehyde)

Carboxylic Acids

OH stretch

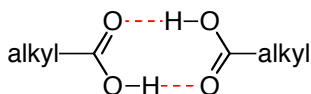
- 'free' OH (ca. 3520 cm^{-1}) is observed only in the vapor phase or in very dilute ($<0.01\text{ M}$) solution in a non-polar solvent
- Otherwise, acids exist as dimers



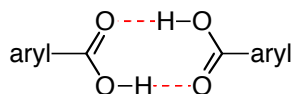
Intense, OH stretching in the $3300\text{--}2500\text{ cm}^{-1}$ region centered near 3000 cm^{-1}

C=O stretch

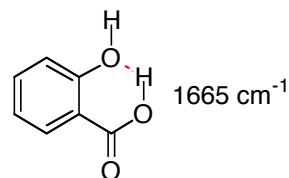
- monomer: 1760 cm^{-1} for aliphatic acids
- dimer: Hydrogen bonding reduces the frequency of the asymmetric C=O stretch, especially when intramolecular



$1720\text{--}1706\text{ cm}^{-1}$



$1710\text{--}1680\text{ cm}^{-1}$



1665 cm^{-1}

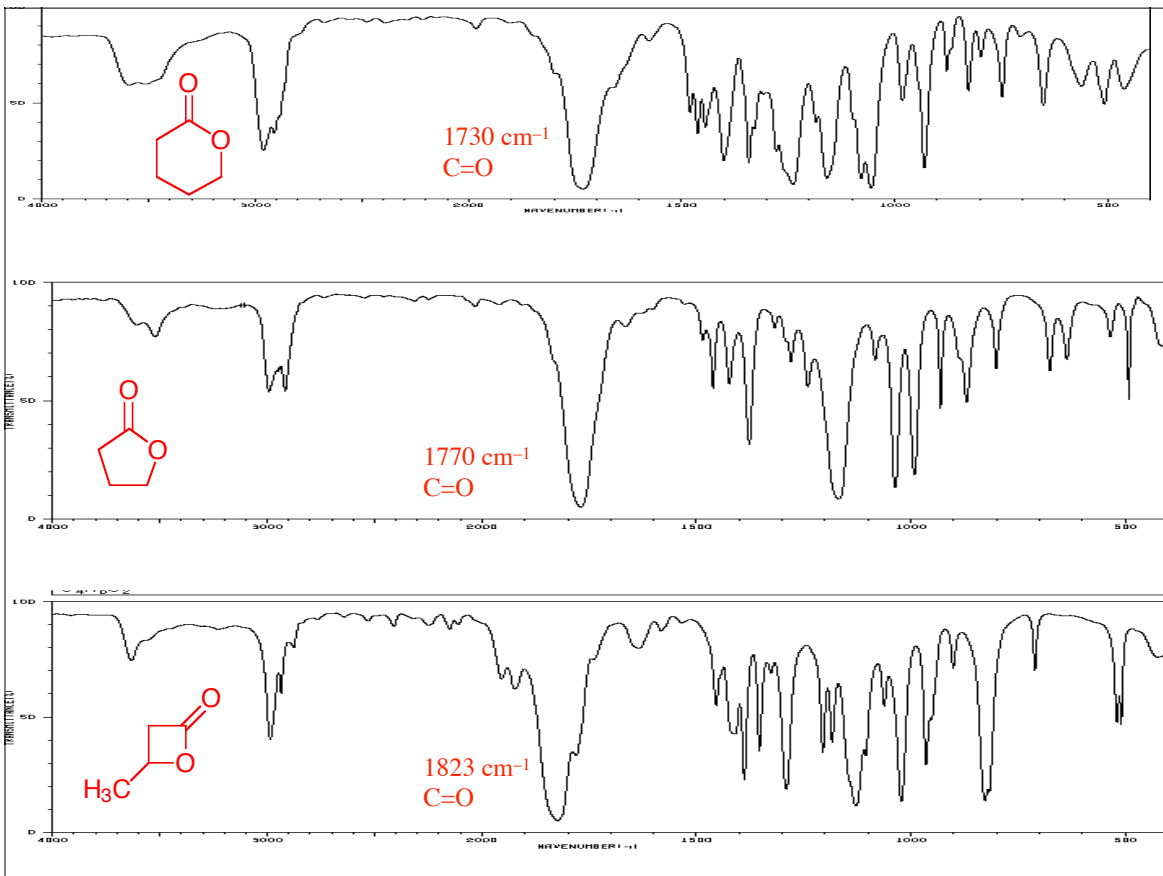
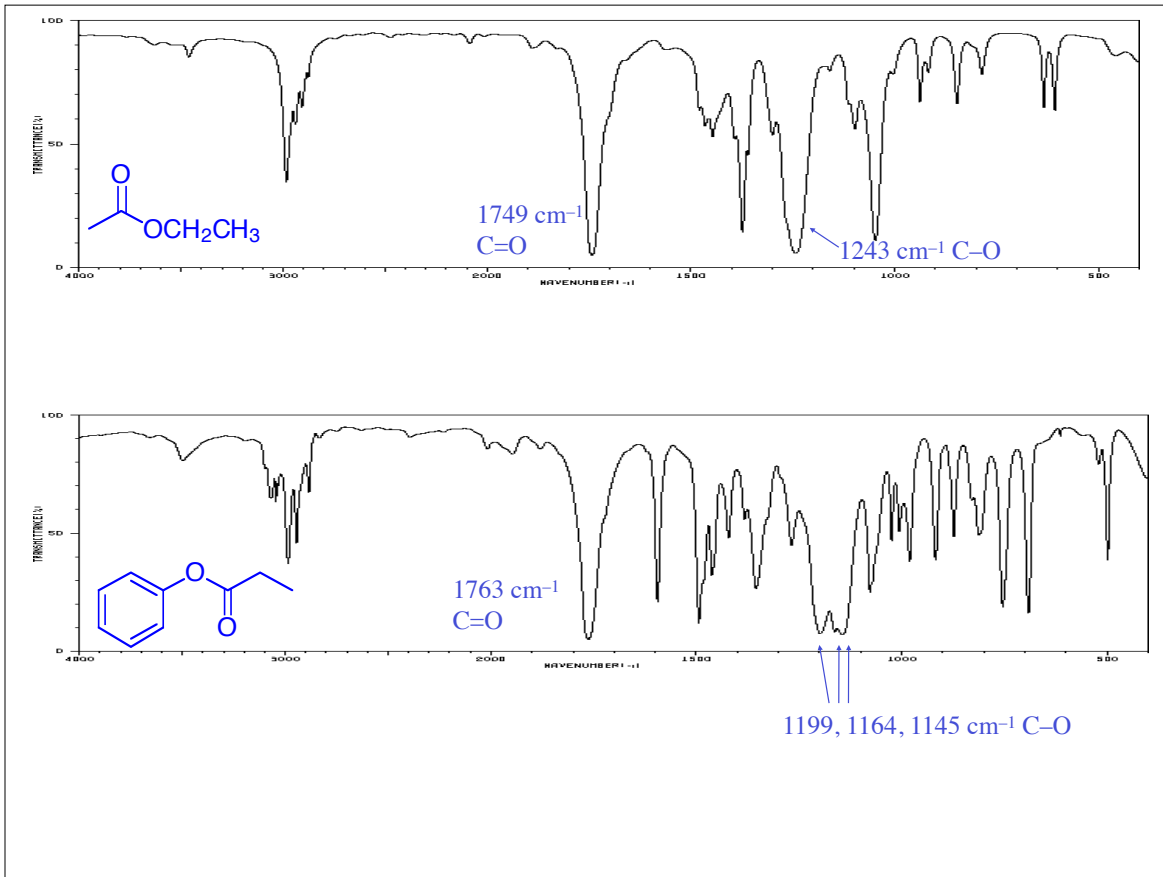
Esters

C=O stretch

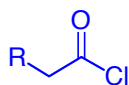
- saturated aliphatic esters: C=O: $1750\text{--}1735\text{ cm}^{-1}$
- formates, α,β -unsaturated, and benzoate esters: $1730\text{--}1715\text{ cm}^{-1}$
- phenyl or vinyl esters: $1770\text{--}1780\text{ cm}^{-1}$

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

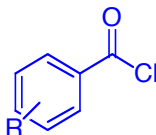
- saturated aliphatic esters (except acetates): C–O: $1210\text{--}1163\text{ cm}^{-1}$
- acetates: 1240 cm^{-1}
- α,β -unsaturated esters: $1300\text{--}1160\text{ cm}^{-1}$
- benzoate esters: $1310\text{--}1250\text{ cm}^{-1}$



Acid Halides



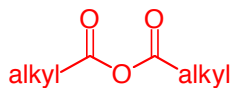
1815–1785 cm^{-1}



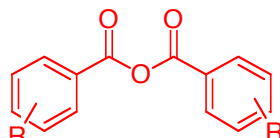
1800–1770 cm^{-1}

Anhydrides

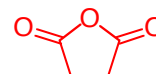
- Two carbonyl stretches (symmetrical and asymmetrical)



1818; 1750 cm^{-1}



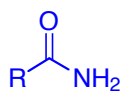
1775; 1720 cm^{-1}



1865; 1782 cm^{-1}

Amides

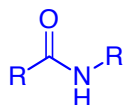
NH stretching:



Two bands

3520 (as), 3400 (s) cm^{-1} (dilute)

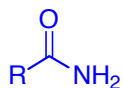
3350 (as), 3180 (s) cm^{-1} (conc)



3500–3400 cm^{-1} (dilute)

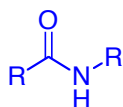
3330–3060 (s) cm^{-1} , multiple bands due to H-bonding (conc)

C=O stretching (Amide I band):



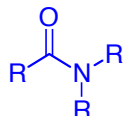
1690 cm^{-1} (dilute)

1650 cm^{-1} (conc) (except CH_3CONH_2 , which absorbs at 1694 cm^{-1})



1680–1700 cm^{-1} (dilute)

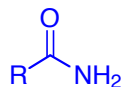
1640 cm^{-1} (conc)



1680–1630 cm^{-1} (H-bonding not possible, unless in protic solvent)

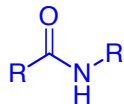
Amides

NH Bending (Amide II band):



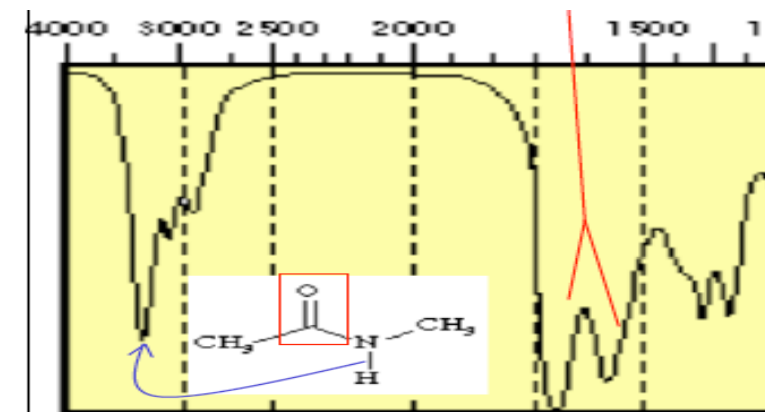
1620-1590 cm^{-1} (dilute)- separate from amide I

1655-1620 cm^{-1} (conc)- overlap with the amide I band

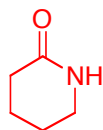


1550-1510 cm^{-1} (dilute)

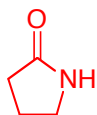
1570-1515 (s) cm^{-1} (conc)



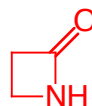
Lactams



1650 cm^{-1}

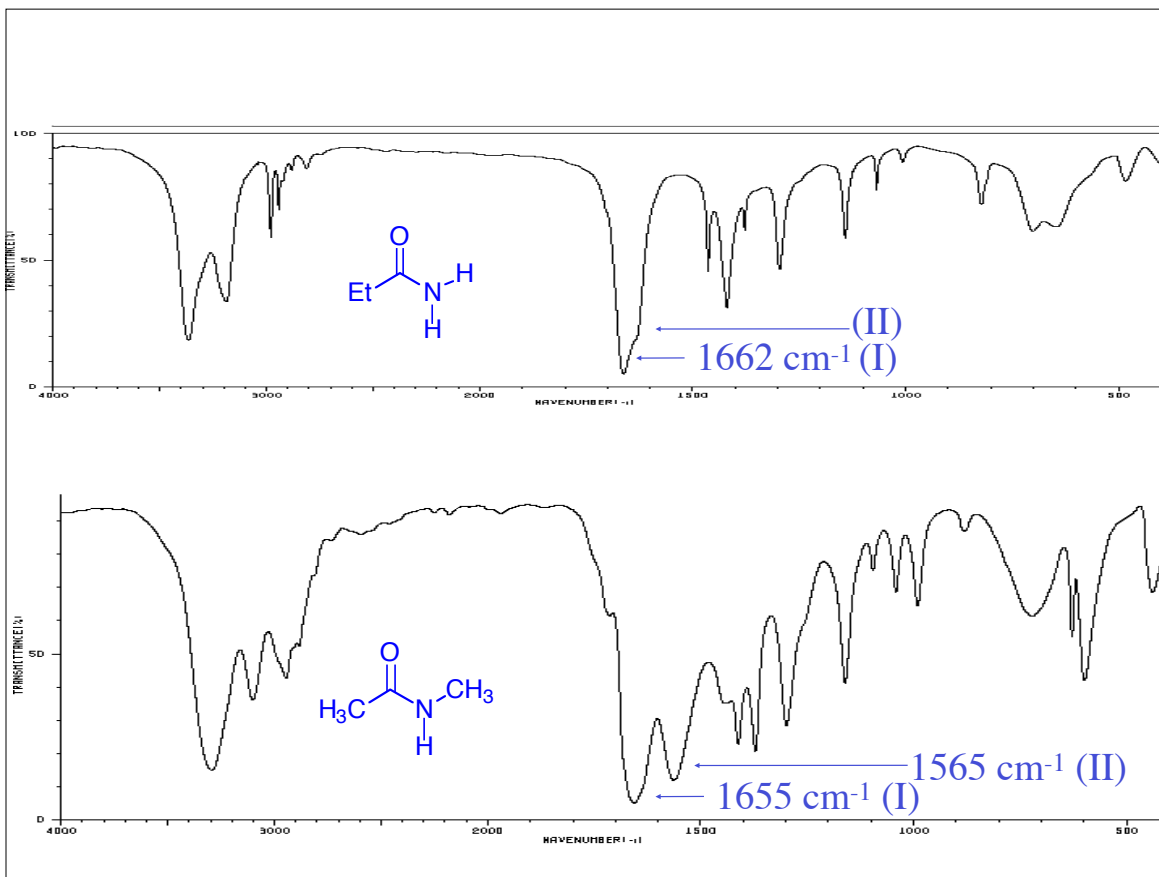


1750-1700 cm^{-1}



1760-1730 cm^{-1}

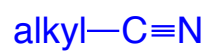
Secondary lactams do not have an NH bending band (Amide band II) near 1550 cm^{-1} . This is a characteristic of s-trans lactams.



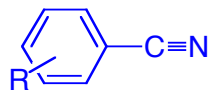
Amines

- NH stretching
 - in dilute solution, primary amines (RNH_2) display 2 bands, near 3500 and 3400 cm^{-1} . These represent 'free' asymmetrical and symmetrical stretches.
 - in dilute soln, secondary amines (R_2NH) display one band near $3350\text{-}3310\text{ cm}^{-1}$.
 - weaker and sharper than OH
 - neat primary aliphatic amines (alkylNH_2) absorb at $3400\text{-}3300$ and $3330\text{-}3250\text{ cm}^{-1}$. Aryl NH_2 absorb at slightly higher frequencies.

Nitriles



2260-2240 cm^{-1}



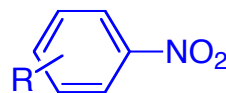
2240-2222 cm^{-1}

Nitro compounds

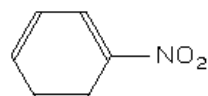
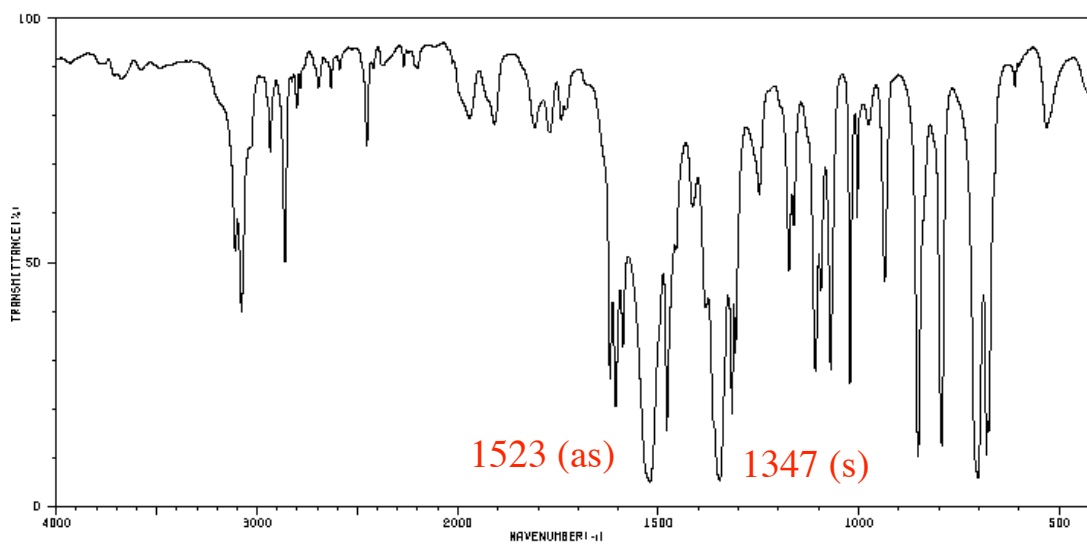
- 2 bands from the asymmetrical and symmetrical stretching of the N=O bond



1550 cm^{-1} and 1372 cm^{-1}

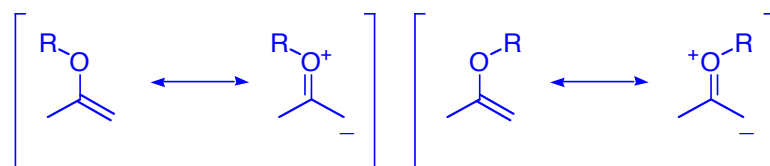


1550-1500 cm^{-1} and 1360-1290 cm^{-1}



Vinyl alkyl ethers: C=C stretch at 1660-1610 cm^{-1}

- often a doublet



trans: $\sim 1620 \text{ cm}^{-1}$

cis: $\sim 1640 \text{ cm}^{-1}$

- vinyl ethers- wagging shifted to lower frequency



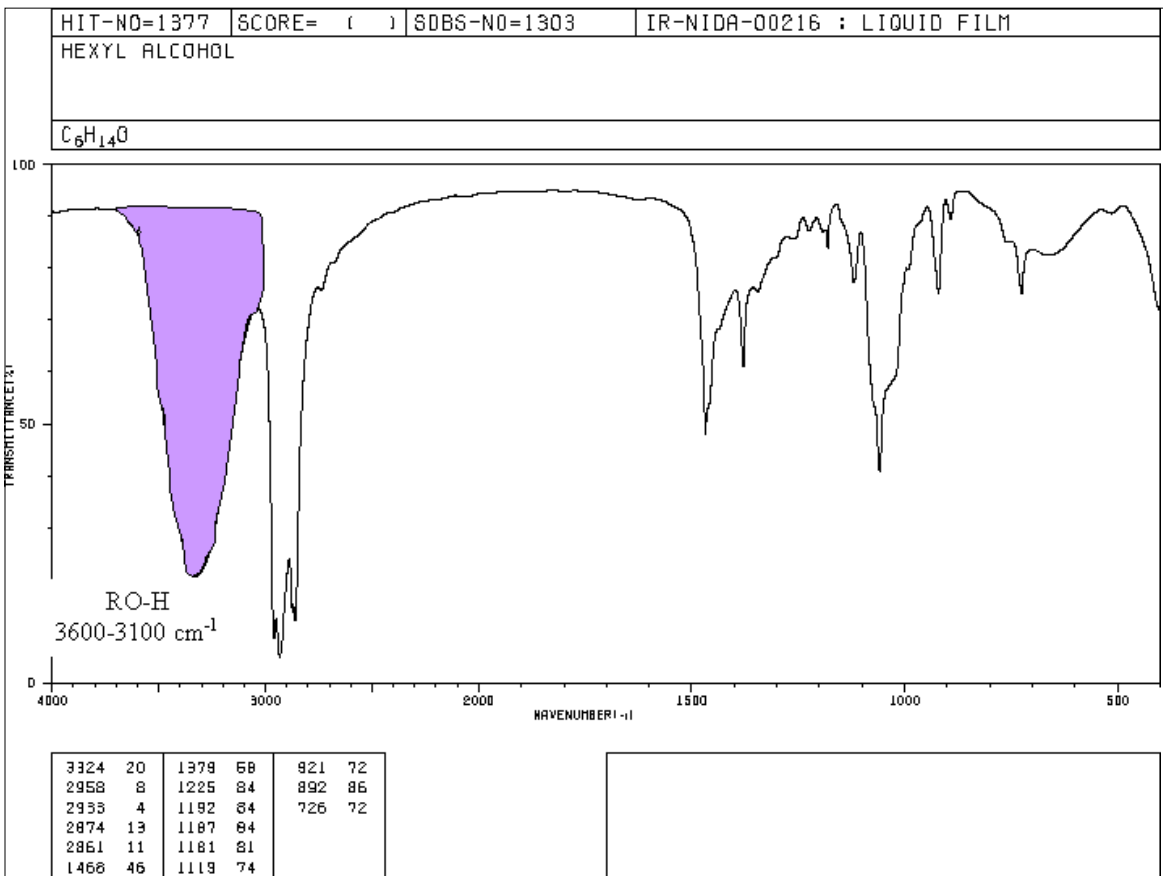
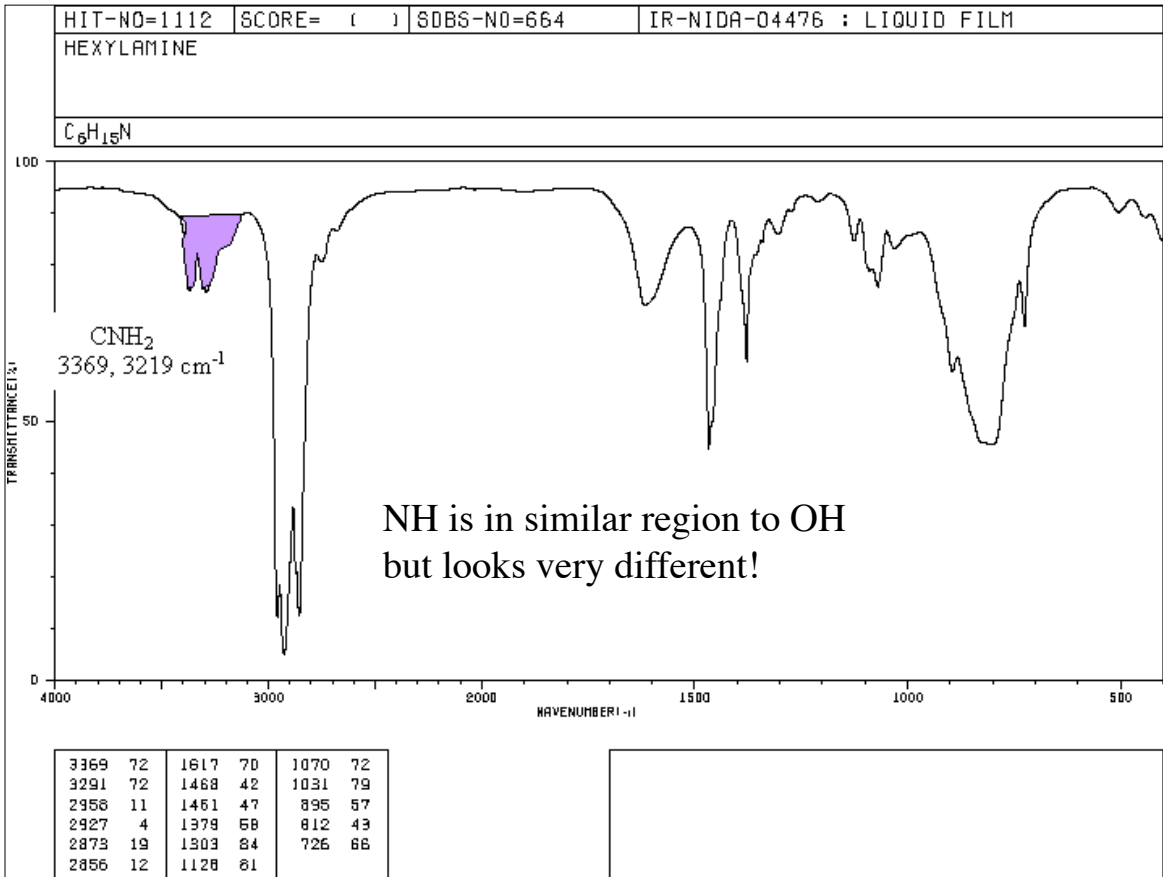
terminal wag: 813 cm^{-1}
trans CH wag: 960 cm^{-1}

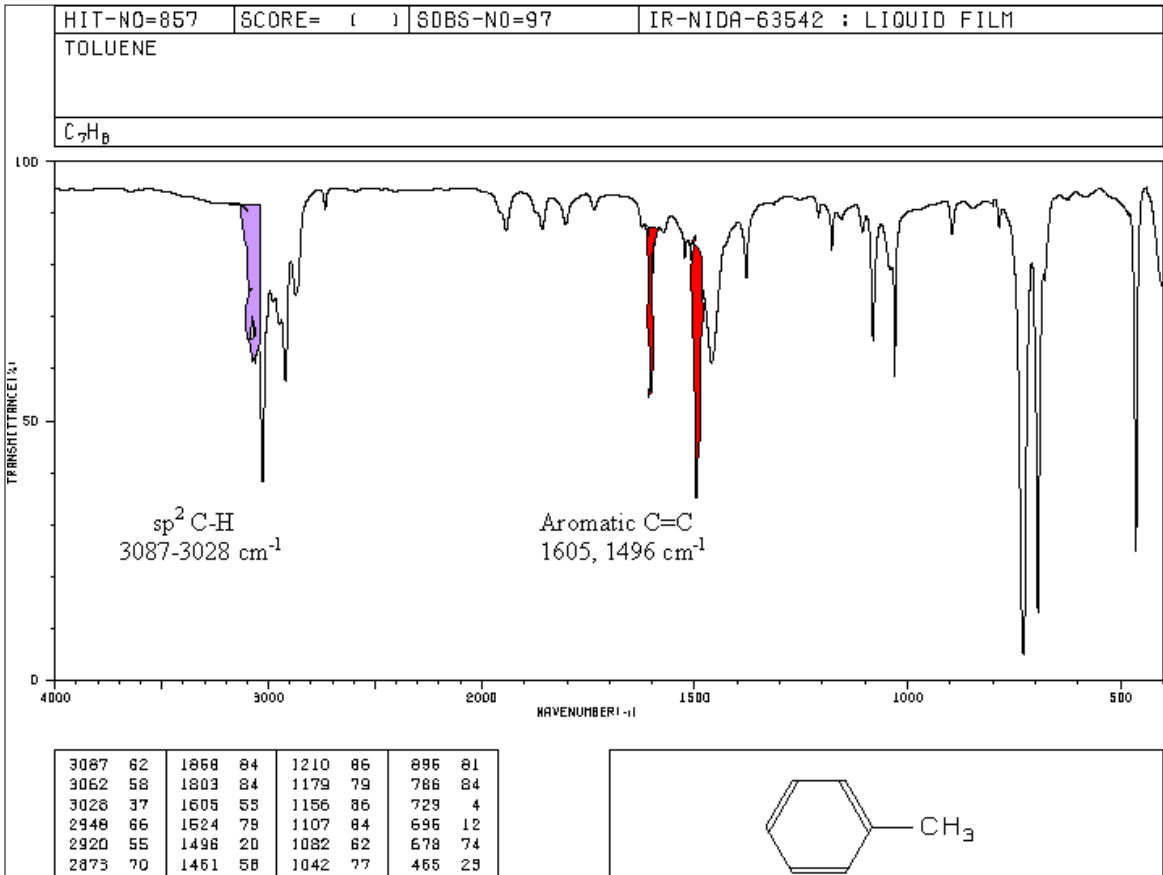
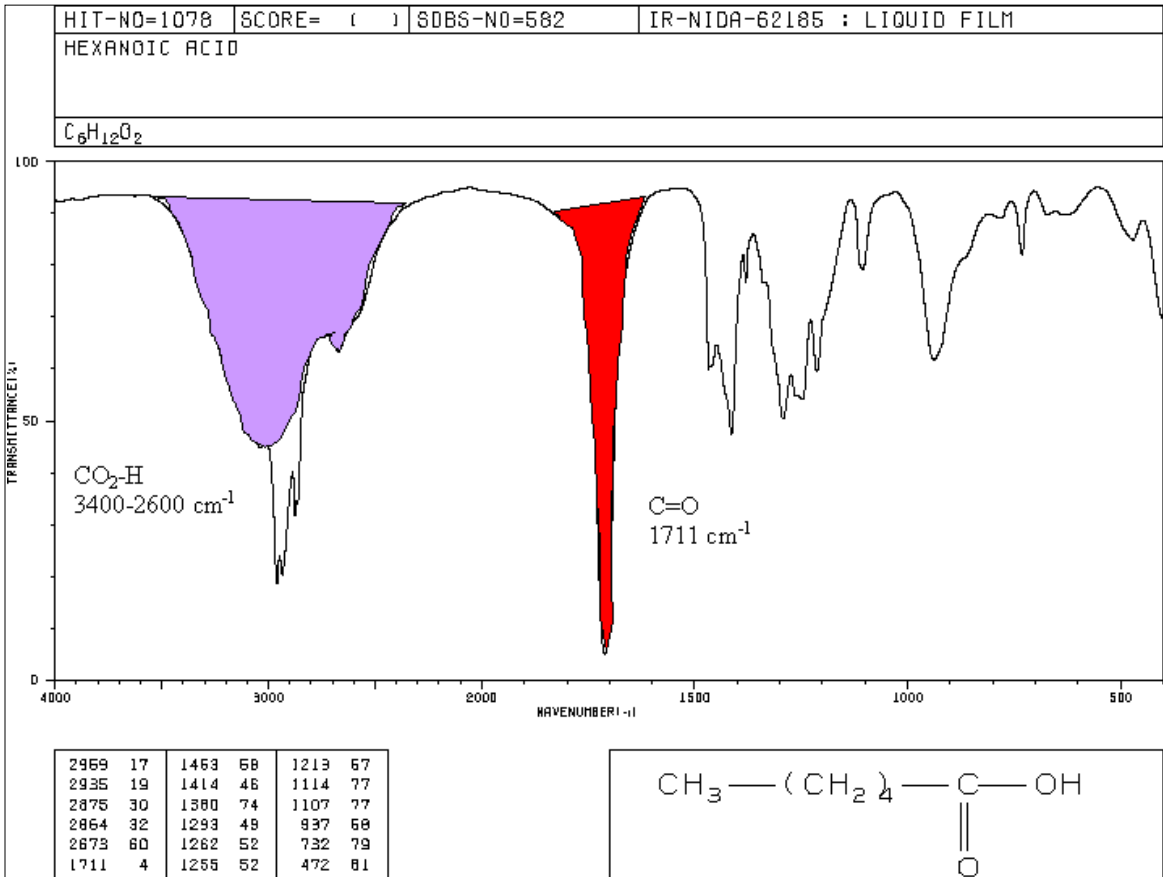


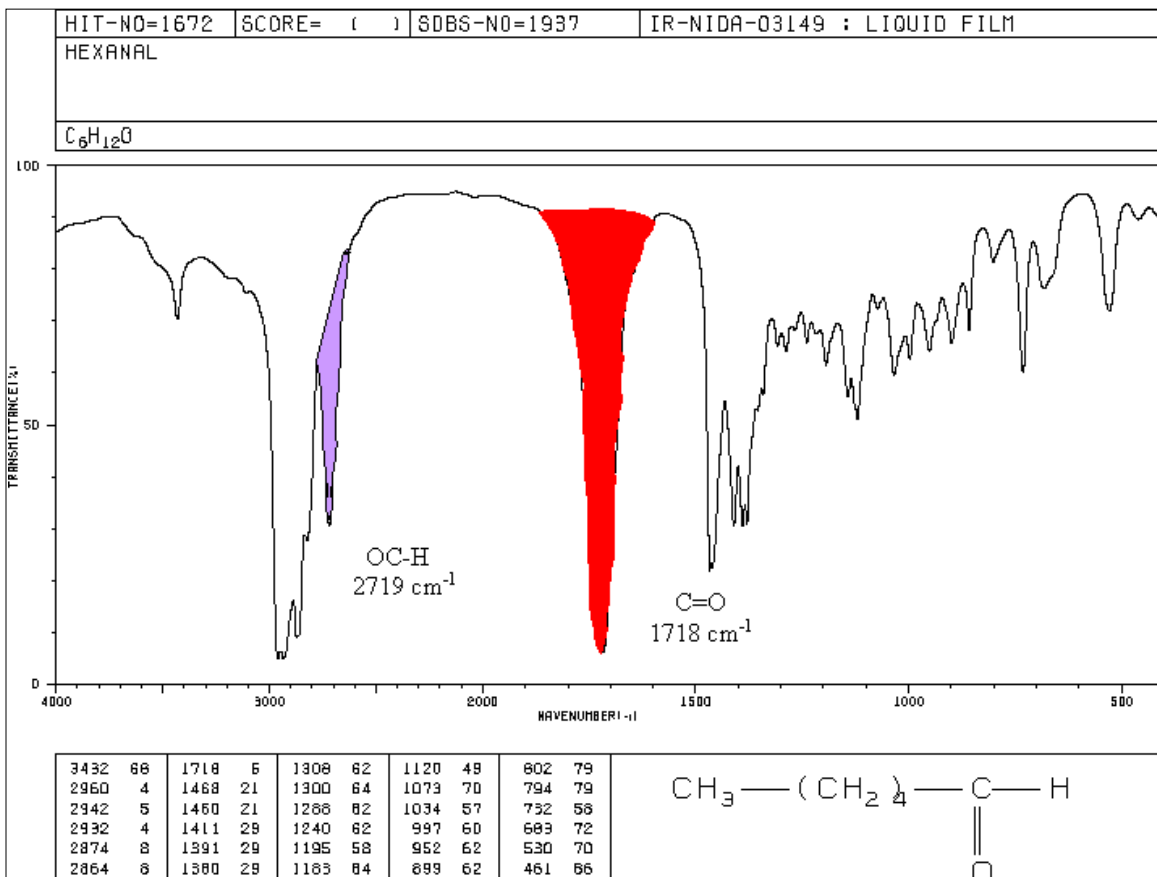
terminal wag: 909 cm^{-1}
trans CH wag: 1000 cm^{-1}

Amines

- NH stretching
 - in dilute solution, primary amines (RNH_2) display 2 bands, near 3500 and 3400 cm^{-1} . These represent 'free' asymmetrical and symmetrical stretches.
 - in dilute soln, secondary amines (R_2NH) display one band near 3350 - 3310 cm^{-1} .
 - weaker and sharper than OH
- neat primary aliphatic amines (alkylNH_2) absorb at 3400 - 3300 and 3330 - 3250 cm^{-1} . Aryl NH_2 absorb at slightly higher frequencies.



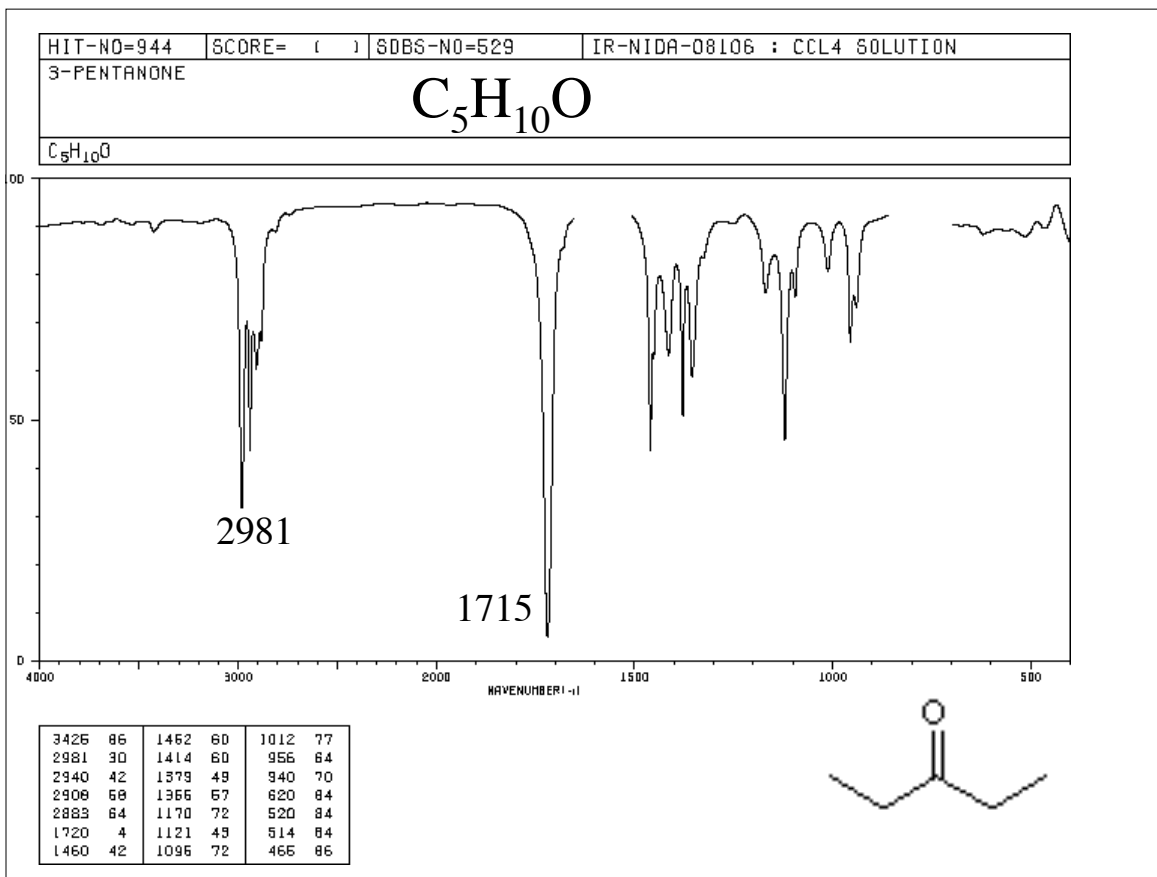




Infrared spectra: It is important to remember that the absence of an absorption band can often provide more information about the structure of a compound than the presence of a band. Be careful to avoid focusing on selected absorption bands and overlooking others. Use the examples linked to the table to see the profile and intensity of bands. Remember that the absence of a band may provide more information than the presence of an absorption band.

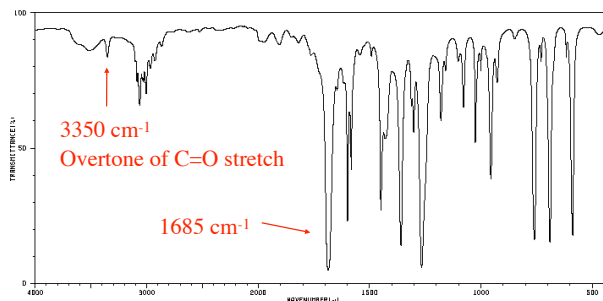
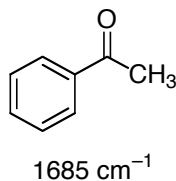
Look for absorption bands in decreasing order of importance:

1. the C-H absorption(s) between 3100 and 2850 cm⁻¹. An absorption above 3000 cm⁻¹ indicates C=C, either alkene or aromatic. Confirm the aromatic ring by finding peaks at 1600 and 1500 cm⁻¹ and C-H out-of-plane bending to give substitution patterns below 900 cm⁻¹. Confirm alkenes with an absorption generally at 1640-1680 cm⁻¹. C-H absorption between 3000 and 2850 cm⁻¹ is due to aliphatic hydrogens.
2. the carbonyl (C=O) absorption between 1690-1760cm⁻¹; this strong band indicates either an aldehyde, ketone, carboxylic acid, ester, amide, anhydride or acyl halide. The an aldehyde may be confirmed with C-H absorption from 2840 to 2720 cm⁻¹.
3. the O-H or N-H absorption between 3200 and 3600 cm⁻¹. This indicates either an alcohol, N-H containing amine or amide, or carboxylic acid. For -NH₂ a doublet will be observed.
4. the C-O absorption between 1080 and 1300 cm⁻¹. These peaks are normally rounded like the O-H and N-H peak in 3. and are prominent. Carboxylic acids, esters, ethers, alcohols and anhydrides all containing this peak.
5. the CC and CN triple bond absorptions at 2100-2260 cm⁻¹ are small but exposed.
6. a methyl group may be identified with C-H absorption at 1380 cm⁻¹. This band is split into a doublet for isopropyl(gem-dimethyl) groups.
7. structure of aromatic compounds may also be confirmed from the pattern of the weak overtone and combination tone bands found from 2000 to 1600 cm⁻¹.

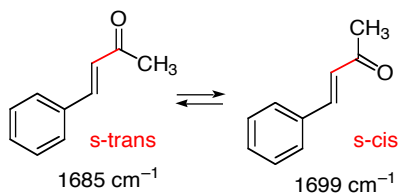


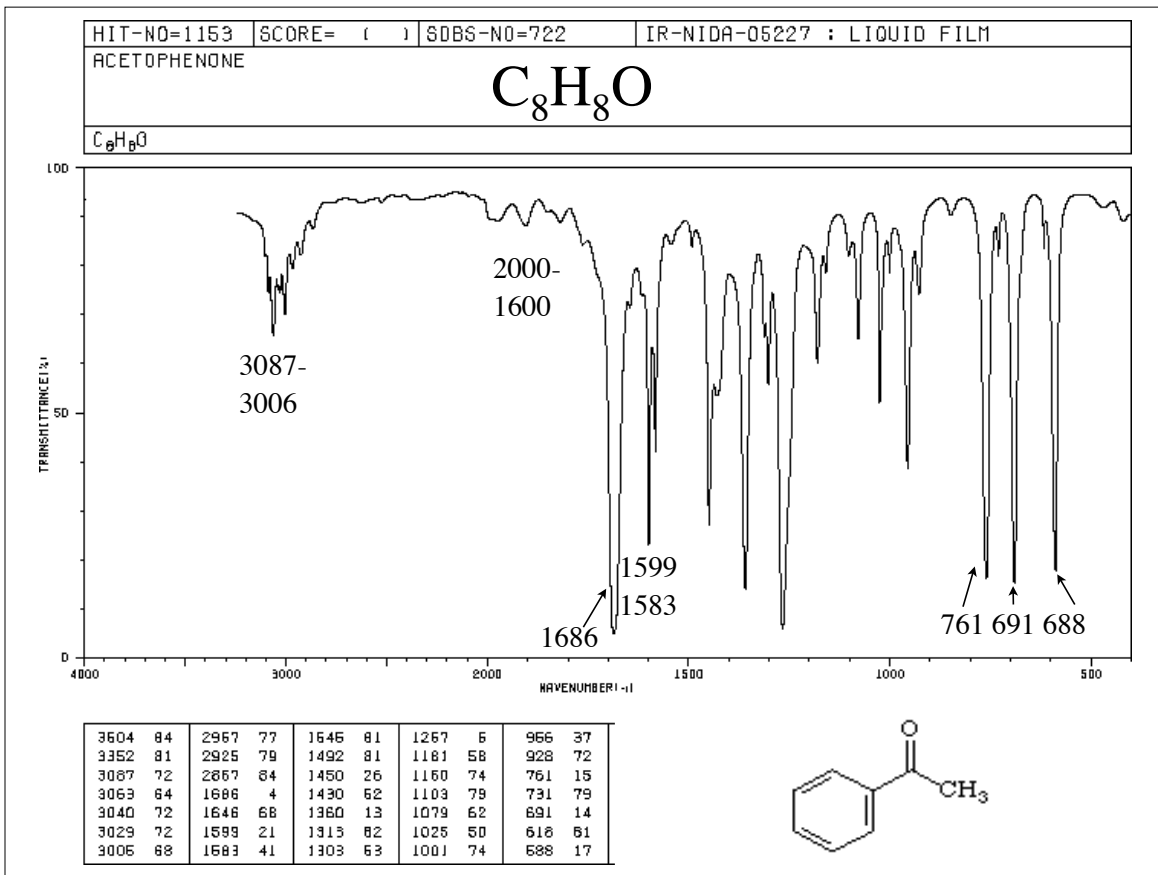
Ketones

- **aliphatic**: 'normal' position of a neat aliphatic ketone is 1715 cm^{-1}
- **conjugation**: shifts position to lower frequency
alkene or phenyl group causes absorption in the $1685\text{-}1666\text{ cm}^{-1}$ region. For α,β -unsaturated carbonyls, 2 absorptions may be observed



- For α,β -unsaturated carbonyls, 2 absorptions may be observed

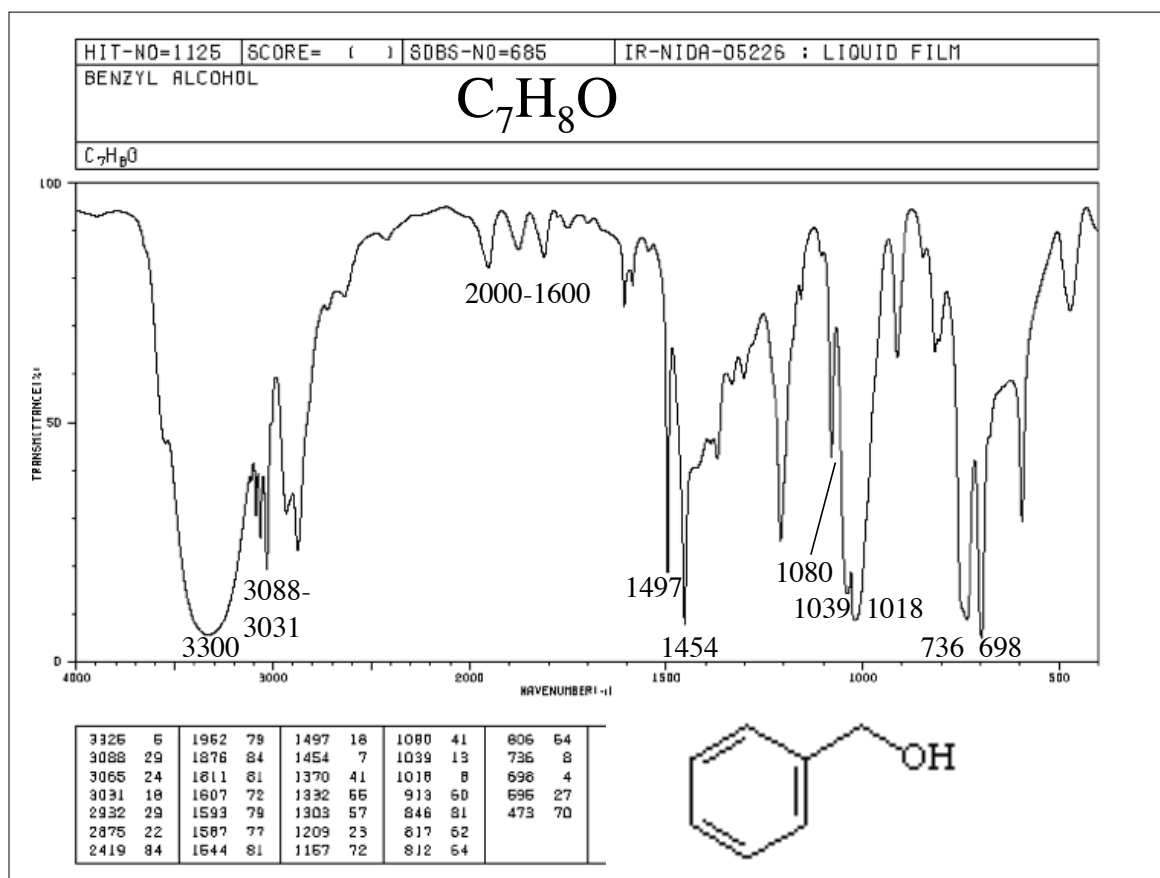
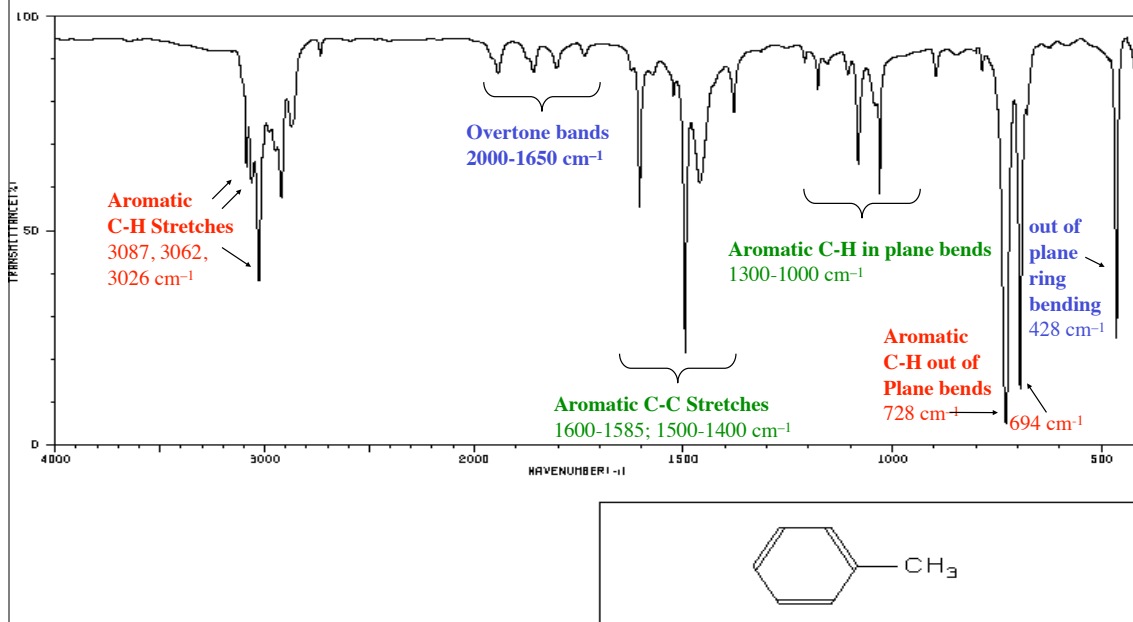




Mononuclear Aromatic Hydrocarbons (benzene)

- Out of plane bending of aromatic C-H bonds: most informative
 - 900–675 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 cm^{-1}
- **C=C** stretch: 1600-1585; 1500-1400 cm^{-1}
- **C=C** out of plane ring bending: 600-420 cm^{-1}

Mononuclear Aromatics



Alcohols and Phenols

- Strongly dependent on hydrogen-bonding
 - non-hydrogen bonded OH groups absorb strongly in the 3700-3584 cm^{-1} range.
 - vapor phase; dilute, non polar solvent; very hindered
- Intermolecular hydrogen bonding occurs as conc. increases;
 - accompanied by a shift to lower freq. (3550-3200 cm^{-1}), at the expense of the free OH band
 - typically at 3300 cm^{-1}
 - Pronounced for intramolecular H-bonding

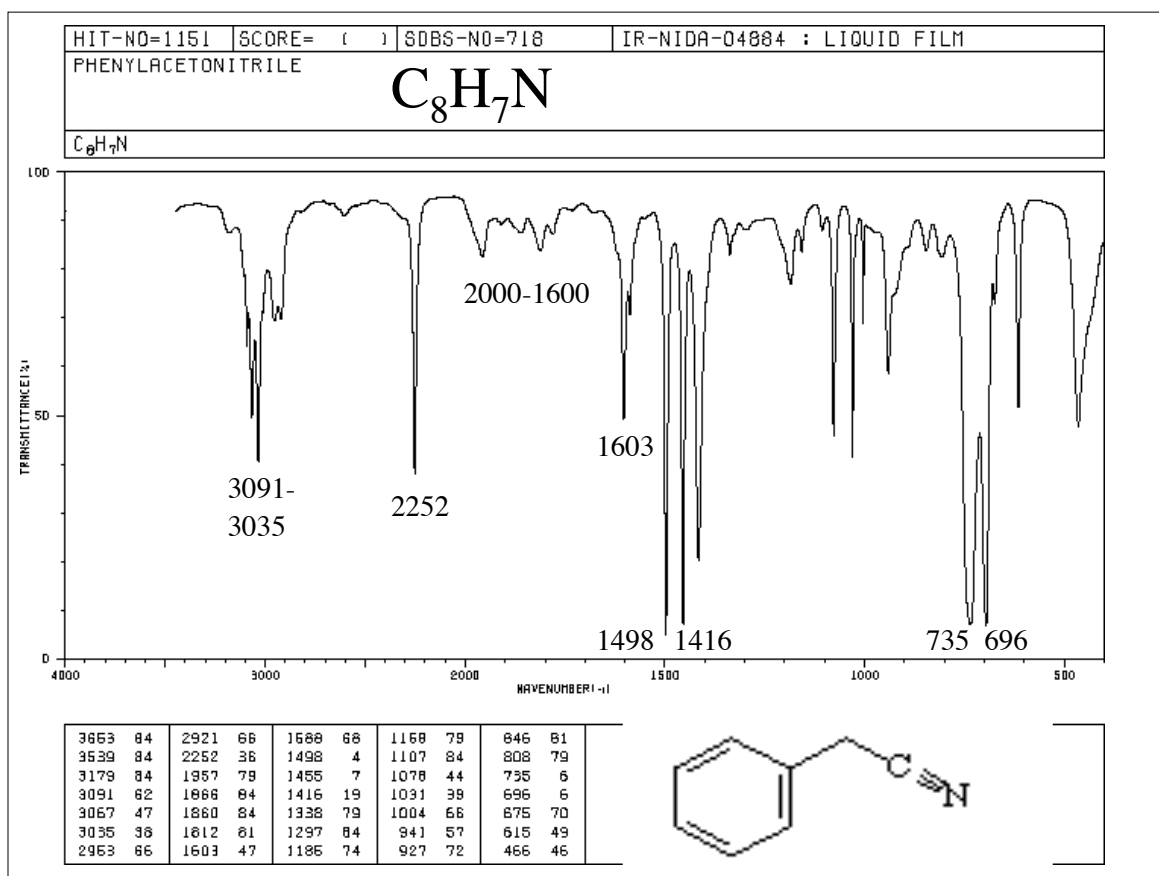
C–O stretching Vibrations

- Alcohols (1260-1000 cm^{-1})
- Phenols (1800-1260 cm^{-1})

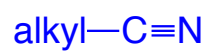
primary alcohol: 1050-1085 cm^{-1}

secondary alcohol: 1085-1125 cm^{-1}

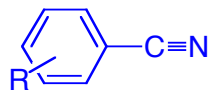
tertiary alcohol: 1125-1200 cm^{-1}



Nitriles

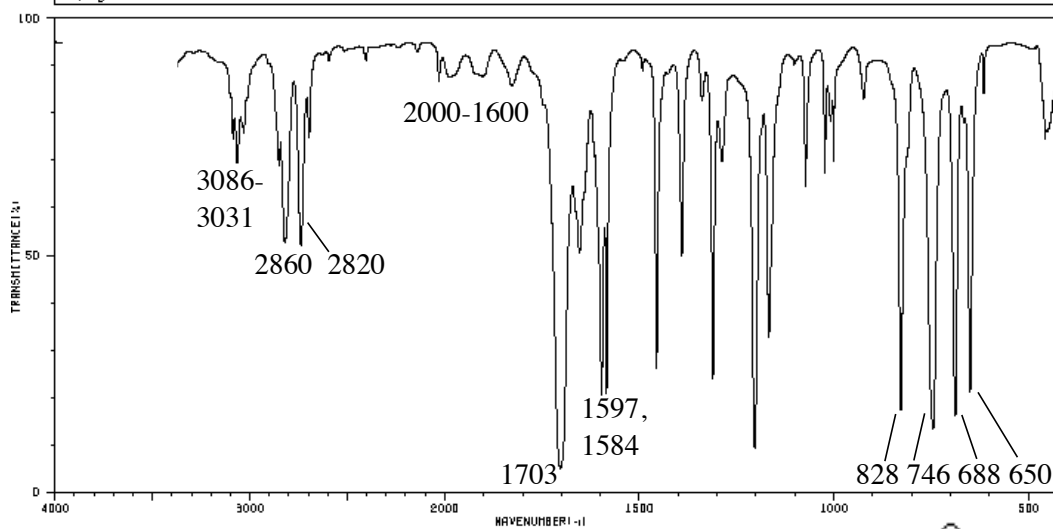


2260-2240 cm^{-1}

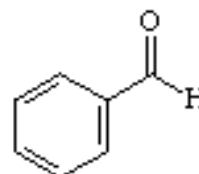


2240-2222 cm^{-1}

HIT-NO=1117	SCORE= ()	SDBS-NO=672	IR-NIDA-05223 ; LIQUID FILM
BENZALDEHYDE			
C₇H₆O			
C ₇ H ₆ O			

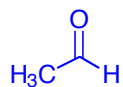


3086	72	1981	84	1597	20	1204	8	628	16
3065	66	1916	84	1584	20	1168	31	746	13
3031	72	1909	84	1456	25	1073	62	688	15
2850	66	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	66	615	61
2696	72	1664	49	1288	68	924	79	467	72

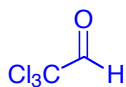


Aldehydes

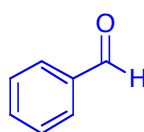
C=O stretch



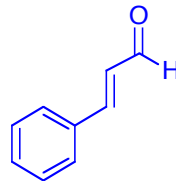
1730 cm^{-1}



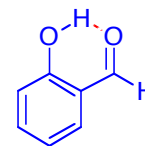
1768 cm^{-1}



1703 cm^{-1}



1678 cm^{-1}



1666 cm^{-1}

C-H stretch

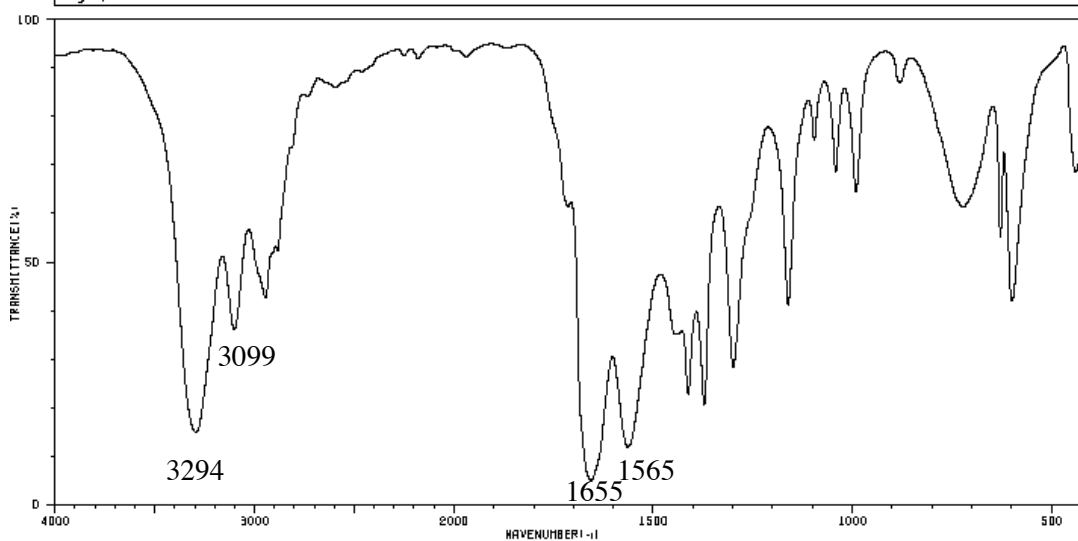
2830–2695 cm^{-1} Often, two bands are observed (the other is a result of an overtone of the C-H bend of the aldehyde)

HIT-NO=2452 SCORE= () SDBS-NO=4002 IR-NIDA-63942 : LIQUID FILM

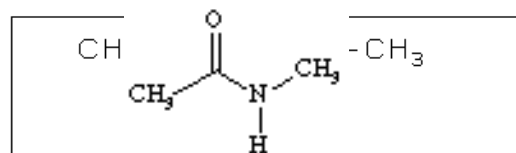
N-METHYLACETAMIDE

C₃H₇NO

C₃H₇NO

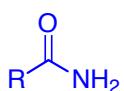


3294	14	1372	20	721	68
3099	35	1299	26	629	53
2946	41	1161	39	599	41
2697	84	1098	72	440	66
1655	4	1042	66		
1563	11	991	62		
1412	21	881	84		



Amides

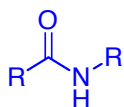
NH stretching:



Two bands

3520 (as), 3400 (s) cm^{-1} (dilute)

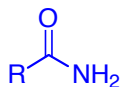
3350 (as), 3180 (s) cm^{-1} (conc)



3500–3400 cm^{-1} (dilute)

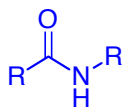
3330–3060 (s) cm^{-1} , multiple bands due to H-bonding (conc)

C=O stretching
(Amide I band):



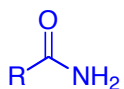
1690 cm^{-1} (dilute)

1650 cm^{-1} (conc) (except CH_3CONH_2 , which absorbs at 1694 cm^{-1})



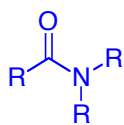
1680–1700 cm^{-1} (dilute)

1640 cm^{-1} (conc)



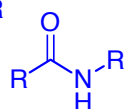
1680–1630 cm^{-1} (H-bonding not possible, unless in protic solvent)

NH Bending
(Amide II band):



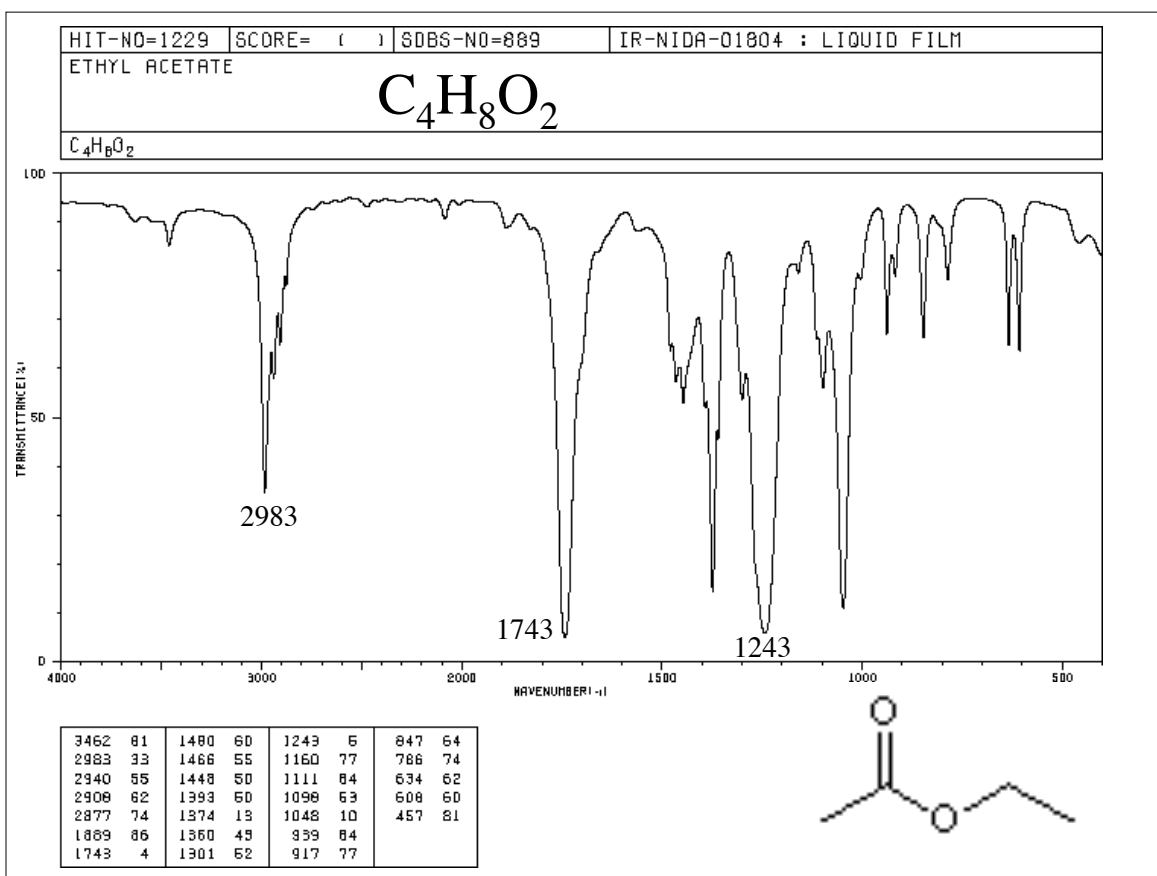
1620–1590 cm^{-1} (dilute)- separate from amide I

1655–1620 cm^{-1} (conc)- overlap with the amide I band



1550–1510 cm^{-1} (dilute)

1570–1515 (s) cm^{-1} (conc)



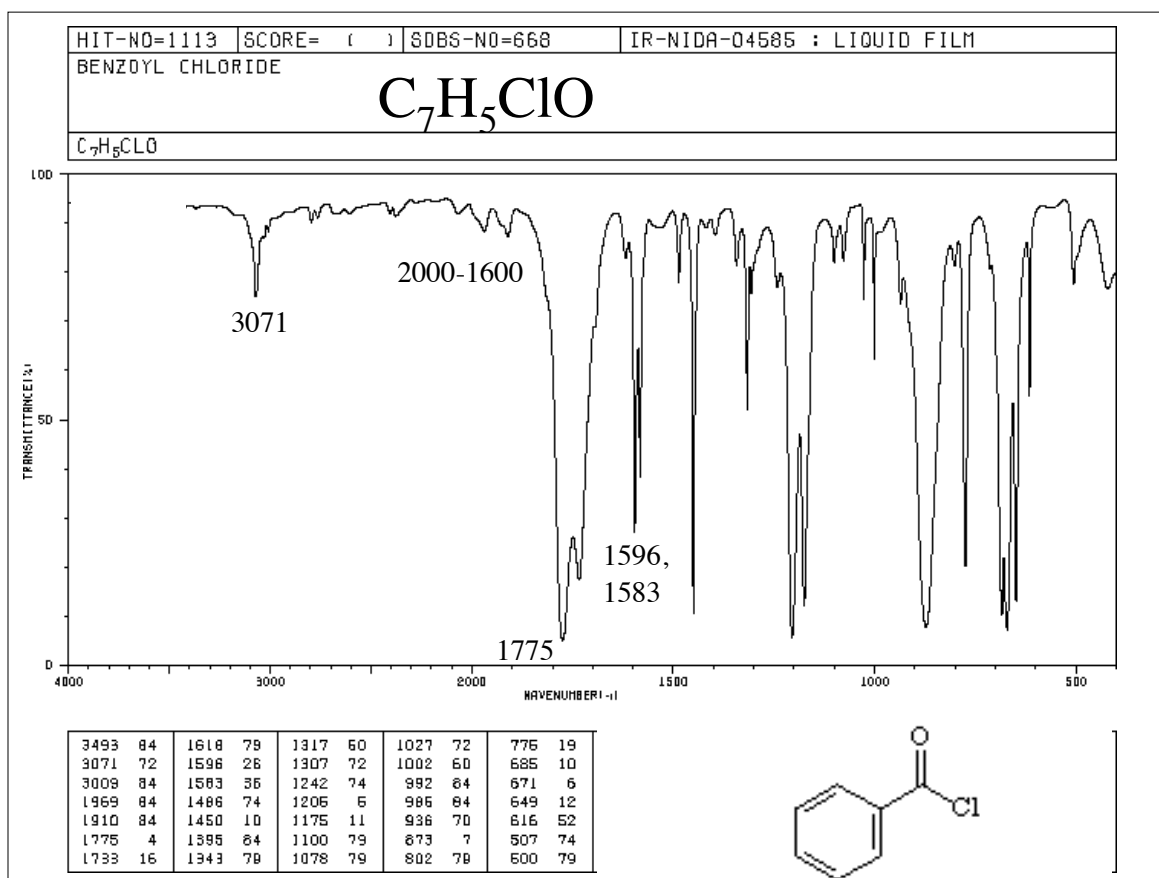
Esters

C=O stretch

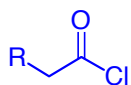
- saturated aliphatic esters: C=O: 1750–1735 cm^{-1}
- formates, α,β -unsaturated, and benzoate esters: 1730–1715 cm^{-1}
- phenyl or vinyl esters: 1770–1780 cm^{-1}

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

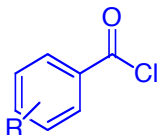
- saturated aliphatic esters (except acetates): C–O: 1210–1163 cm^{-1}
- acetates: 1240 cm^{-1}
- α,β -unsaturated esters: 1300–1160 cm^{-1}
- benzoate esters: 1310–1250 cm^{-1}



Acid Halides



1815–1785 cm^{-1}



1800–1770 cm^{-1}

$\text{C}_{12}\text{H}_{22}\text{O}_2$

IR: 2926, 2856, 1728, 1645, 1436, 1197, 1175, 819 cm^{-1}

^{13}C NMR

166.5, s 29.0, t

150.7, d 28.9, t

119.0, d 28.8, t

50.6, q 22.5, t

31.7, t 13.9, q

29.3, t

29.1, t

^1H NMR

6.14, dt, 1H, $J = 7.5, 11.5$ Hz

5.68, d, 1H, $J = 11.5$ Hz

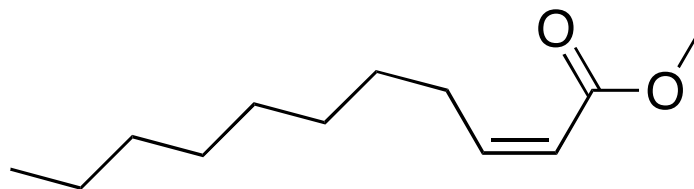
3.61, s, 3H

2.57, dt, 2H, $J = 7.5, 7.4$ Hz

1.35, m, 2H

1.18, m, 10H

0.80, m, 3H



$C_7H_{12}O_2$

IR: 2980, 2890, 1775, 1470, 1370, 1350, 1190, 1020, 980, 925 cm^{-1}

^{13}C NMR

13.1, q

17.9, t

27.3, t

28.1, t

36.9, t

80.1, d

176.6, s

1H NMR

0.96, t, $J = 6.8$, 3H

1.4-1.9, m, 6H

2.4-2.6, m, 2H

4.5, m, 1H

