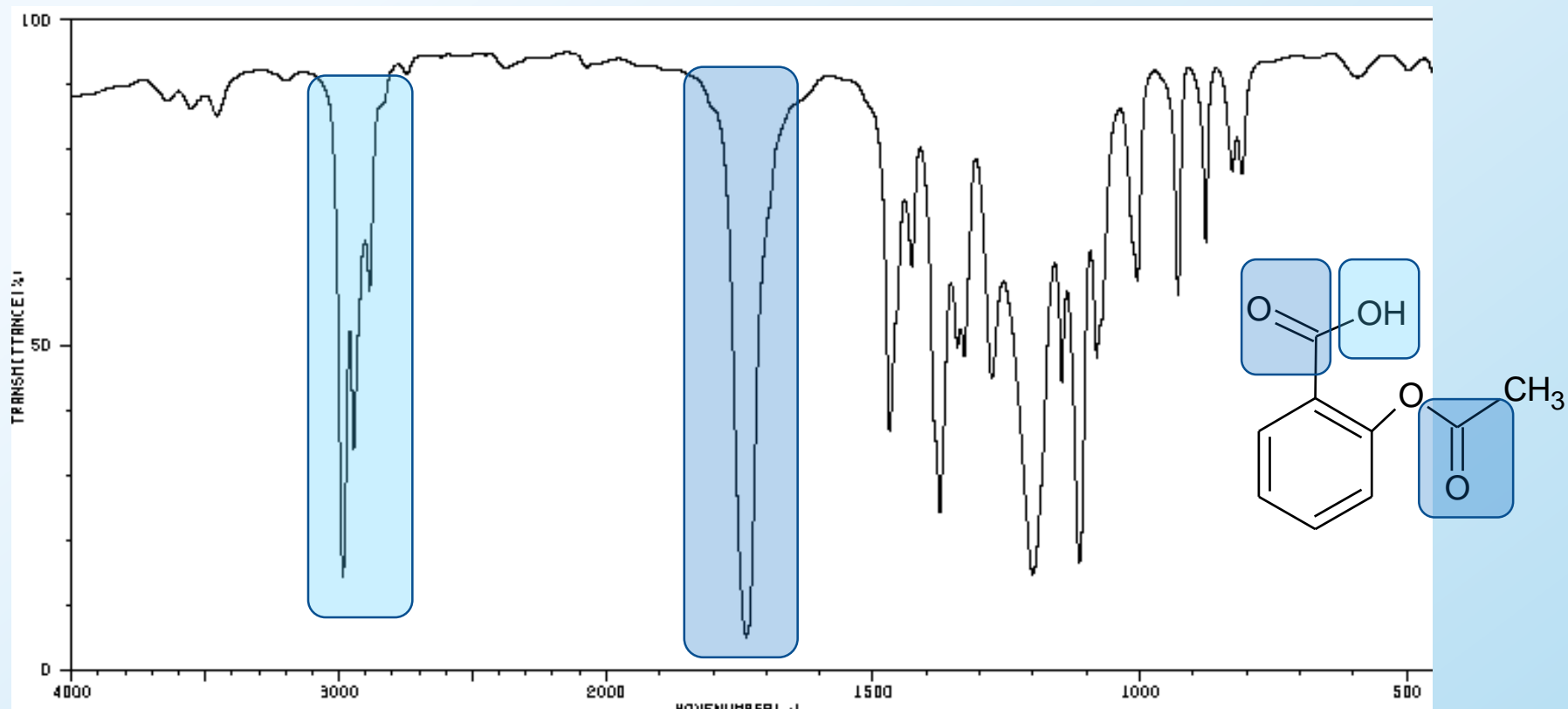


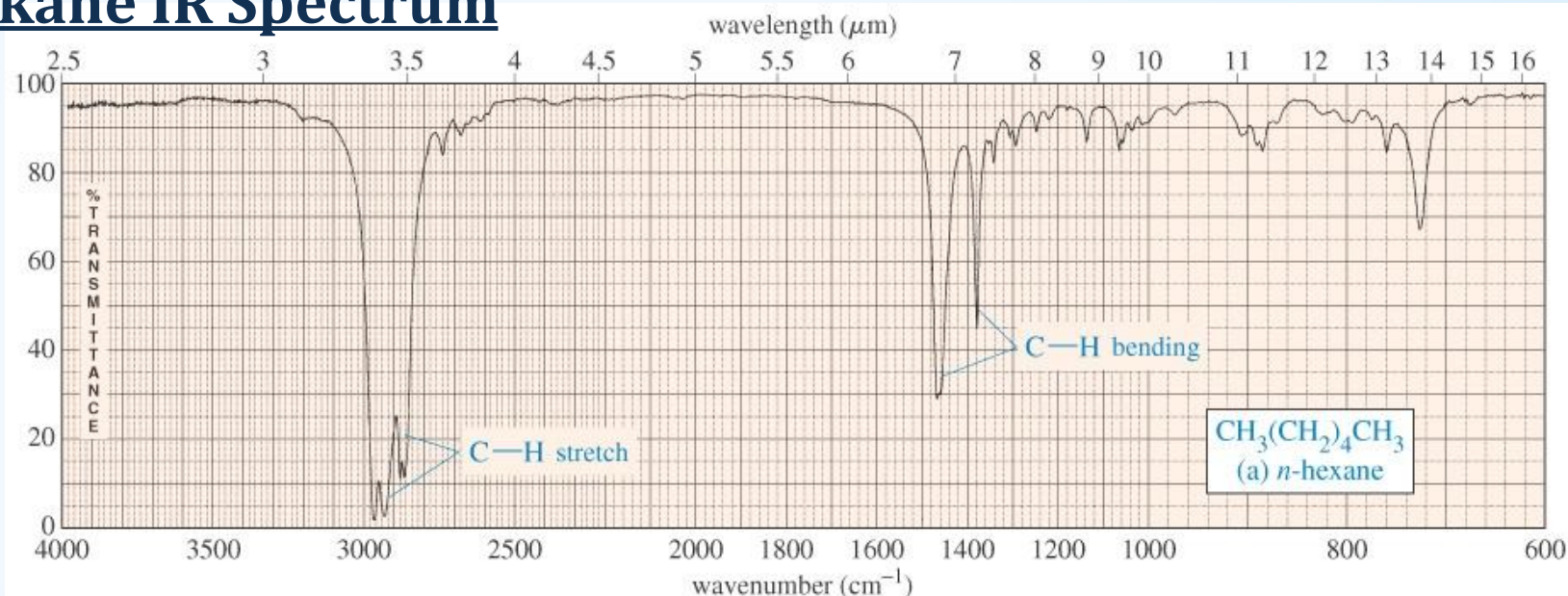
# IR – Functional Groups

Sapna Gupta

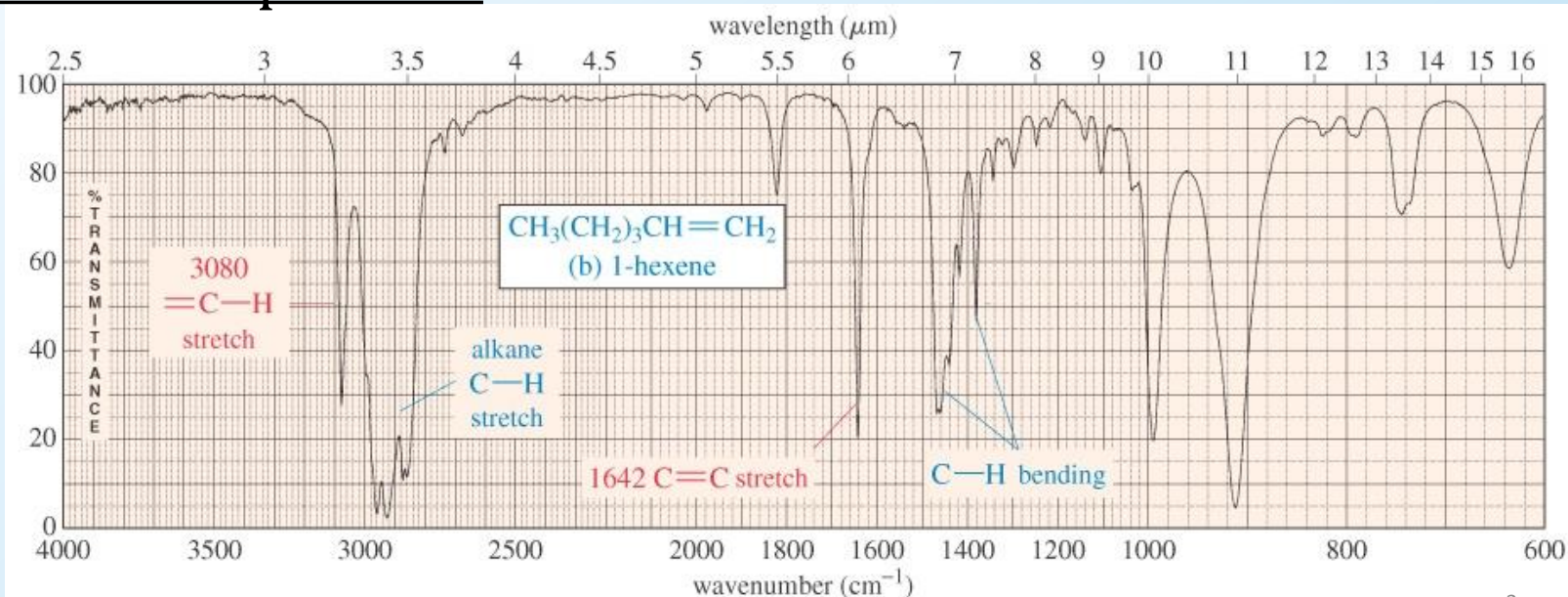
# IR Spectrum of Aspirin



## An Alkane IR Spectrum

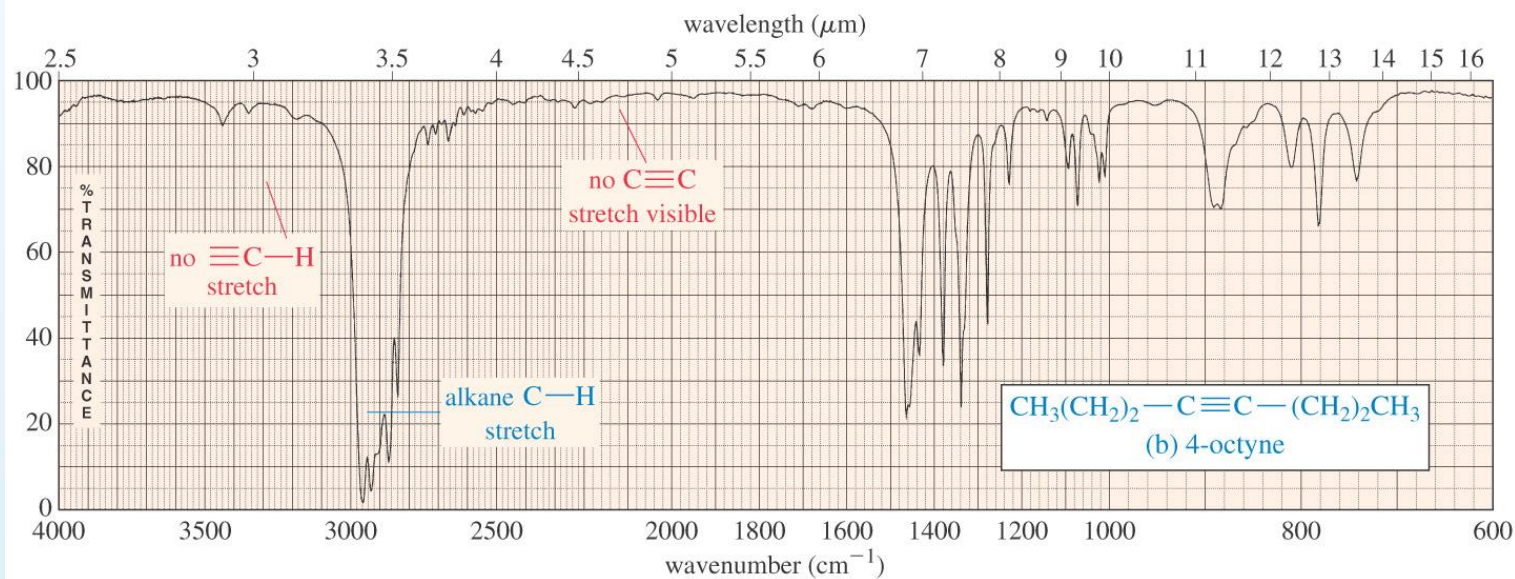
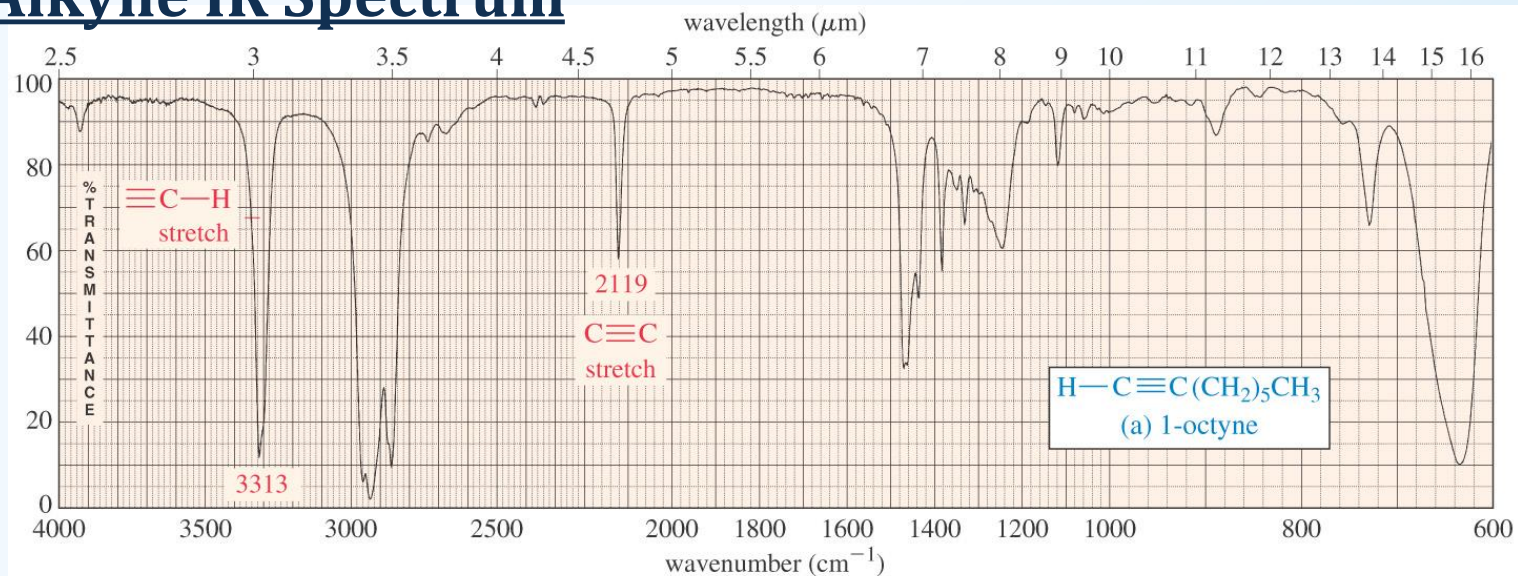


## An Alkene IR Spectrum





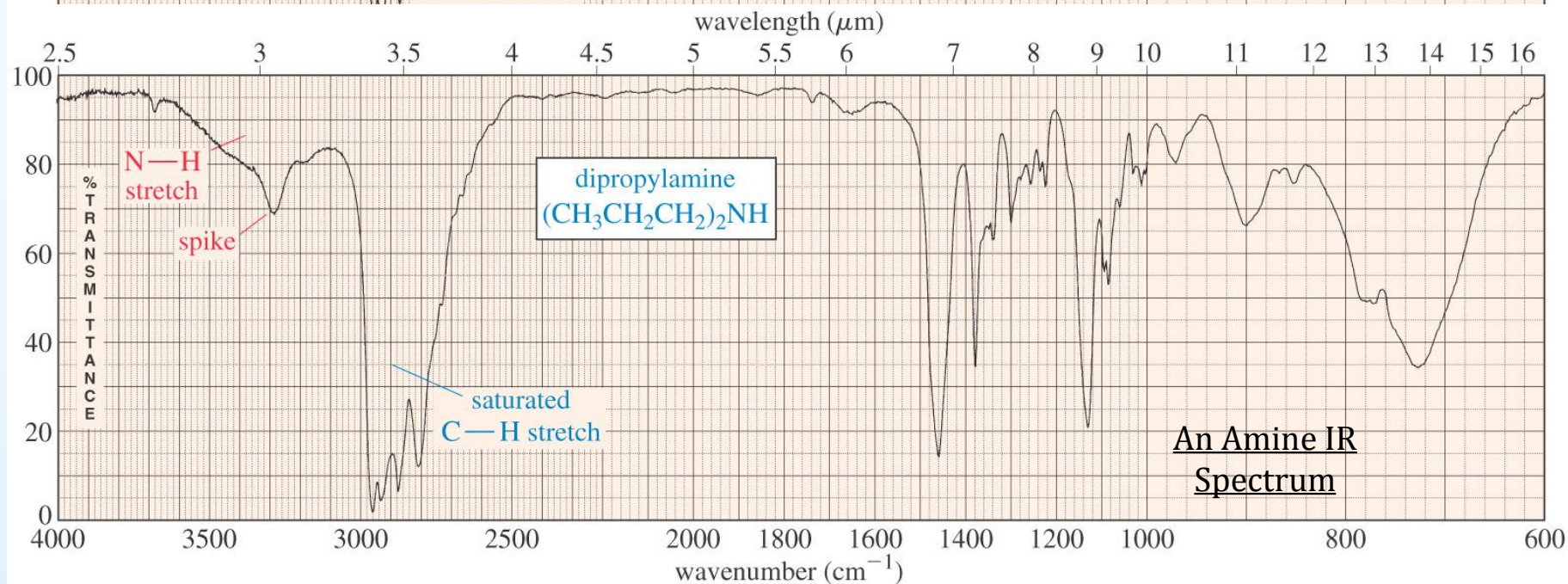
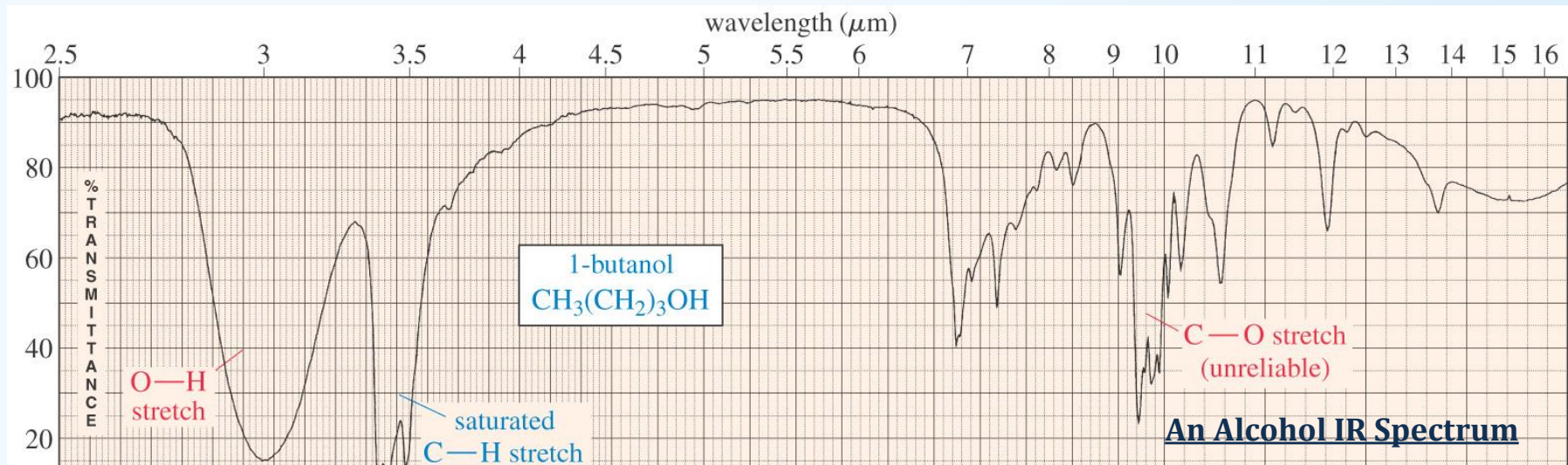
# An Alkyne IR Spectrum



# O-H and N-H Stretching

- Both of these occur around  $3300\text{ cm}^{-1}$ , but they look different.
  - Alcohol O-H, broad with rounded tip.
  - Secondary amine ( $\text{R}_2\text{NH}$ ), broad with one sharp spike.
  - Primary amine ( $\text{RNH}_2$ ), broad with two sharp spikes.
  - No signal for a tertiary amine ( $\text{R}_3\text{N}$ ).



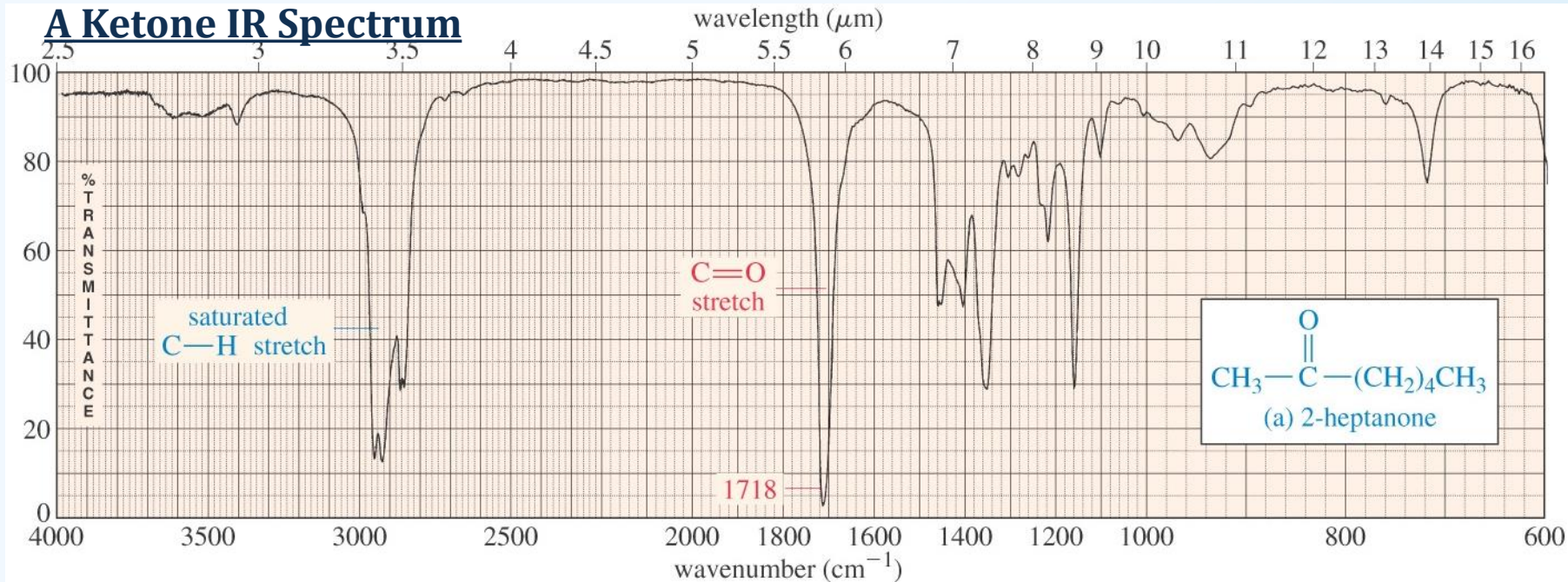


# Carbonyl Stretching

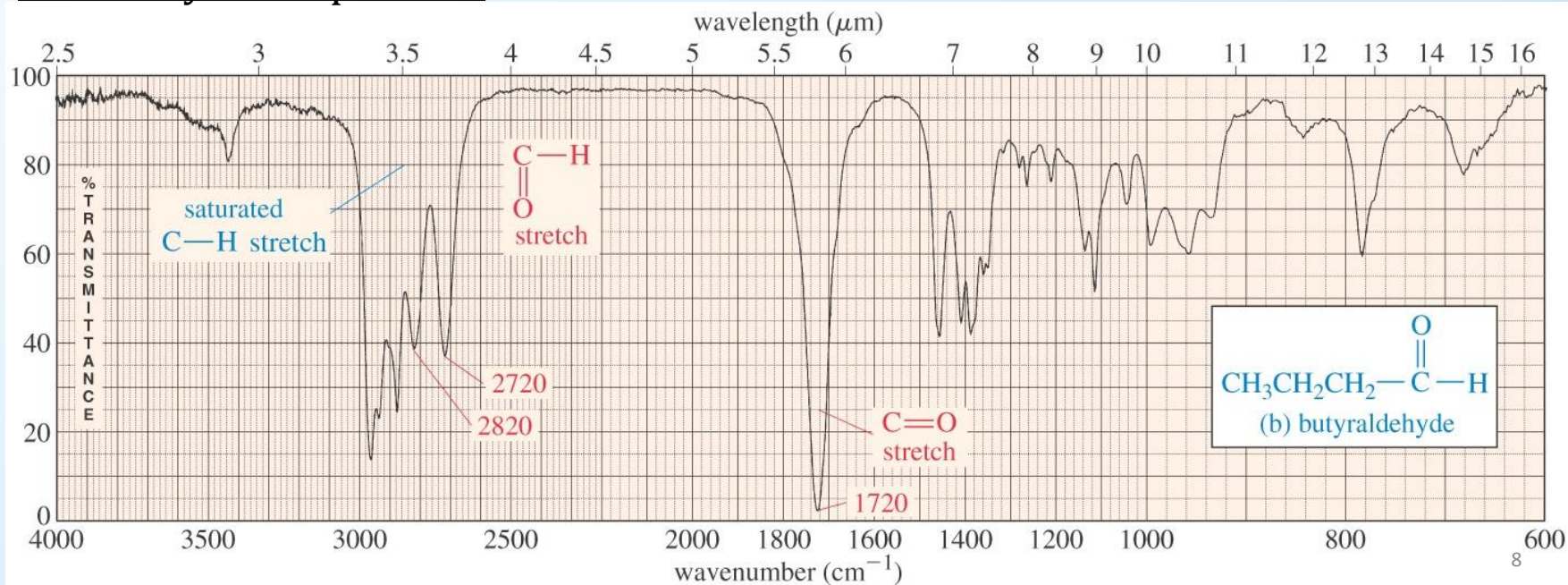
- The C=O bond of simple ketones, aldehydes, and carboxylic acids absorb around  $1710\text{ cm}^{-1}$ .
- Usually, it's the strongest IR signal.
- Carboxylic acids will have O-H also.
- Aldehydes have two C-H signals around  $2700$  and  $2800\text{ cm}^{-1}$ .



## A Ketone IR Spectrum

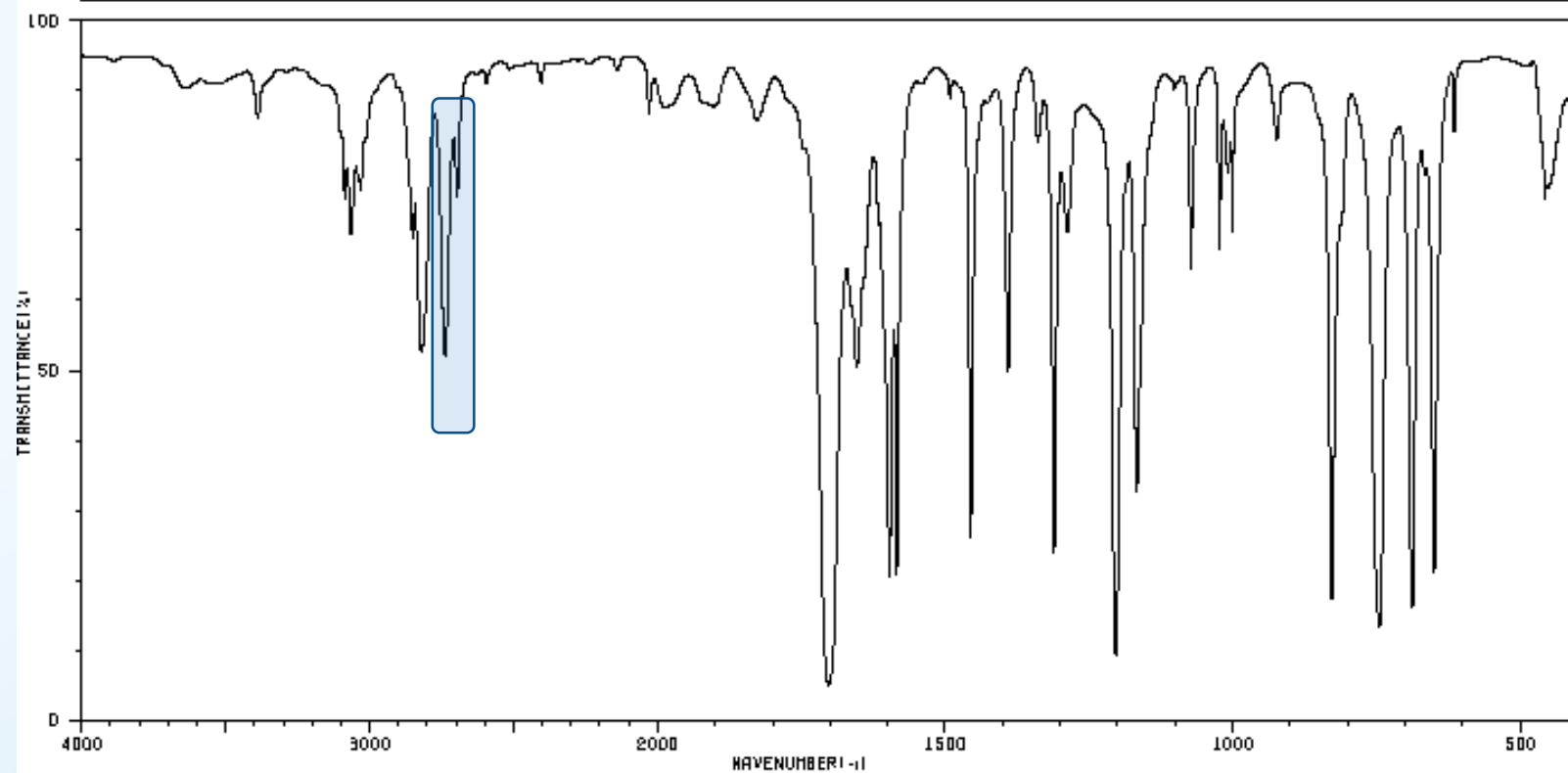


## An Aldehyde IR Spectrum

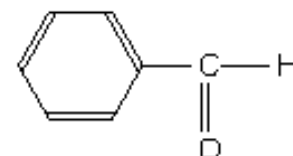




HIT-NO=1117	SCORE= ( )	SDBS-NO=672	IR-NIDA-05223 : LIQUID FILM
BENZALDEHYDE			
$C_7H_6O$			



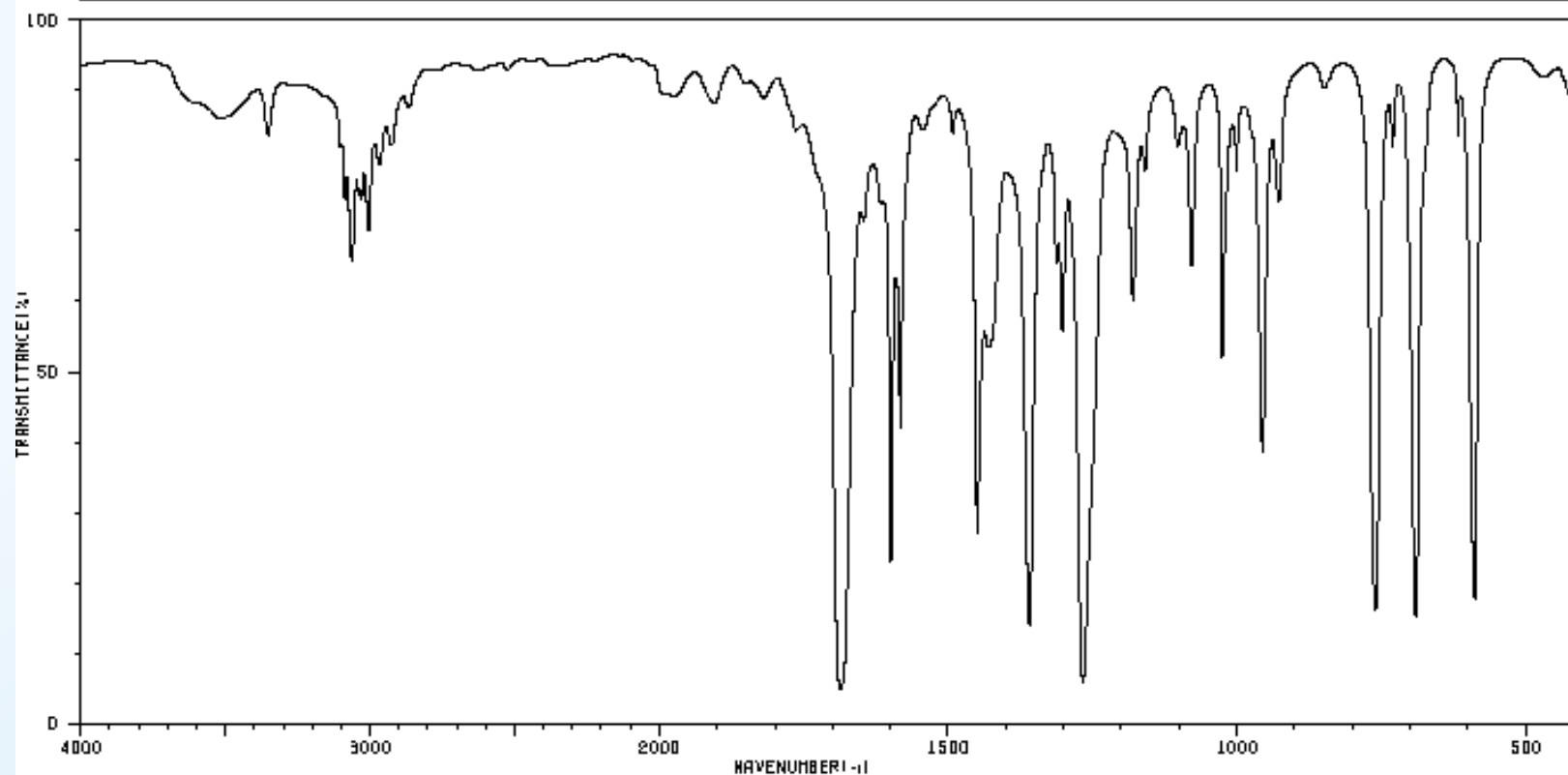
3086	72	1981	84	1697	20	1204	8	828	16
3065	86	1916	84	1584	20	1168	31	746	13
3031	72	1909	84	1456	25	1073	62	688	15
2850	66	1901	84	1391	47	1023	64	667	74
2820	50	1828	81	1339	79	1008	74	650	20
2736	50	1703	4	1311	23	1001	66	615	61
2696	72	1664	48	1288	68	924	78	467	72



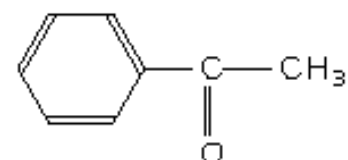
HIT-NO=1153 SCORE= ( ) SDBS-NO=722 IR-NIDA-05227 : LIQUID FILM

ACETOPHENONE

$C_8H_8O$



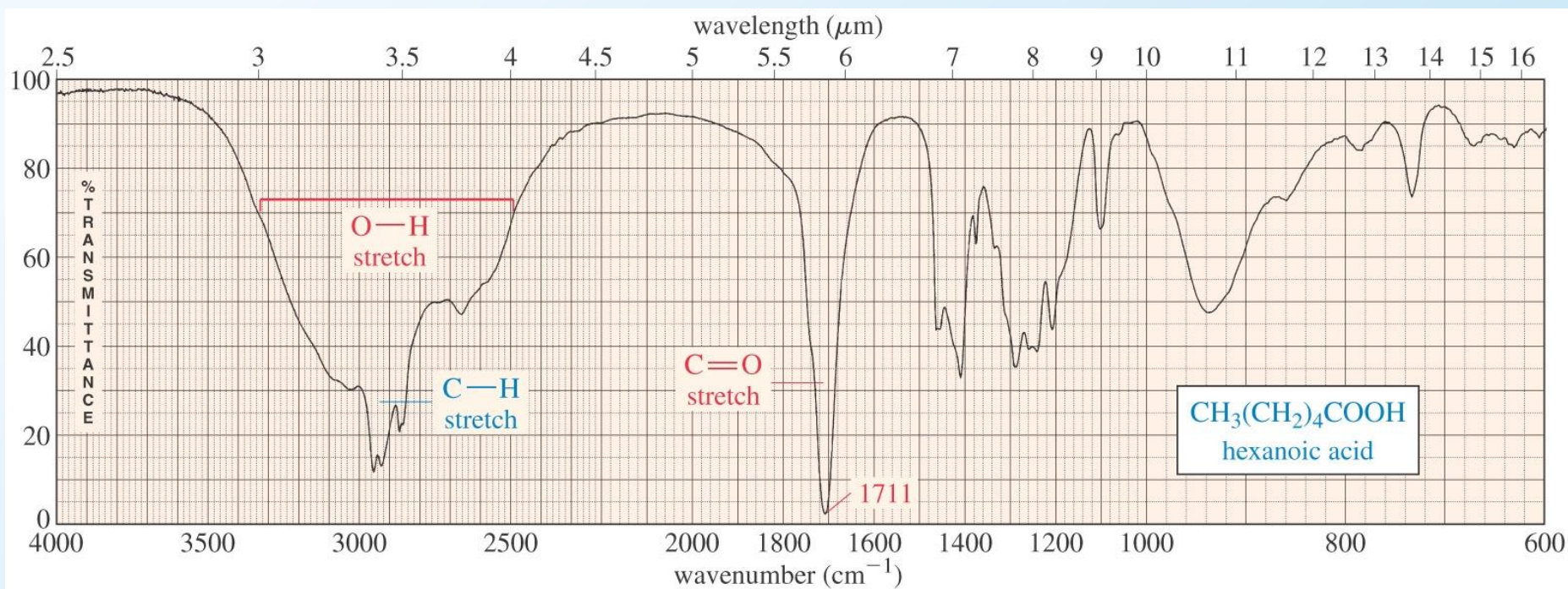
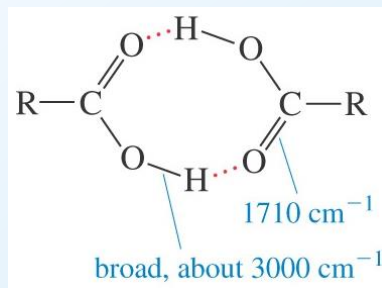
3504	84	2967	77	1646	81	1267	6	966	37
3352	81	2925	79	1492	81	1181	58	928	72
3087	72	2867	84	1450	26	1160	74	761	15
3063	84	1686	4	1430	62	1103	79	731	79
3040	72	1646	68	1360	13	1079	62	691	14
3029	72	1599	21	1313	82	1025	50	616	61
3006	68	1583	41	1303	63	1001	74	588	17





# O-H Stretch of a Carboxylic Acid

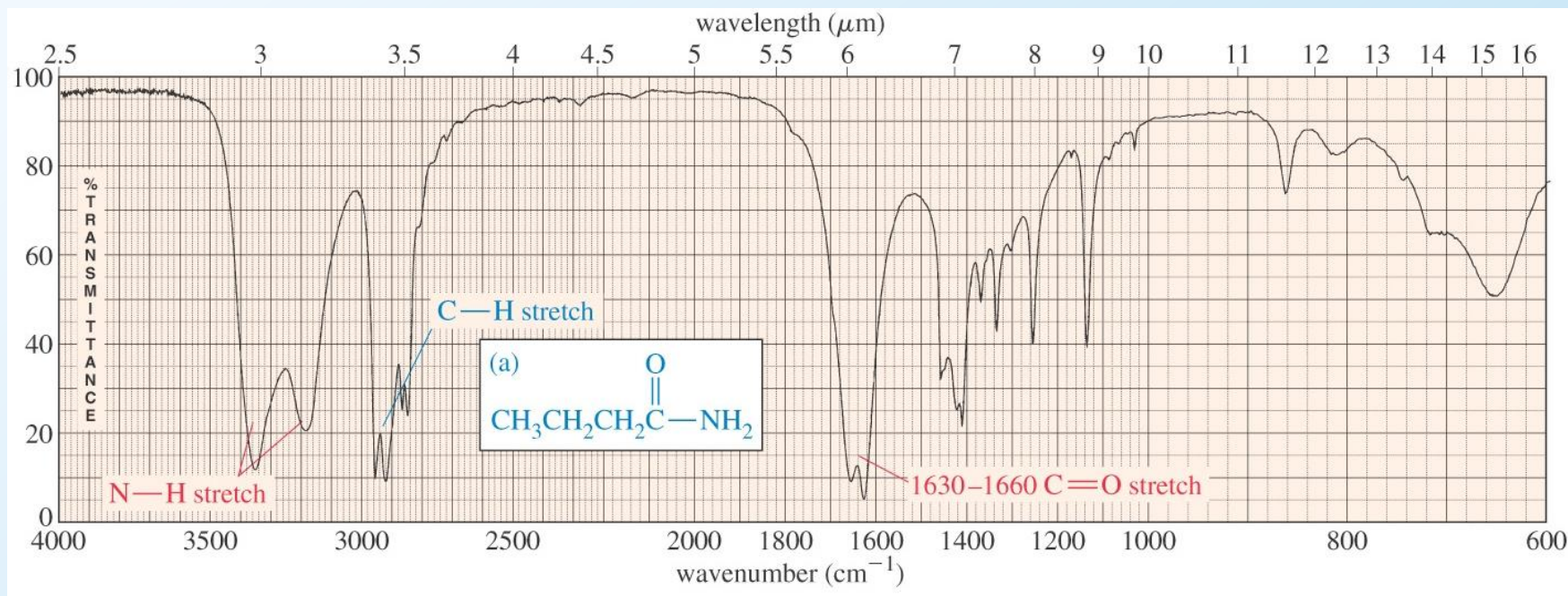
This O-H absorbs broadly,  $2500\text{--}3500\text{ cm}^{-1}$ , due to strong hydrogen bonding.



# Variations in C=O Absorption

- Conjugation of C=O with C=C lowers the stretching frequency to  $\sim 1680\text{ cm}^{-1}$ .
- The C=O group of an amide absorbs at an even lower frequency, 1640-1680  $\text{cm}^{-1}$ .
- The C=O of an ester absorbs at a higher frequency,  $\sim 1730\text{-}1740\text{ cm}^{-1}$ .
- Carbonyl groups in small rings (5 C's or less) absorb at an even higher frequency.

## An Amide IR Spectrum

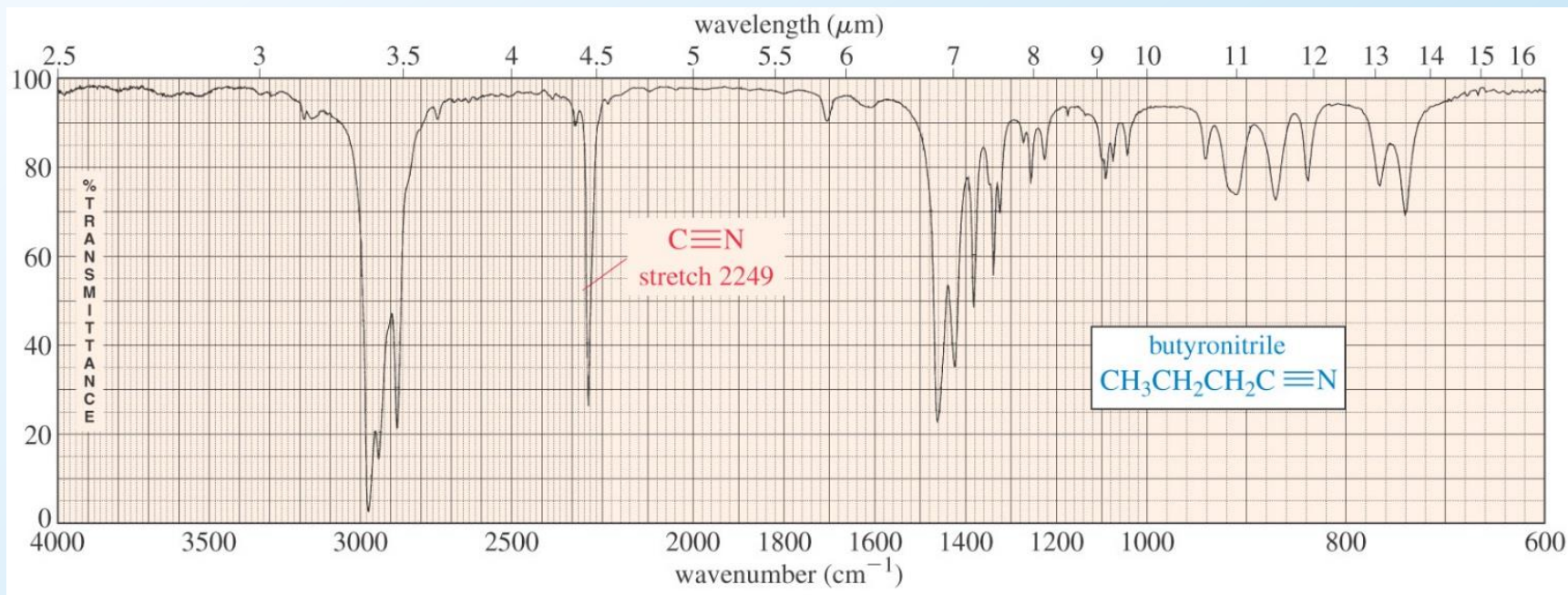




# Carbon - Nitrogen Stretching

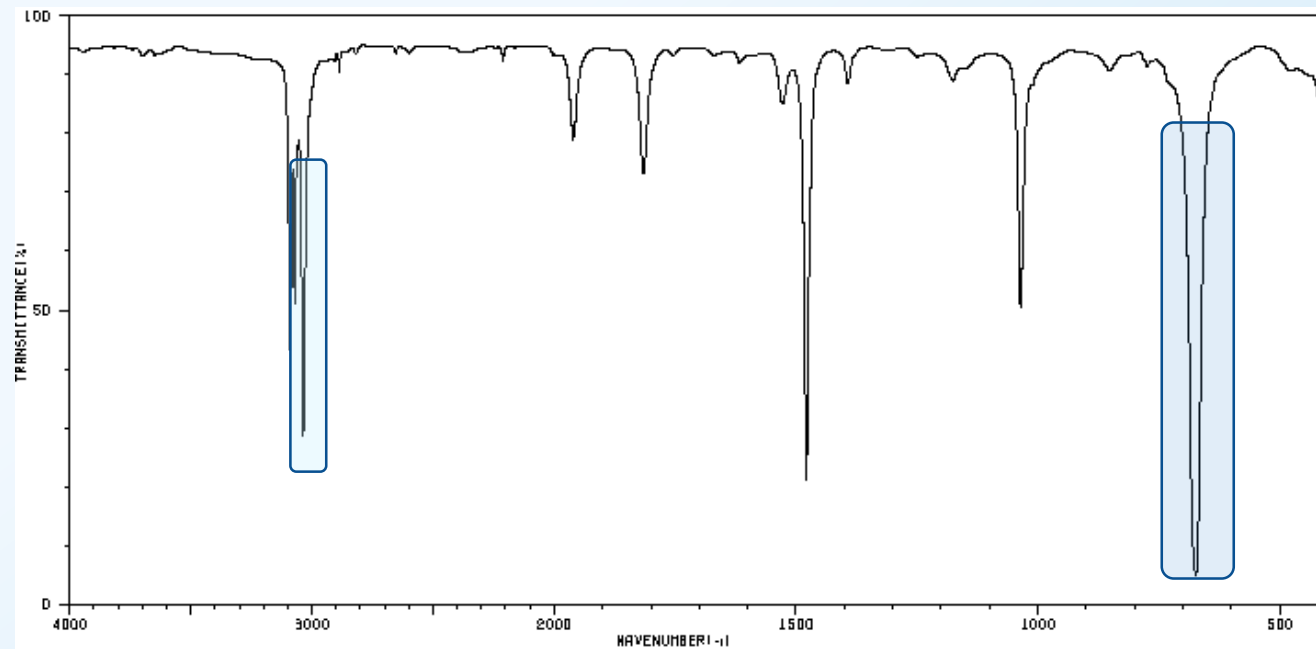
- C - N absorbs around  $1200\text{ cm}^{-1}$ .
- C = N absorbs around  $1660\text{ cm}^{-1}$  and is much stronger than the C = C absorption in the same region.
- C  $\equiv$  N absorbs strongly just *above*  $2200\text{ cm}^{-1}$ . The alkyne C  $\equiv$  C signal is much weaker and is just *below*  $2200\text{ cm}^{-1}$ .

## A Nitrile IR Spectrum

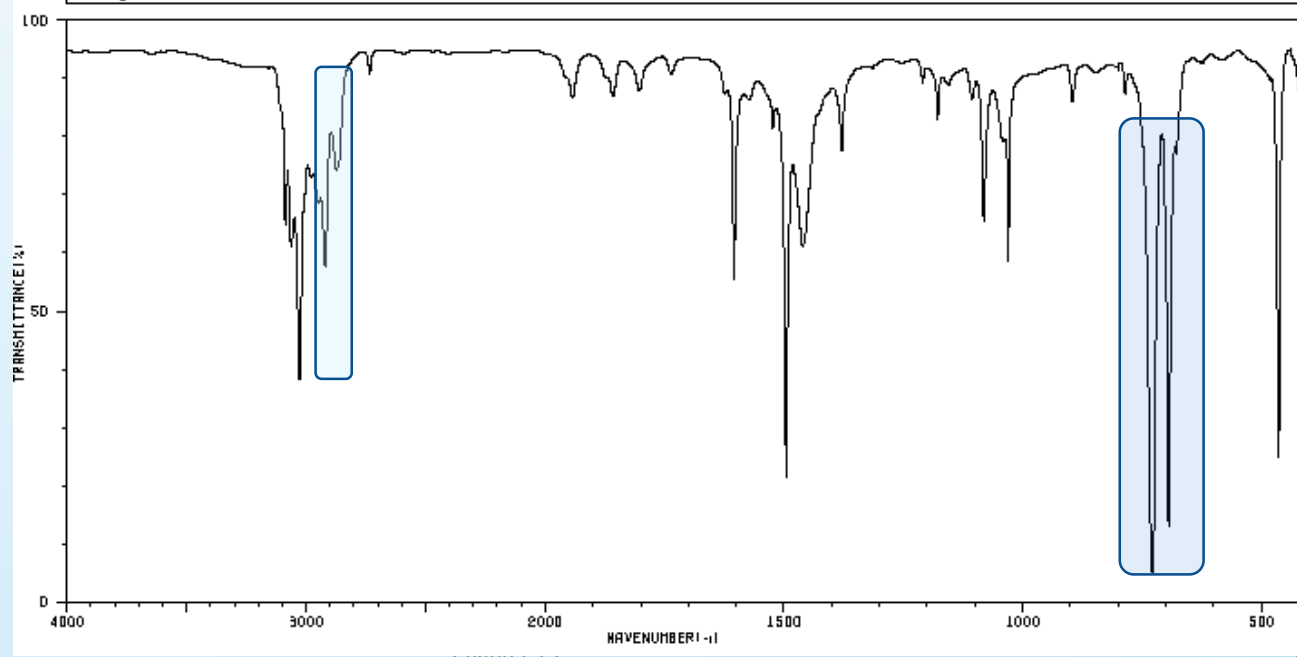


# Aromatic

Benzene

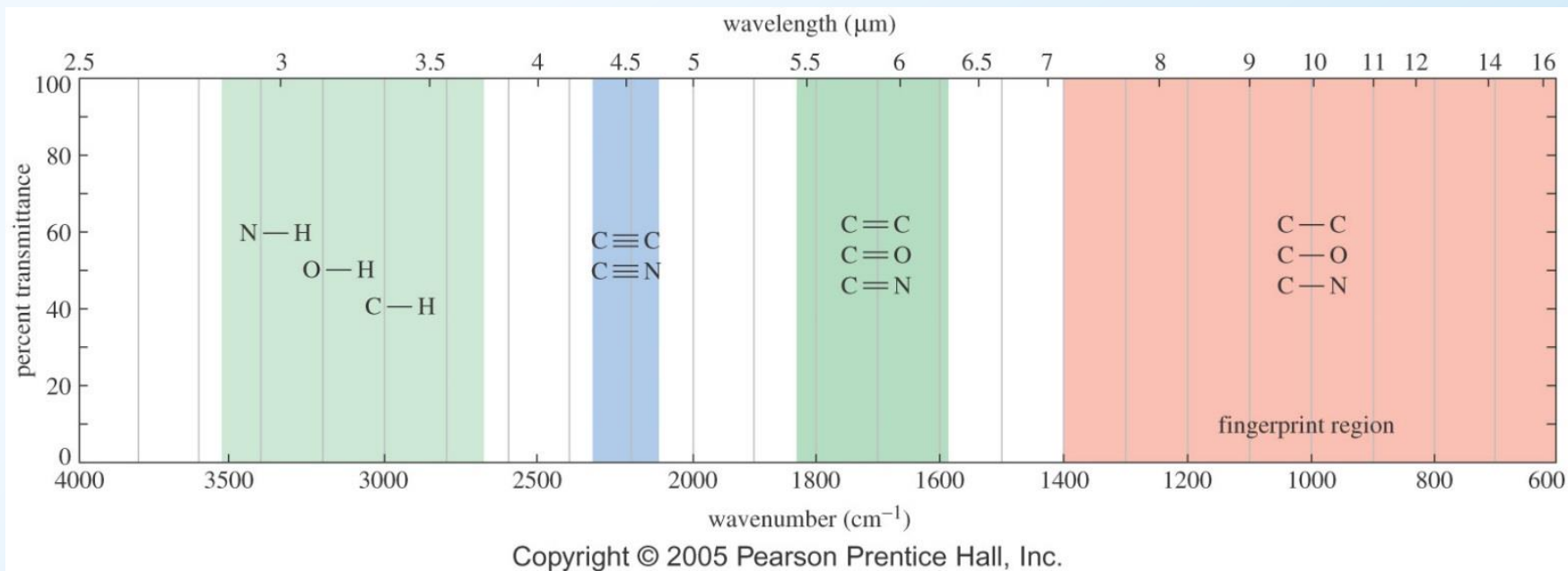


Methylbenzene  
(Mono substituted  
Benzene)





# Summary of IR Absorptions



Here is the table I have given you in class

Group	Frequency Range (cm <sup>-1</sup> )	Intensity <sup>a</sup>
<b>A. Alkyl</b>		
C—H (stretching)	2853–2962	(m–s)
Isopropyl, —CH(CH <sub>3</sub> ) <sub>2</sub>	1380–1385	(s)
	and 1365–1370	(s)
<i>tert</i> -Butyl, —C(CH <sub>3</sub> ) <sub>3</sub>	1385–1395	(m)
	and ~ 1365	(s)
<b>B. Alkenyl</b>		
C—H (stretching)	3010–3095	(m)
C=C (stretching)	1620–1680	(v)
R—CH=CH <sub>2</sub>	985–1000	(s)
	and 905–920	(s)
R <sub>2</sub> C=CH <sub>2</sub>	880–900	(s)
<i>cis</i> -RCH=CHR	675–730	(s)
<i>trans</i> -RCH=CHR	960–975	(s)
(out-of-plane C—H bendings)		
<b>C. Alkynyl</b>		
≡C—H (stretching)	~ 3300	(s)
C≡C (stretching)	2100–2260	(v)
<b>D. Aromatic</b>		
Ar—H (stretching)	~ 3030	(v)
Aromatic substitution type (C—H out-of-plane bendings)		
Monosubstituted	690–710	(very s)
<i>o</i> -Disubstituted	and 730–770	(very s)
<i>m</i> -Disubstituted	735–770	(s)
	680–725	(s)
	and 750–810	(very s)
<i>p</i> -Disubstituted	800–860	(very s)
<b>E. Alcohols, Phenols, and Carboxylic Acids</b>		
O—H (stretching)		
Alcohols, phenols (dilute solutions)	3590–3650	(sharp, v)
Alcohols, phenols (hydrogen bonded)	3200–3550	(broad, s)
Carboxylic acids (hydrogen bonded)	2500–3000	(broad, v)
<b>F. Aldehydes, Ketones, Esters, and Carboxylic Acids</b>		
C=O (stretching)	1630–1780	(s)
Aldehydes	1690–1740	(s)
Ketones	1680–1750	(s)
Esters	1735–1750	(s)
Carboxylic acids	1710–1780	(s)
Amides	1630–1690	(s)
<b>G. Amines</b>		
N—H	3300–3500	(m)
<b>H. Nitriles</b>		
C≡N	2220–2260	(m)

<sup>a</sup>Abbreviations: s = strong, m = medium, w = weak, v = variable, ~ = approximately.



# Strengths and Limitations of IR

- IR alone cannot determine a structure.
- Some signals may be ambiguous.
- The functional group is usually indicated.
- The *absence* of a signal is definite proof that the functional group is absent.
- Correspondence with a known sample's IR spectrum confirms the identity of the compound.