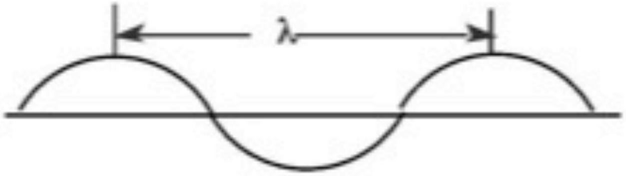
Introduction to Infrared Spectroscopy

Electromagnetic Radiation

- Electromagnetic radiation: light and other forms of radiant energy
- Wavelength (λ): the distance between consecutive identical points on a wave
- Frequency (ν): the number of full cycles of a wave that pass a point in a second
- Hertz (Hz): the unit in which radiation frequency is reported; s^{-1} (read “per second”)

Electromagnetic Radiation

- Wavelength



Unit	Relation to Meter
Meter (m)	----
Millimeter (mm)	1 mm = 10^{-3} m
Micrometer (μm)	1 μm = 10^{-6} m
Nanometer (nm)	1 nm = 10^{-9} m
Angstrom (Å)	1 Å = 10^{-10} m

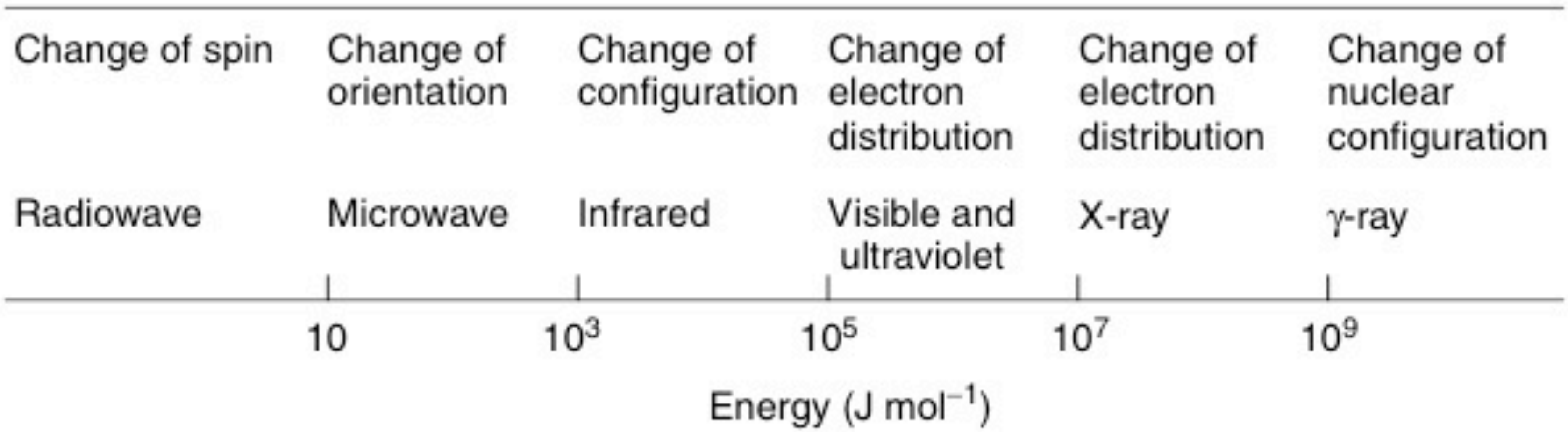


Figure 1.1 Regions of the electromagnetic spectrum. From Stuart, B., *Biological Applications of Infrared Spectroscopy*, ACOL Series, Wiley, Chichester, UK, 1997. © University of Greenwich, and reproduced by permission of the University of Greenwich.

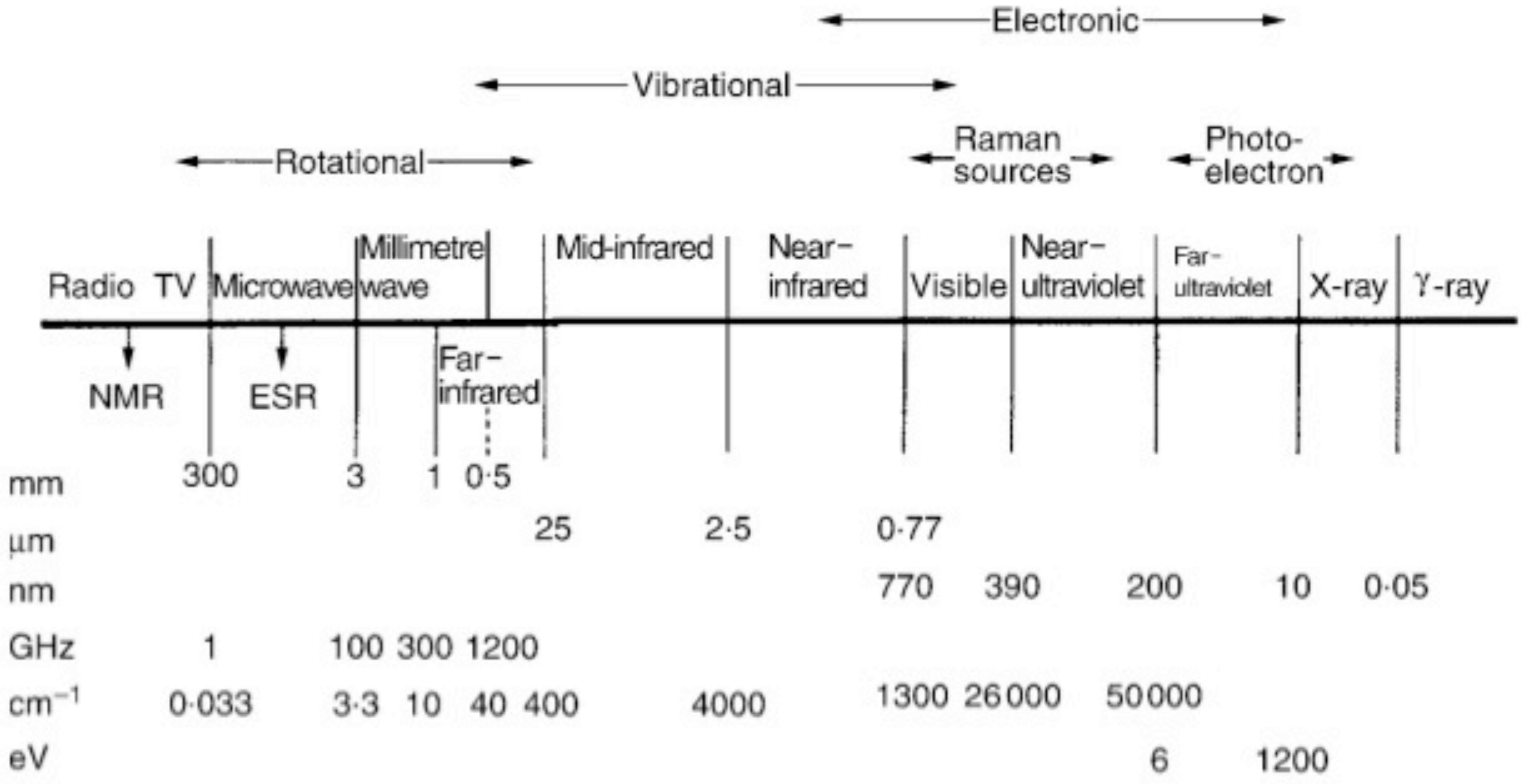


Figure 3.1 Regions of the electromagnetic spectrum

Table 1 Spectral Regions of Electromagnetic Radiation

Electromagnetic radiation type	Wavelength (m)	Wavenumber (cm^{-1})	Frequency (Hz)
γ-ray	Less than 1.0×10^{-10}	Greater than 100,000,000	Greater than 3.0×10^{18}
X-Ray	1.0×10^{-10} to 1.0×10^{-8}	1,000,000 to 100,000,000	3.0×10^{16} to 3.0×10^{18}
Ultraviolet			
Far	1.0×10^{-8} to 2.0×10^{-7} (10 to 200 nm)	50,000 to 1,000,000	1.5×10^{15} to 3.0×10^{16}
Near	2.0×10^{-7} to 4.0×10^{-7} (200 to 400 nm)	25,000 to 50,000	7.5×10^{14} to 1.5×10^{15}
Visible	4.0×10^{-7} to 7.5×10^{-7} (400 to 750 nm)	13,350 to 25,000	4.0×10^{14} to 7.5×10^{14}
Infrared			
Near	7.5×10^{-7} to 2.5×10^{-6} (0.75 to 2.5 μm)	4,000 to 13,350	1.2×10^{14} to 4.0×10^{14}
Mid	2.5×10^{-6} to 2.5×10^{-5} (2.5 to 25 μm)	400 to 4000	1.2×10^{13} to 1.2×10^{14}
Far	2.5×10^{-5} to 4.0×10^{-4} (25 to 400 μm)	25 to 400	7.5×10^{11} to 1.2×10^{13}
Microwave	4.0×10^{-4} to 1.0×10^{0} (0.04 to 100 cm)	0.01 to 25	3.0×10^{8} to 7.5×10^{11}
Radiowave	Greater than 1	Less than 0.01	Less than 3.0×10^{8}

Molecular Spectroscopy

- Molecular spectroscopy: the study of which frequencies of electromagnetic radiation are absorbed or emitted by substances and the correlation between these frequencies and specific types of molecular structure
- we study three types of molecular spectroscopy

Region of the Electromagnetic Spectrum	Absorption of Electromagnetic Radiation Results in Transition Between
infrared	vibrational energy levels
radio frequency	nuclear spin energy levels
ultraviolet-visible	electronic energy levels

Infrared Spectroscopy

- **The vibrational IR extends from 2.5×10^{-6} m (2.5 μm) to 2.5×10^{-5} m (25 μm)**
  - the frequency of IR radiation is commonly expressed in wavenumbers (ν)
  - wavenumber: the number of waves per centimeter, cm^{-1} (read reciprocal centimeters)
  - expressed in wavenumbers, the vibrational IR extends from 4000 cm^{-1} to 400 cm^{-1}

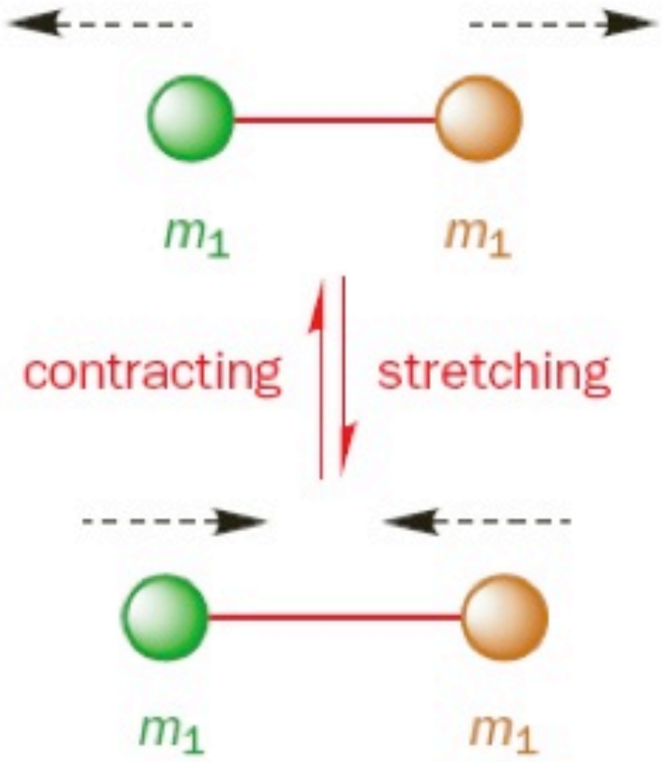
$$\nu = \frac{10^{-2}\ \mathrm{m} \bullet \mathrm{cm}^{-1}}{2.5 \times 10^{-6}\ \mathrm{m}} = 4000\ \mathrm{cm}^{-1} \qquad \dot{\nu} = \frac{10^{-2}\ \mathrm{m} \bullet \mathrm{cm}^{-1}}{2.5 \times 10^{-5}\ \mathrm{m}} = 400\ \mathrm{cm}^{-1}$$

Infrared Spectroscopy

- The IR region covers
  - 7.8 x 10^{-7} m (just above the visible region) to
  - 2.0 x 10^{-3} m (just below the microwave region)
- Organic chemistry uses mainly the vibrational IR, which covers
  - 2.5 x 10^{-6} m (2.5 μm) to 2.5 x 10^{-5} m (25 μm)
- Absorption of IR radiation in this region causes bonds to change from a lower vibrational energy level to a higher one

Molecular Vibrations

- Atoms joined by covalent bonds undergo continual vibrations relative to each other.
- The energies associated with these vibrations are quantized; within a molecule, only specific vibrational energy levels are allowed.
- The energies associated with transitions between vibrational energy levels for most covalent bonds are from 2 to 10 kcal/mol (8.4 to 42 kJ/mol).



bond vibration in the infrared

Hooke's law describes the movement of two masses attached to a spring. You may have met it if you have studied physics. You need not be concerned here with its derivation, just the result.

Infrared Spectroscopy: When an organic compound absorbs radiation with a wavelength of λ= 2–15 microns (**infrared radiation**, 4000–600 cm^{-1}), specific vibrational modes, mostly stretching and bending motions, are excited. The frequency at which this occurs can be approximated by Hooke's Law, and is dependent on the mass of the atoms and the bond strength (the force constant).

$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}} \qquad \text{where,}$$

$\bar{\nu}$ = frequency in cm^{-1}

c = velocity of light, $3 \times 10^{10}\ \text{cm}/_{\text{sec}}$

K = force constant in $\text{dynes}/_{\text{cm}}$

$\mu = \frac{m_1 m_2}{m_1 + m_2}$ the reduced mass

Molecular Vibrations

$$\bar{\nu} = 4.12 \sqrt{\frac{K}{\mu}}$$

K = force constant of bond

μ = reduced mass

- From this equation, we see that the position of a stretching vibration depends on
  - the strength of the vibrating bond
  - the masses of the atoms connected by the bond
  - The stronger the bond and the lighter the atoms connected by the bond, the higher the wavenumber of the vibration.

- The intensity of absorption is not governed by this equation; it depends primarily on the polarity of the vibrating bond.

Molecular Vibrations

- For a molecule to absorb IR radiation, the bond undergoing vibration
  - must be polar and
  - its vibration must cause a periodic change in the bond dipole moment
- Covalent bonds which do not meet these criteria are said to be IR inactive
  - the C-C double and triple bonds of symmetrically substituted alkenes and alkynes, for example, do not absorb IR radiation because they are not polar bonds

Molecular Vibrations

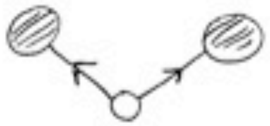
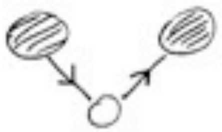
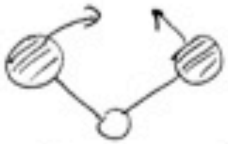
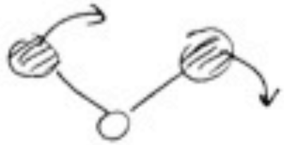
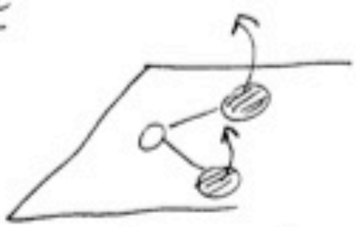
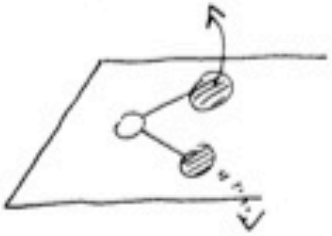
- Consider two covalently bonded atoms as two vibrating masses connected by a spring
- As the bond vibrates, its energy continually changes from kinetic to potential and vice versa
- The total energy (KE + PE) is proportional to the frequency of vibration

Molecular Vibrations

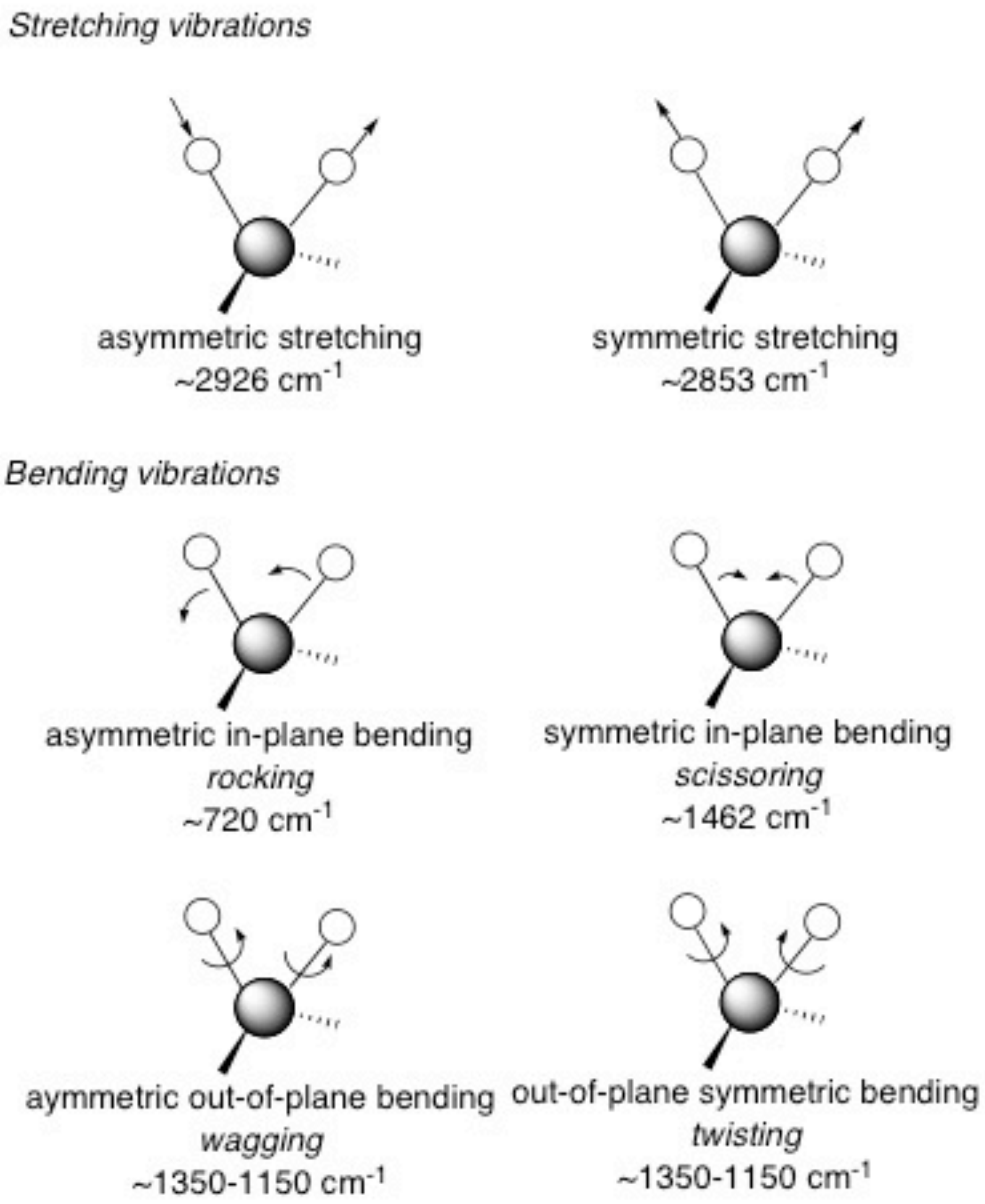
- For even a relatively small molecule, a large number of vibrational energy levels exist and patterns of IR absorption can be very complex (For a nonlinear molecule containing *n* atoms, there are $3n$ -6 allowed fundamental vibrations).

- The simplest vibrational motions are bending and stretching

VIBRATIONAL - ROTATIONAL MODES

	SYMMETRICAL	ANTISYMMETRICAL	
IN PLANE			
STRETCHING			4000 - 1500 cm^{-1} VIBRATIONS OF VALENCE noted ν
BENDING	 (scissoring)	 (rocking)	1500 - 650 cm^{-1} VIBRATIONS OF DEFORMATION noted $\delta_{in\ \&\ out}$
OUT OF PLANE			
TWISTING	 (wagging)		

ν are related to functional groups
δ are related to specific molecule



Stretching vibrations

asymmetric stretching
~2926 cm^{-1}

symmetric stretching
~2853 cm^{-1}

Bending vibrations

asymmetric in-plane bending
rocking
~720 cm^{-1}

symmetric in-plane bending
scissoring
~1462 cm^{-1}

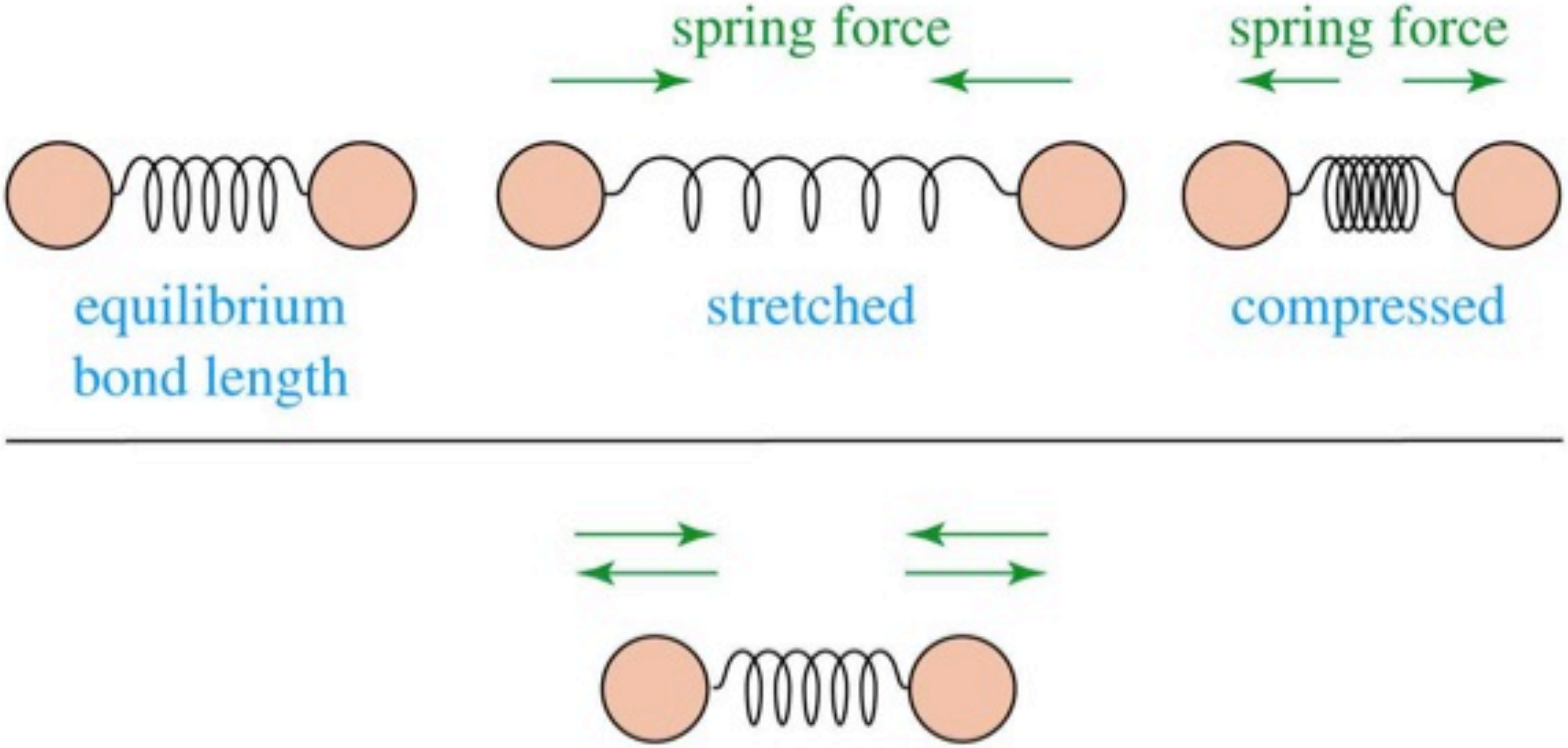
aymmetric out-of-plane bending
wagging
~1350-1150 cm^{-1}

out-of-plane symmetric bending
twisting
~1350-1150 cm^{-1}

Figure 2. Some of the vibrational modes for a CH_2 group.

Molecular Vibrations

Covalent bonds vibrate at only
certain allowable frequencies



Two types of molecular vibrations

Stretching: rhythmical movement along the bond axis

Bending: change in bond angle between bonds with common atom (twisting, rocking, torsional)

Each atom has 3 degrees of freedom (x, y, z coordinates to describe the position of the atom in space)

A molecule has as many degrees of freedom as the total degree of freedom of its individual atoms

A molecule of n atoms has **3n** degrees of freedom

For non-linear molecules:

3 degrees of freedom describe **rotation** and

3 degrees of freedom describe **translation**

The remaining **3n-6** are **vibrational** - these are observed in IR

For non-linear molecules:

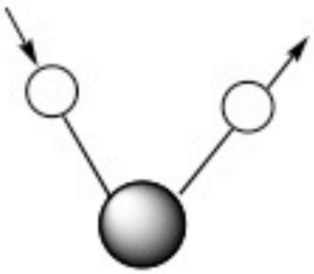
3 degrees of freedom describe **rotation** and

3 degrees of freedom describe **translation**

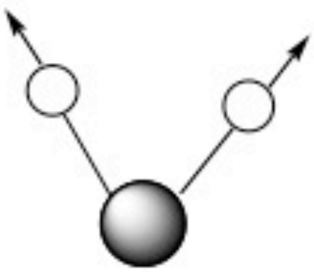
The remaining **3n-6** are **vibrational** - these are observed in IR

For linear molecules: **3n-5**

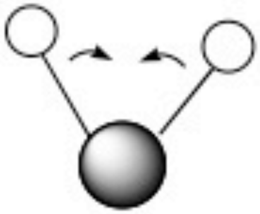
Since only 2 degrees of freedom are required to describe rotation



asymmetric stretching
~3756 cm^{-1}



symmetric stretching
~3652 cm^{-1}

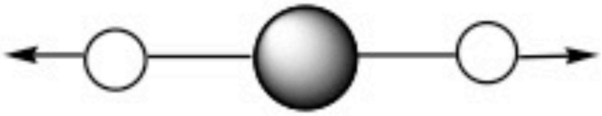


scissoring
~1596 cm^{-1}

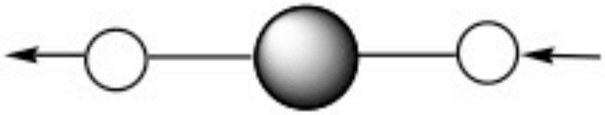
3n-6

$3 \times 3 - 6 = 3$

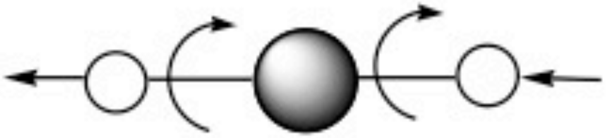
H_2O



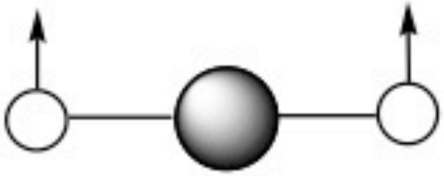
symmetric stretching
~1340 cm^{-1}



asymmetric stretching
~2350 cm^{-1}



bending
scissoring
~667 cm^{-1}



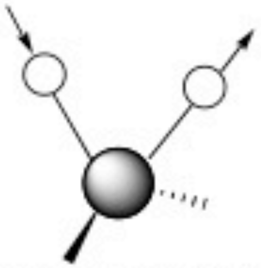
bending
scissoring
~667 cm^{-1}

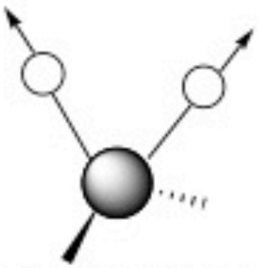
3n-5

3x3 - 5 = 4

CO_2

stretching


asymmetric stretching
~2926 cm^{-1}

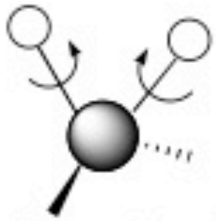

symmetric stretching
~2853 cm^{-1}

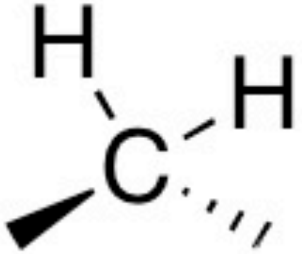
bending


in-plane bending
rocking
~720 cm^{-1}


in-plane bending
scissoring
~1462 cm^{-1}


out-of-plane bending
wagging
~1350-1150 cm^{-1}


out-of-plane bending
twisting
~1350-1150 cm^{-1}



IR bands

position

mass

Light atoms -
High frequency

bond strength

Strong bonds -
High frequency

IR bands

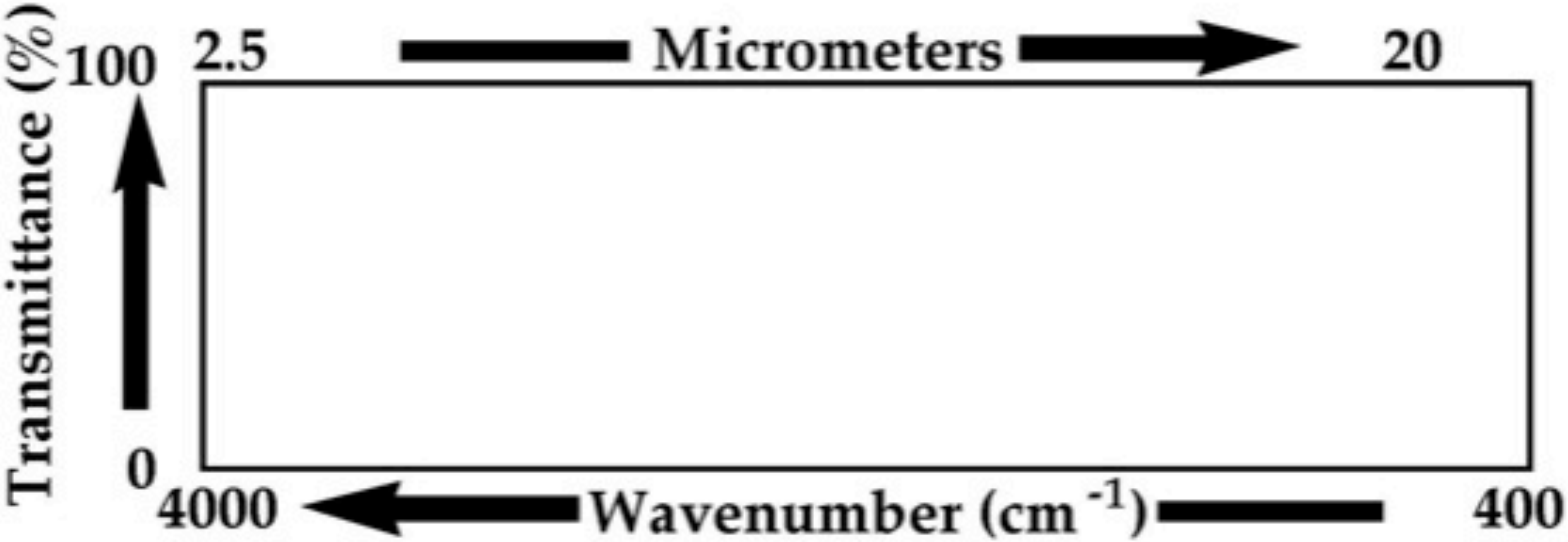
position	**mass**	Light atoms - High frequency
	bond strength	Strong bonds - High frequency
strength	**polarity**	Polar bonds give strong bands

IR bands

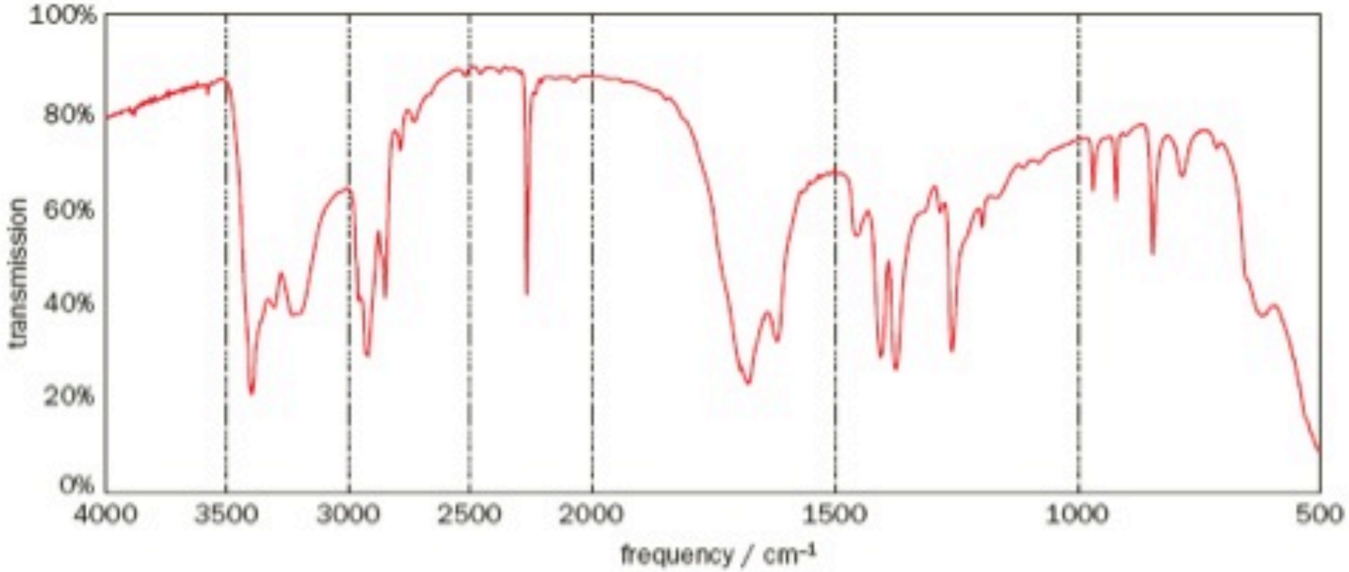
position	**mass**	Light atoms - High frequency
	bond strength	Strong bonds - High frequency
strength	**polarity**	Polar bonds give strong bands
width	**hydrogen bonding**	Broad bands

Infrared Spectroscopy

- For the IR spectra recorded in this text, calibrations are



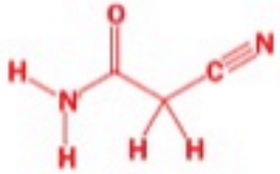
A typical IR spectrum



There are four important regions of the infrared spectrum

▶

IR spectra are plotted 'upside down' because they record **transmission** (the amount of light reaching the detector) rather than absorbance.



cyanoacetamide
(spectrum taken as a Nujol mull)

The regions of the infrared spectrum

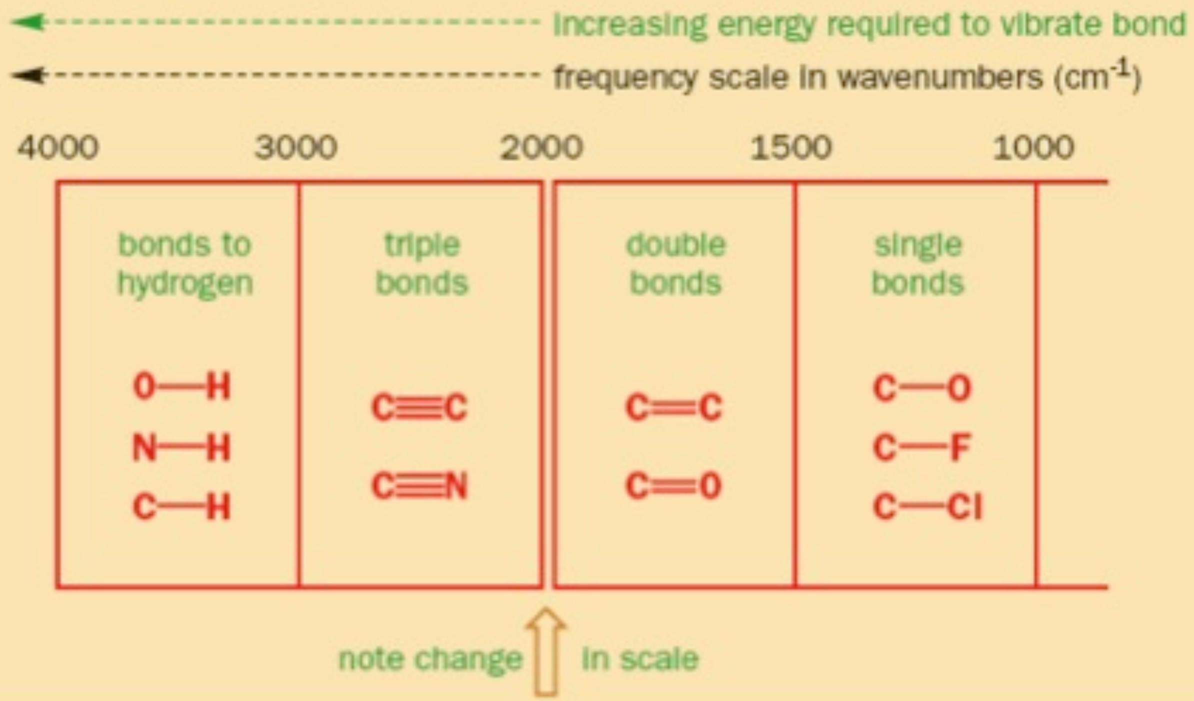


Table 1.

Bond type	Absorption region, cm^{-1}
C-C, C-O, C-N	1300 - 800
C=C, C=O, C=N, N=O	1900 - 1500
C≡C, C≡N	2300 - 2000
C-H, O-H, N-H	3800 - 2700

Carbon-Carbon Bond Stretching

Stronger bonds absorb at higher frequencies:

C-C 1200 cm^{-1}

C=C 1660 cm^{-1}

C ≡ C 2200 cm^{-1} (weak or absent if internal)

Carbon-Carbon Bond Stretching

Conjugation lowers the frequency:

isolated C=C	1640-1680 cm^{-1}
conjugated C=C	1620-1640 cm^{-1}
aromatic C=C	approx. 1600 cm^{-1}

Stretching Frequencies

Bond		**Bond Energy [kcal (kJ)]**		**Stretching Frequency (cm^{-1})**	
		Frequency dependence on atomic masses			
C—H	↓ heavier atoms	100 (420)		3000	↓ $\bar{\nu}$ decreases
C—D		100 (420)		2100	
C—C		83 (350)		1200	
		Frequency dependence on bond energies			
C—C		83 (350)	↓ stronger bond	1200	↓ $\bar{\nu}$ increases
C═C		146 (611)		1660	
C≡C		200 (840)		2200	

Frequency decreases with increasing atomic weight

Frequency increases with increasing bond energy

$$\bar{\nu} = \frac{1}{2\pi c}\left[\frac{f}{M_1 M_2 / (M_1 + M_2)}\right]^{1/2}$$

$M_1 > M_2$, thus $M_1M_2/(M_1+M_2) \approx M_2$

$M_1 = C$

$M_2 = H$

IR region - between visible and microwave

Practical interest for organic chemistry:

4000-400 cm^{-1}

Any two compounds (*except enantiomers*) are **unlikely to have two identical IR spectra** (in the entire spectrum range)

Wavenumbers ($\bar{\nu}$) in cm^{-1}

Proportional to energy

$$E = h\nu$$

You can never deduce the structure of the organic compound based just on the IR spectrum

Unless you have an authentic sample that gives IDENTICAL IR spectrum as your sample

You can never deduce the structure of the organic compound based just on the IR spectrum

Unless you have an authentic sample that gives IDENTICAL IR spectrum as your sample

So what is the value of IR?

Certain groups of atoms produce bands at or near the same frequency regardless of the rest of the molecule

IR - “functional group spectroscopy”!

Because IR is not the only spectroscopic tool used for structure determination of a compound, detailed analysis of the IR spectrum is not required

You only consider the major bands, and disregard all others.

IR radiation at <100cm^{-1} is absorbed and converted into the molecular rotation, this energy is quantized, therefore molecular rotation spectrum consists of discrete lines

10,000-100cm^{-1} is absorbed and converted into energy of molecular vibration; this energy is also quantized, but single vibrational energy change is accompanied by a number of rotational energy changes

Thus the vibrational spectrum appears as bands rather than lines

Vibrational-rotational (IR) spectrum 400-4000cm^{-1}

♦ Infrared Spectroscopy: An Instrumental Method for Detecting Functional Groups

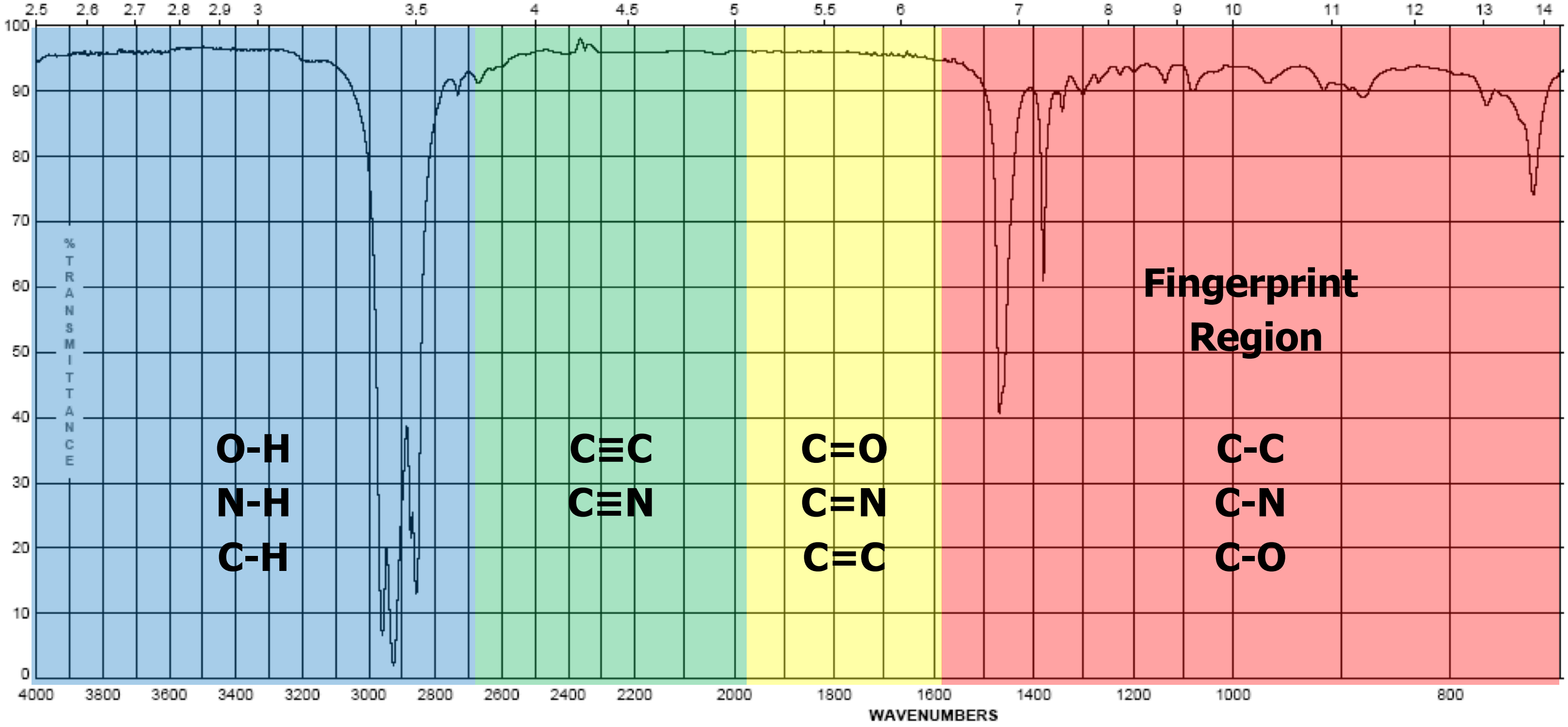
- Electromagnetic radiation in the infrared (IR) frequency range is absorbed by a molecule at certain characteristic frequencies
  - ➡ Energy is absorbed by the bonds in the molecule and they vibrate faster
  - ➡ The bonds behave like tiny springs connecting the atoms
    - ★ The bonds can absorb energy and vibrate faster only when the added energy is of a particular resonant frequency
  - ➡ The frequencies of absorption are very characteristic of the type of bonds contained in the sample molecule
  - ➡ The type of bonds present are directly related to the functional groups present
  - ➡ A plot of these absorbed frequencies is called an IR spectrum

- **Infrared Spectrometer**
  - An infrared spectrometer detects the frequencies absorbed by the sample molecule
  - Light of all the various IR frequencies is transmitted to the molecule and the frequencies absorbed are recorded
  - The absorption frequencies are specified as wavenumbers in units of reciprocal centimeters (cm^{-1})
    - ★ Alternatively the wavelength (λ) in units of microns (μm) can be specified

$$\overline{\upsilon} = \frac{1}{\lambda} \quad \text{(with } \lambda \text{ in cm)} \qquad \text{or} \qquad \overline{\upsilon} = \frac{10{,}000}{\lambda} \quad \text{(with } \lambda \text{ in } \mu\text{m)}$$

  - The spectrum is a plot of frequency on the horizontal axis versus strength of absorption on the vertical axis

The four primary regions of the IR spectrum



Bonds to H **Triple bonds** **Double bonds** **Single Bonds**

O-H
N-H
C-H

$C\equiv C$
$C\equiv N$

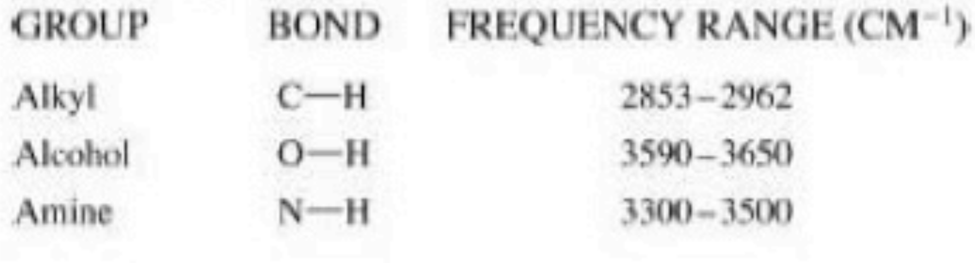
$C=O$
$C=N$
$C=C$

Fingerprint Region

C-C
C-N
C-O

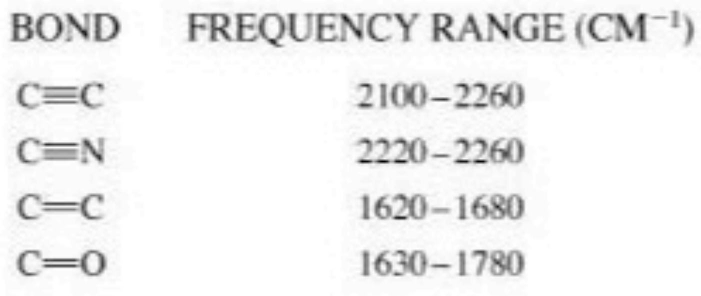
$4000\ cm^{-1}$ **$2700\ cm^{-1}$** **$2000\ cm^{-1}$** **$1600\ cm^{-1}$** **$600\ cm^{-1}$**

- The actual relative frequency of vibration can be predicted
  - Bonds with lighter atoms vibrate faster than those with heavier atoms



GROUP	BOND	FREQUENCY RANGE (CM^{-1})
Alkyl	C—H	2853–2962
Alcohol	O—H	3590–3650
Amine	N—H	3300–3500

- Triple bonds (which are stiffer and stronger) vibrate at higher frequencies than double bonds
  - Double bonds in turn vibrate at higher frequencies than single bonds



BOND	FREQUENCY RANGE (CM^{-1})
C≡C	2100–2260
C≡N	2220–2260
C=C	1620–1680
C=O	1630–1780

- The IR spectrum of a molecule usually contains many peaks
  - These peaks are due to the various types of vibrations available to each of the different bonds
  - Additional peaks result from overtone (harmonic) peaks which are weaker and of lower frequency
  - The IR is a "fingerprint" of the molecule because of the unique and large number of peaks seen for a particular molecule

Group			Frequency Range (cm^{-1})	Intensity[a]
A. Alkyl				
C—H (stretching)			2853–2962	(m–s)
Isopropyl, —CH(CH$_3$)$_2$			1380–1385	(s)
		and	1365–1370	(s)
tert-Butyl, —C(CH$_3$)$_3$			1385–1395	(m)
		and	~1365	(s)
B. Alkenyl				
C—H (stretching)			3010–3095	(m)
C═C (stretching)			1620–1680	(v)
R—CH═CH$_2$	(out-of-plane C—H bendings)		985–1000	(s)
		and	905–920	(s)
R$_2$C═CH$_2$			880–900	(s)
cis-RCH═CHR			675–730	(s)
trans-RCH═CHR			960–975	(s)
C. Alkynyl				
≡C—H (stretching)			~3300	(s)
C≡C (stretching)			2100–2260	(v)
D. Aromatic				
Ar—H (stretching)			~3030	(v)
Aromatic substitution type				
(C—H out-of-plane bendings)				
Monosubstituted			690–710	(very s)
o-Disubstituted		and	730–770	(very s)
m-Disubstituted			735–770	(s)
			680–725	(s)
		and	750–810	(very s)
p-Disubstituted			800–860	(very s)
E. Alcohols, Phenols, and Carboxylic Acids				
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)
F. Aldehydes, Ketones, Esters, and Carboxylic Acids				
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)
G. Amines				
N—H			3300–3500	(m)
H. Nitriles				
C≡N			2220–2260	(m)

[a] Abbreviations: s = strong, m = medium, w = weak, v = variable, ~ = approximately.

♦ Interpreting IR Spectra

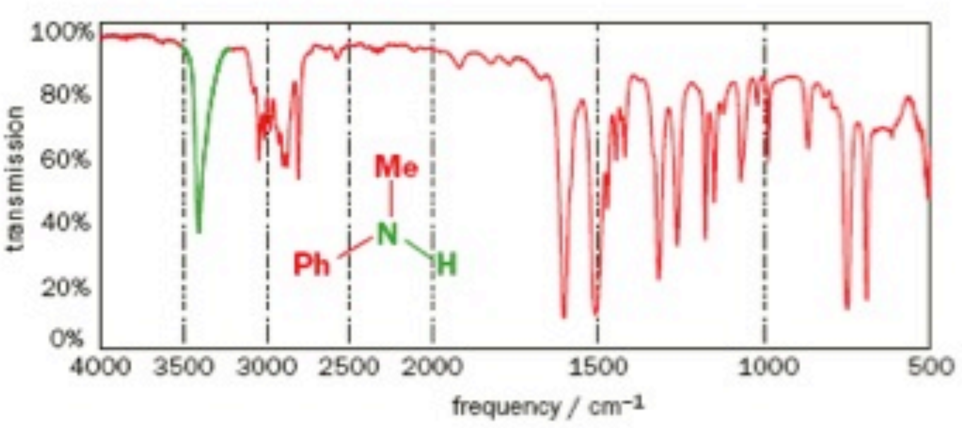
- Generally only certain peaks are interpreted in the IR
  - Those peaks that are large and above 1400 cm^{-1} are most valuable

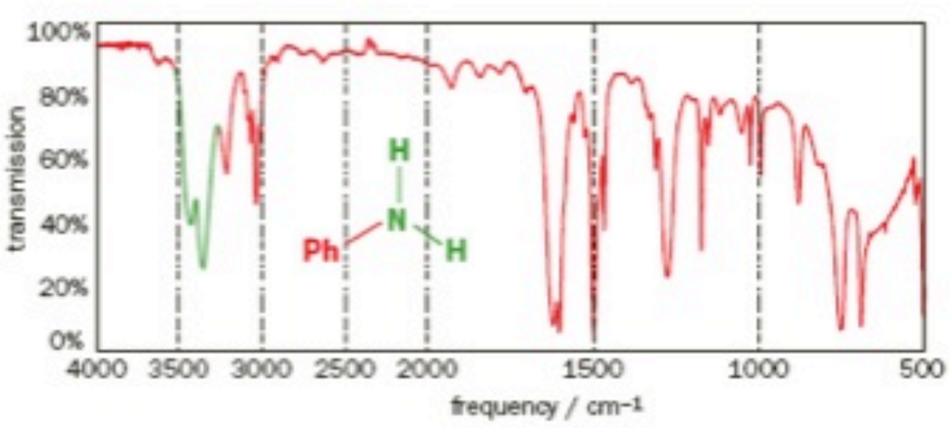
Hydrocarbons

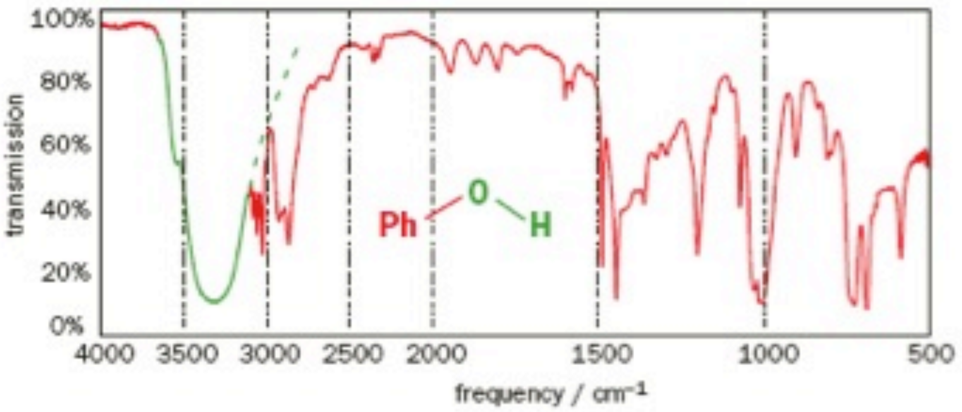
- The C-H stretching regions from 2800-3300 cm^{-1} is characteristic of the type of carbon the hydrogen is attached to
- C-H bonds where the carbon has more *s* character are shorter, stronger and stiffer and thus vibrate at higher frequency
  - C-H bonds at sp centers appear at 3000-3100 cm^{-1}
  - C-H bonds at sp^2 centers appear at about 3080 cm^{-1}
  - C-H bonds at sp^3 centers appear at about 2800-3000 cm^{-1}
- C-C bond stretching frequencies are only useful for multiple bonds
  - C-C double bonds give peaks at 1620-1680 cm^{-1}
  - C-C triple bonds give peaks at 2100-2260 cm^{-1}
  - These peaks are absent in symmetrical double and triple bonds

It is important to make note of peak intensities to show the effect of these factors:

- ***Strong (s)*** – peak is tall, transmittance is low (0-35 %)
- ***Medium (m)*** – peak is mid-height (75-35%)
- ***Weak* (w)** – peak is short, transmittance is high (90-75%)
- **** Broad (br)*** – if the Gaussian distribution is abnormally broad
  *(*this is more for describing a bond that spans many energies)*


100%
80%
60%
40%
20%
0%
transmission
4000 3500 3000 2500 2000 1500 1000 500
frequency / cm⁻¹
Me
N
Ph
H


100%
80%
60%
40%
20%
0%
transmission
4000 3500 3000 2500 2000 1500 1000 500
frequency / cm⁻¹
H
N
Ph
H


100%
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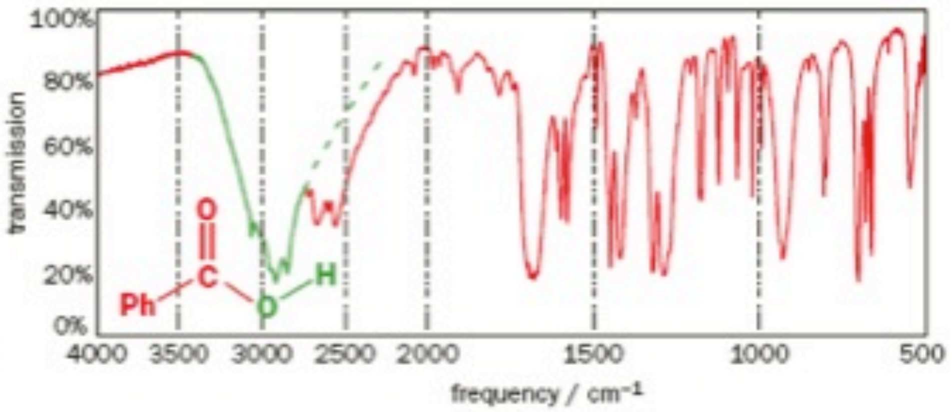
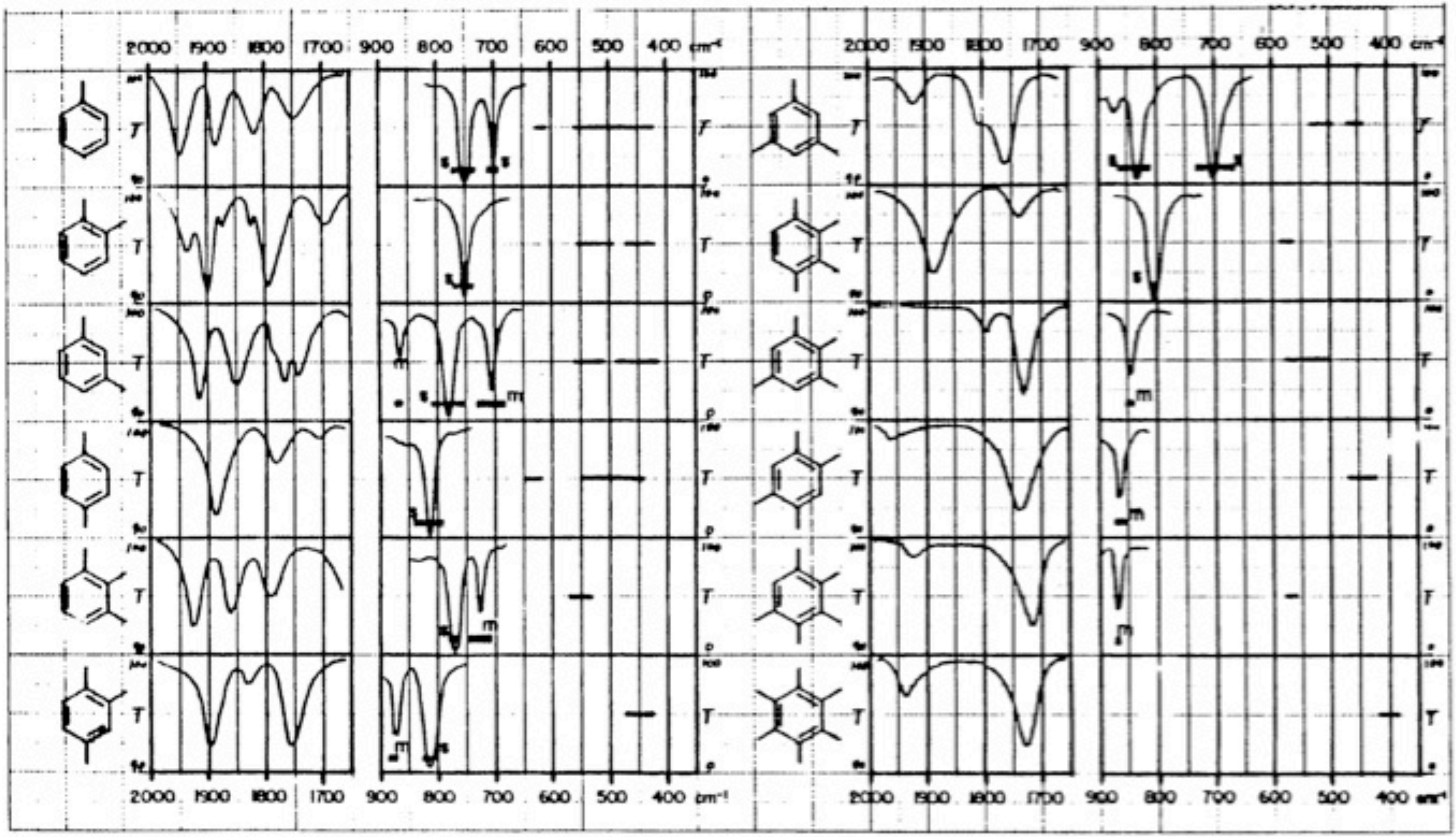
40%
20%
0%
transmission
4000 3500 3000 2500 2000 1500 1000 500
frequency / cm⁻¹
Ph
O
H


100%
80%
60%
40%
20%
0%
transmission
4000 3500 3000 2500 2000 1500 1000 500
frequency / cm⁻¹
O
C
Ph
O
H



INFRARED ABSORPTION CORRELATION CHART (continued)

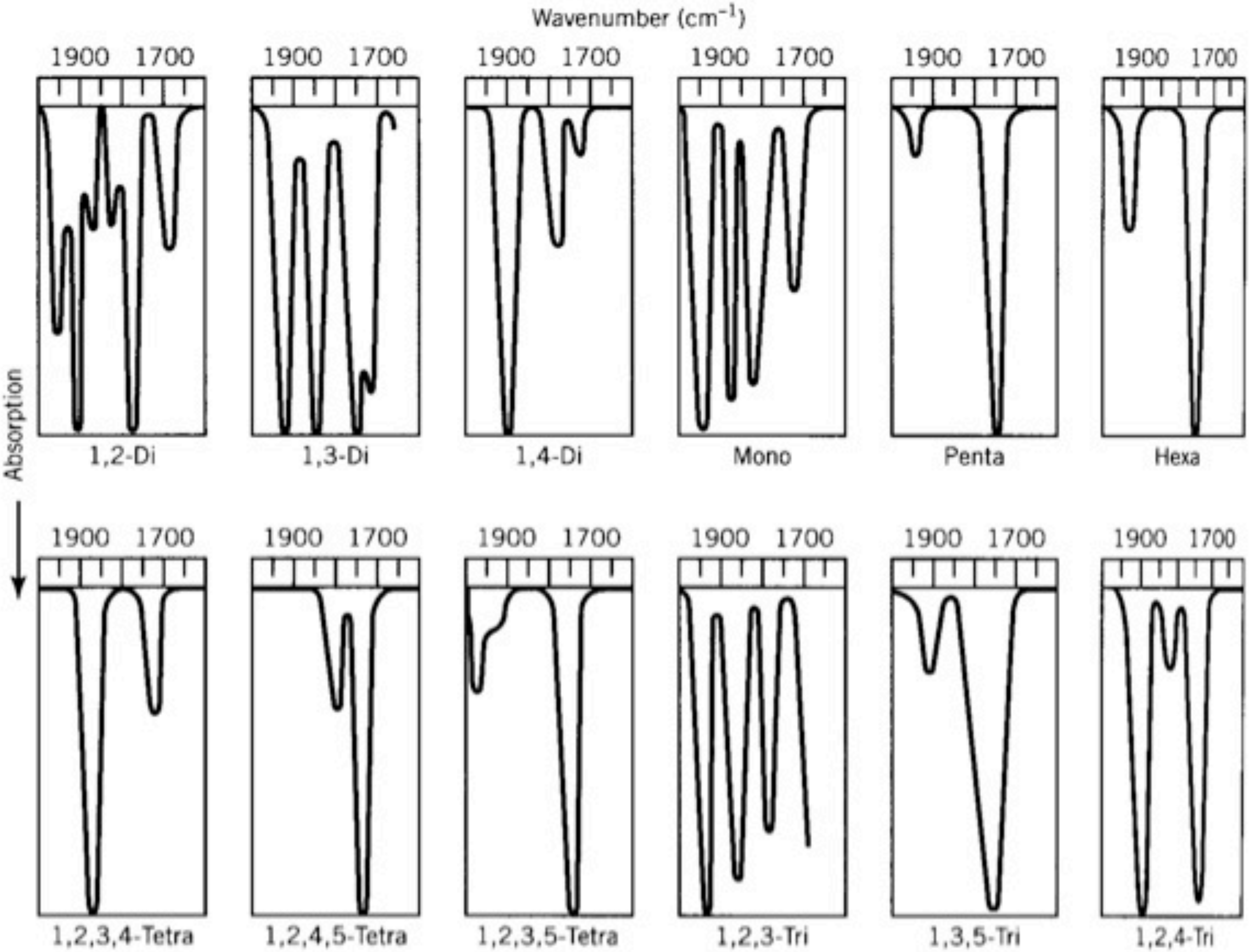
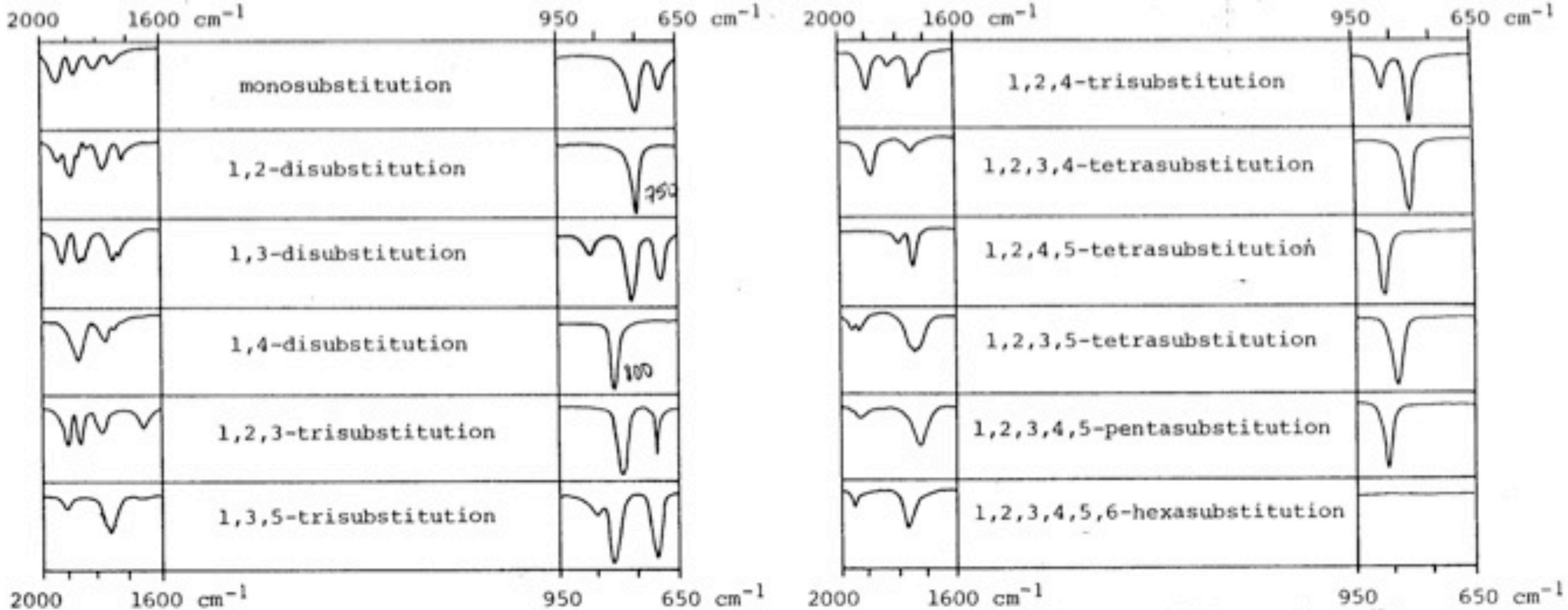


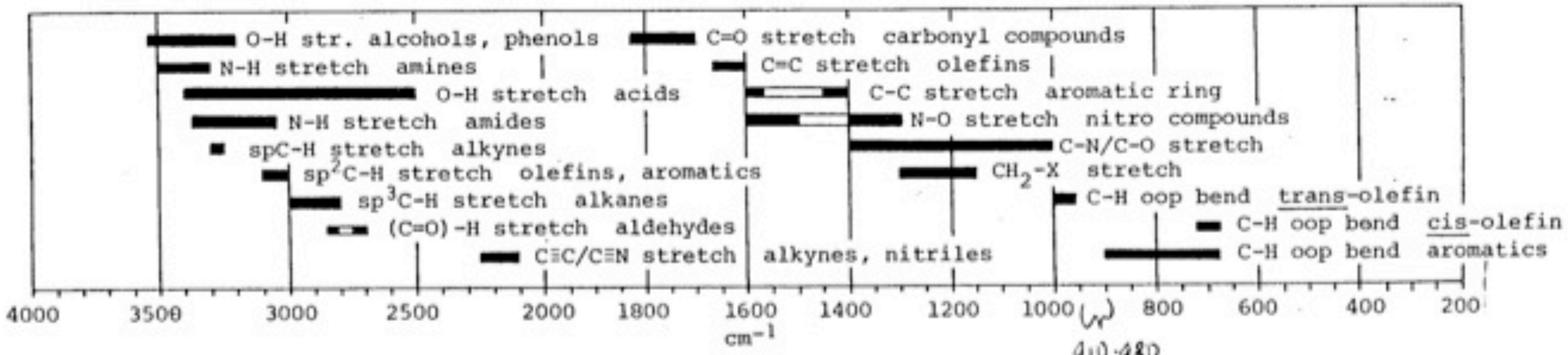
Figure 31.14 Overtones and combination bands of substituted benzenes (from D.W. Mayo, R.M. Pike, and P.K. Trumper, *Microscale Organic Laboratory*, 3rd ed. New York: Wiley, 1994).

TABLE VI. Idealized Patterns Useful for Establishing the Substitution Pattern in Substituted Benzenes



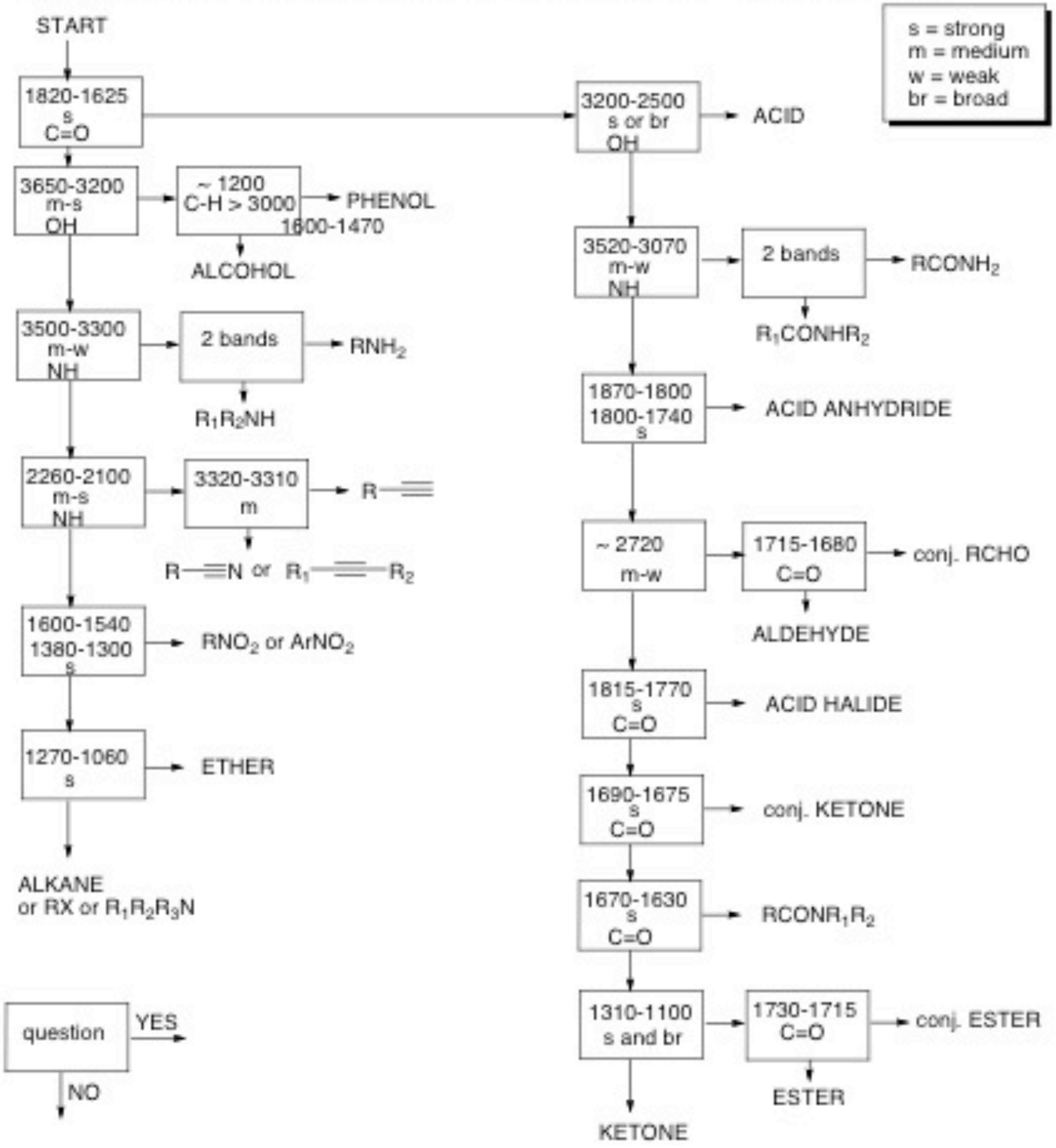
Both regions may be obscured by other absorptions and the best fit for both regions should be sought. Note that the intensity of the absorptions in the 2000 to 1600 cm^{-1} regions are exaggerated for clarity.

TABLE VII. Typical Absorption Regions for Some Common Functional Groups



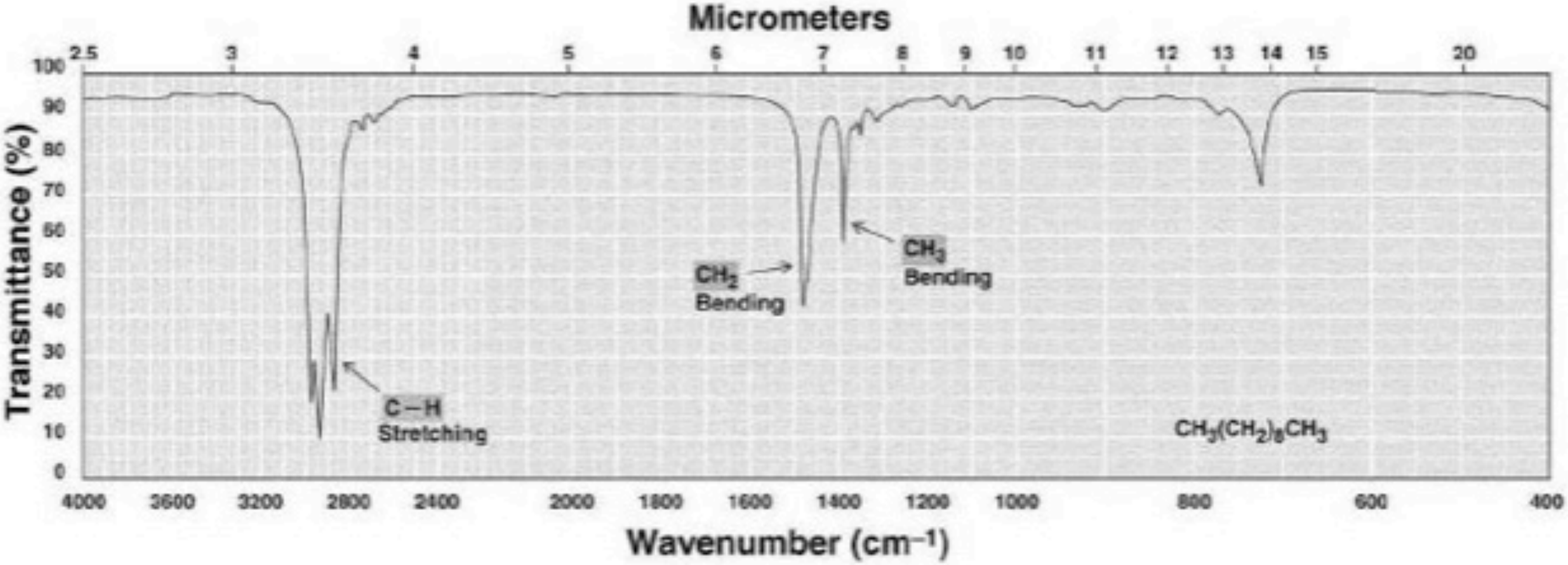
910-980
OH oop bending
carboxylic acids

INTERPRETATION OF INFRARED SPECTRUM - FLOW CHART



Warning: this chart is only a guideline for a rational interpretation of an IR spectrum. It cannot be substituted for solubility and class tests. If the compound is polyfunctional, then care must be taken in using this chart as one functional group might be overlooked.

IR of Alkanes



$C_{10}H_{22}$

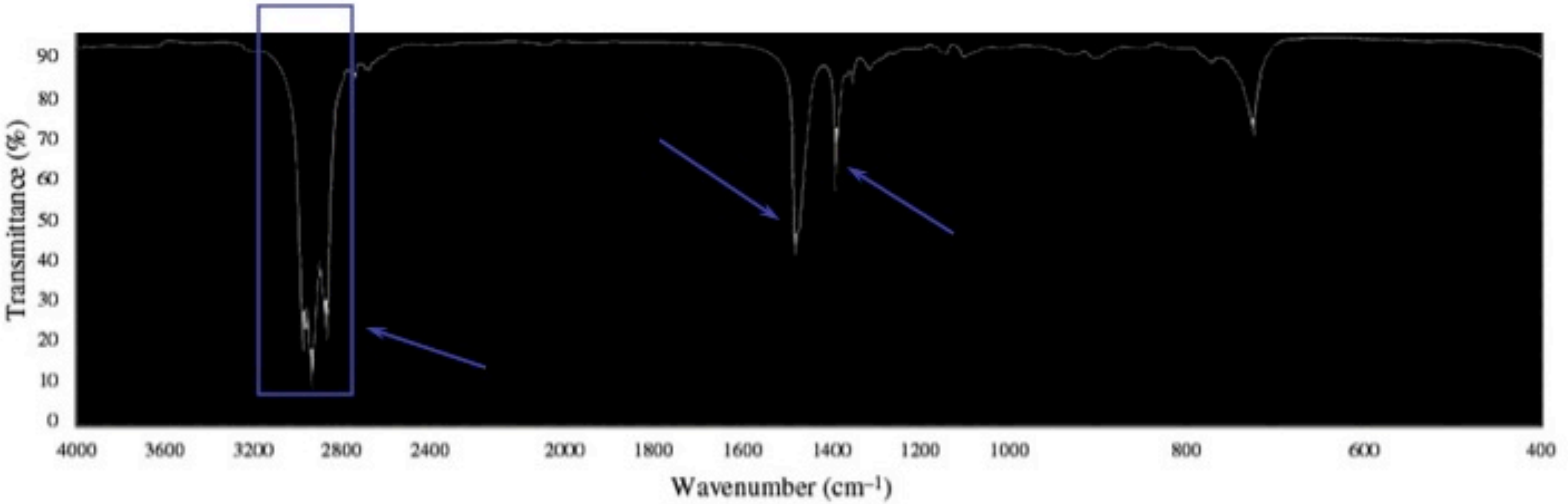
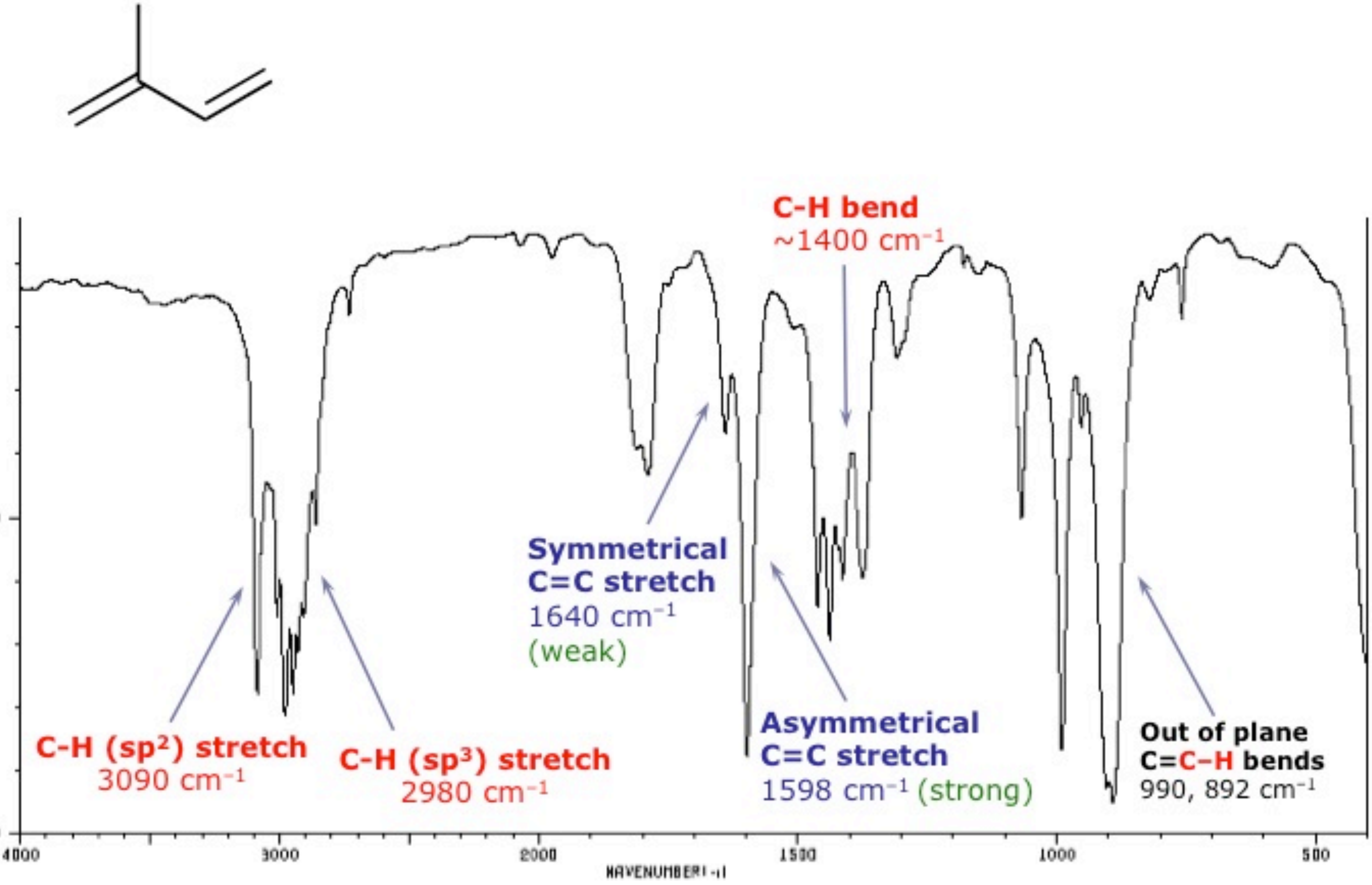


Figure 4.1: IR spectrum of *n*-decane



C-H bend
~1400 cm^{-1}

Symmetrical C=C stretch
1640 cm^{-1}
(weak)

C-H (sp^2) stretch
3090 cm^{-1}

C-H (sp^3) stretch
2980 cm^{-1}

Asymmetrical C=C stretch
1598 cm^{-1} (strong)

Out of plane C=C–H bends
990, 892 cm^{-1}

Figure 4.2: IR spectrum of 2-methyl-1,3-butadiene

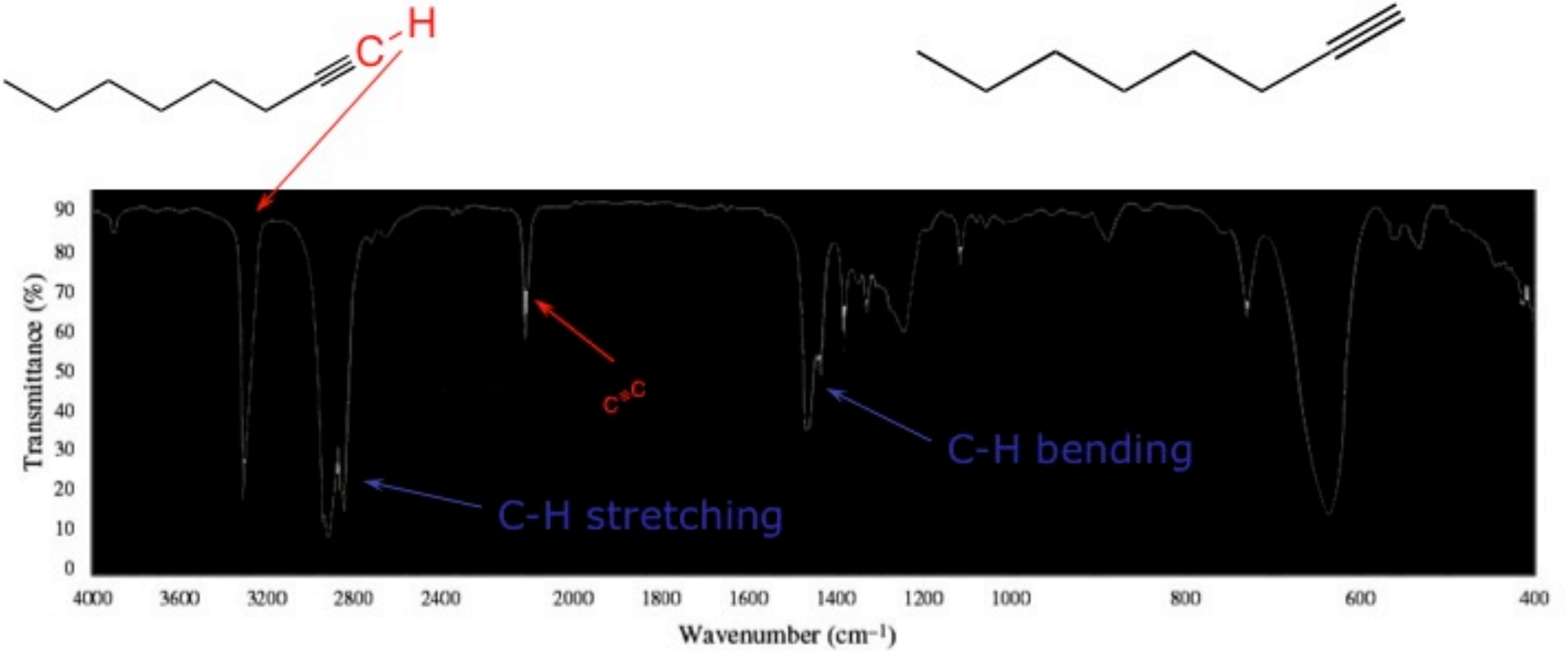
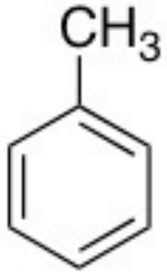


Figure 4.3: IR spectrum of 1-octyne



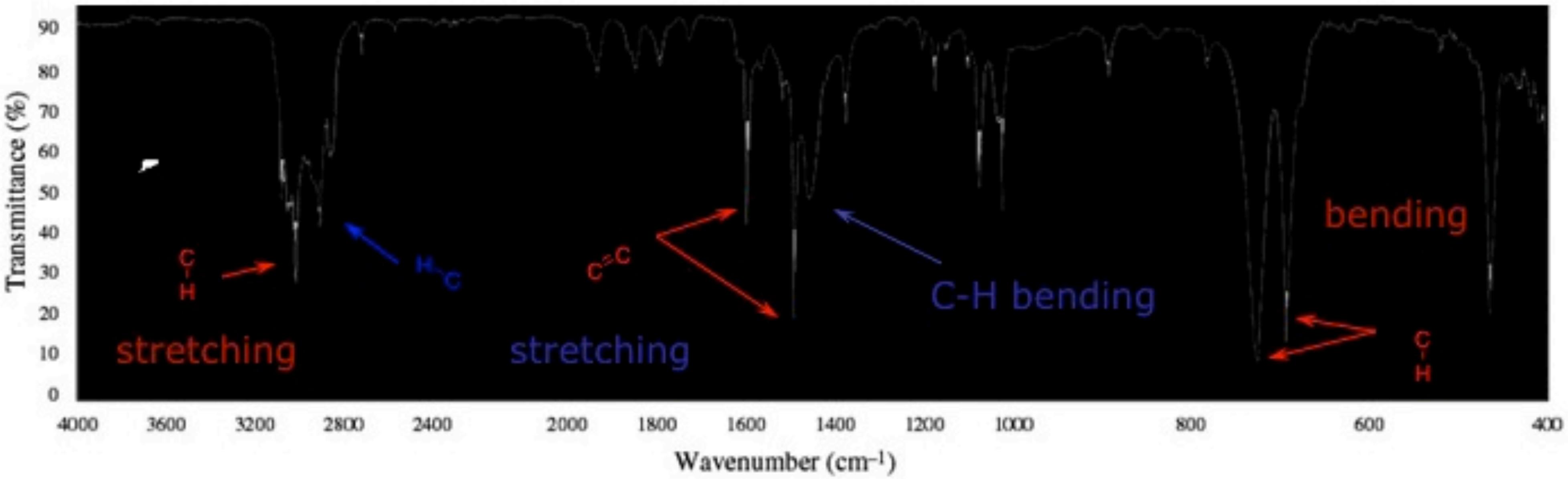
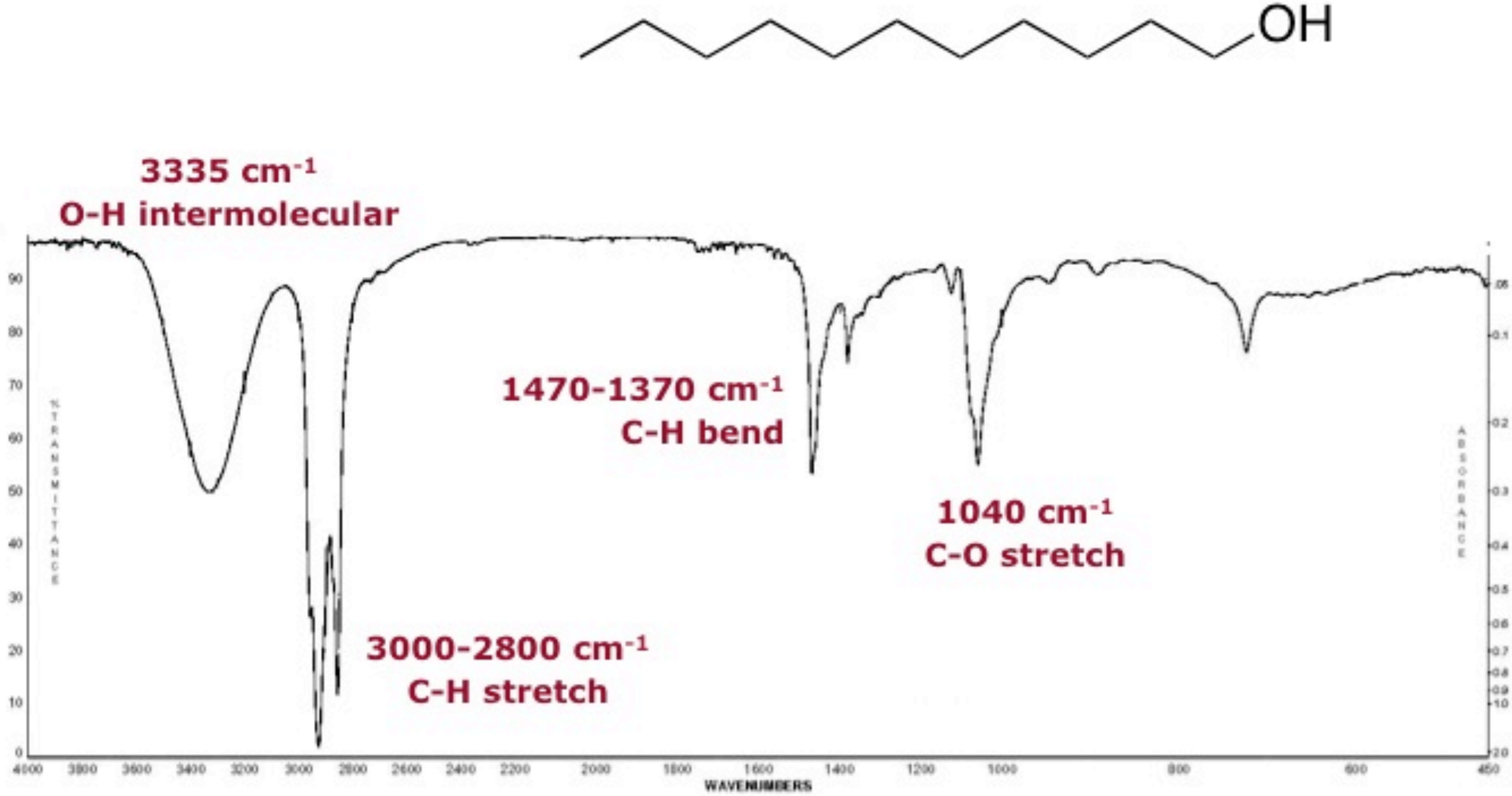


Figure 4.4: IR spectrum of toluene



3335 cm^{-1}
O-H intermolecular

1470-1370 cm^{-1}
C-H bend

1040 cm^{-1}
C-O stretch

3000-2800 cm^{-1}
C-H stretch

Figure 4.5: IR spectrum of 1-undecanol

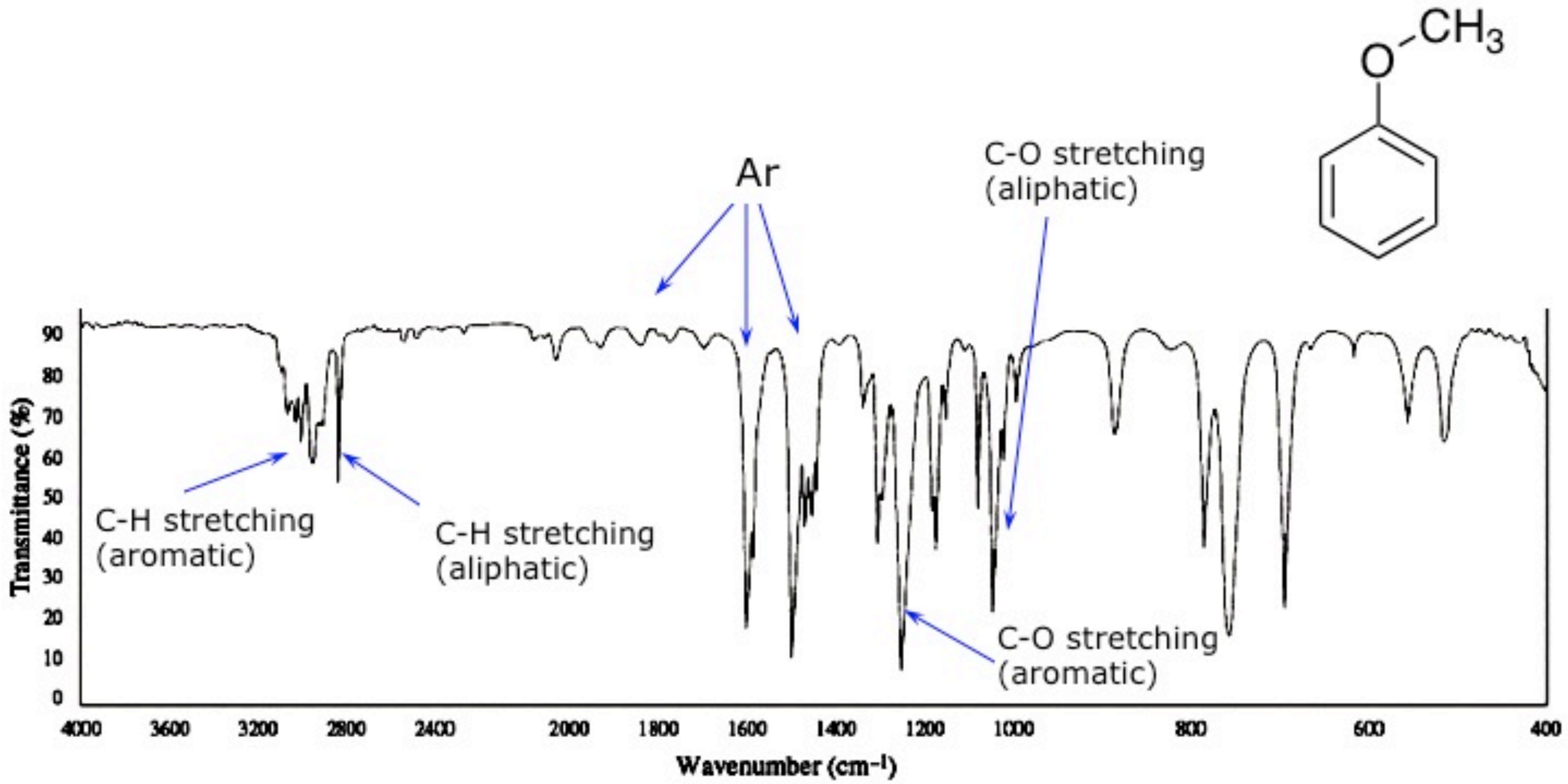


Figure 4.6: IR spectrum of anisole

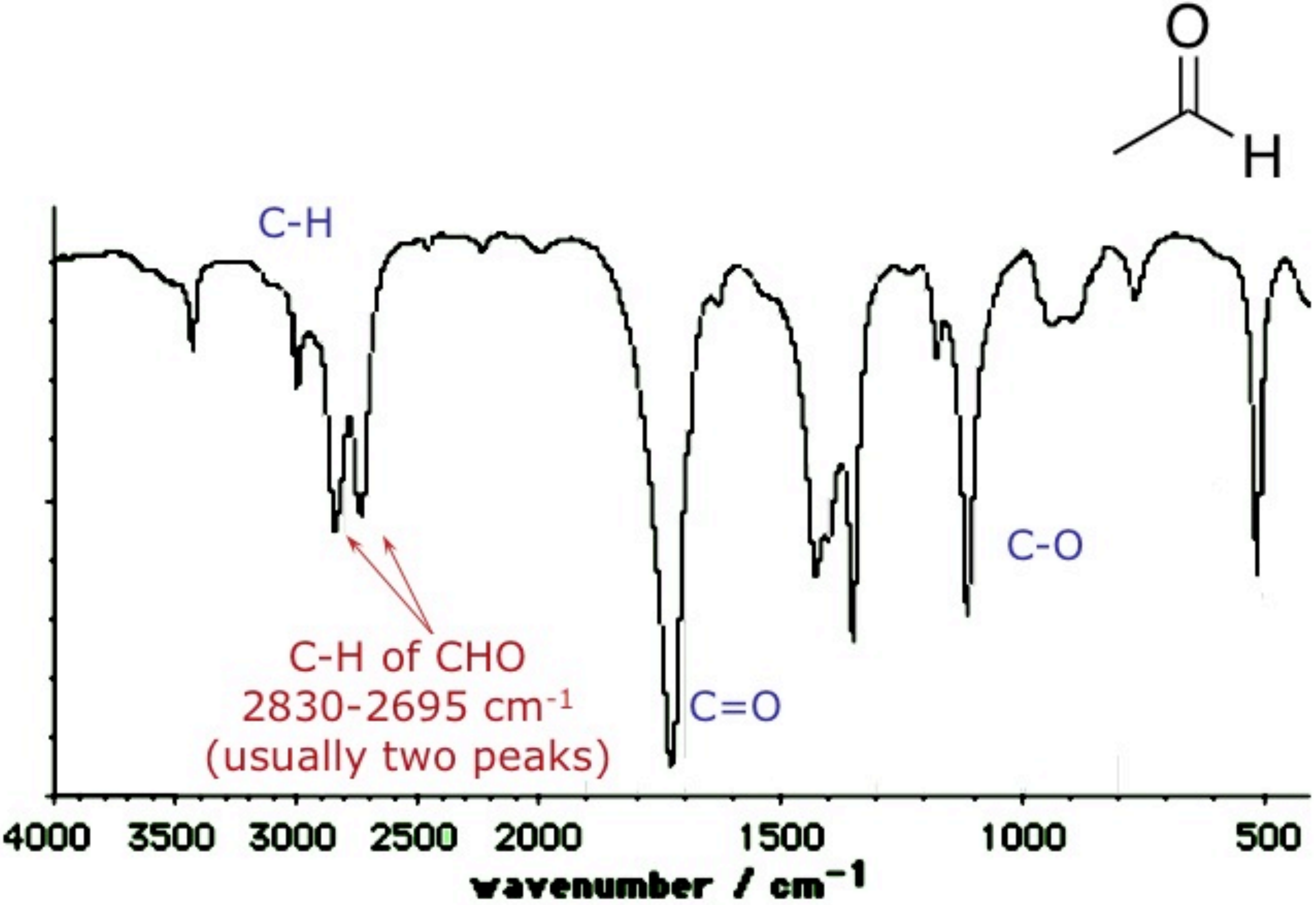


Figure 4.7: IR spectrum of acetaldehyde

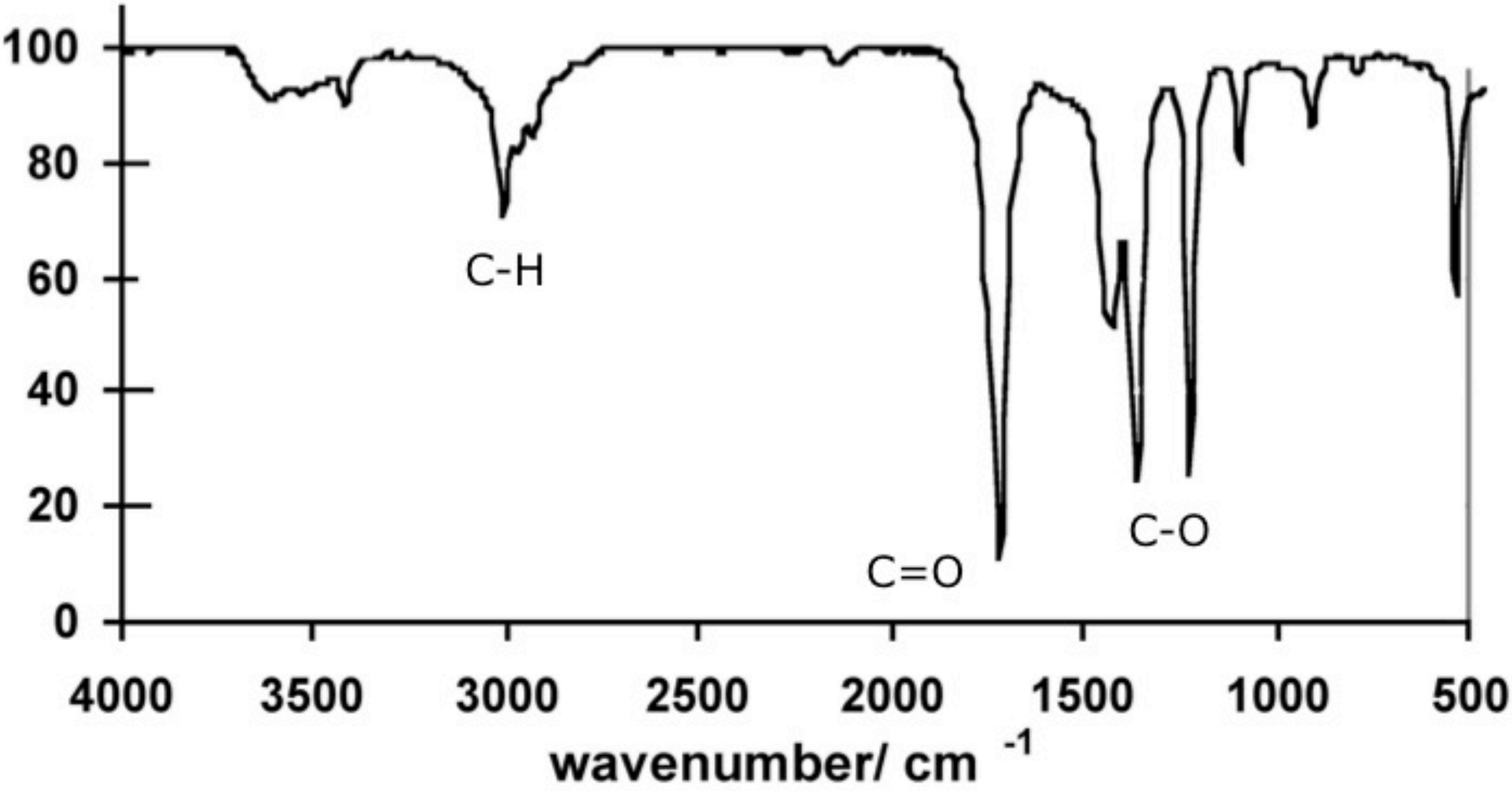


Figure 4.8: IR spectrum of acetone

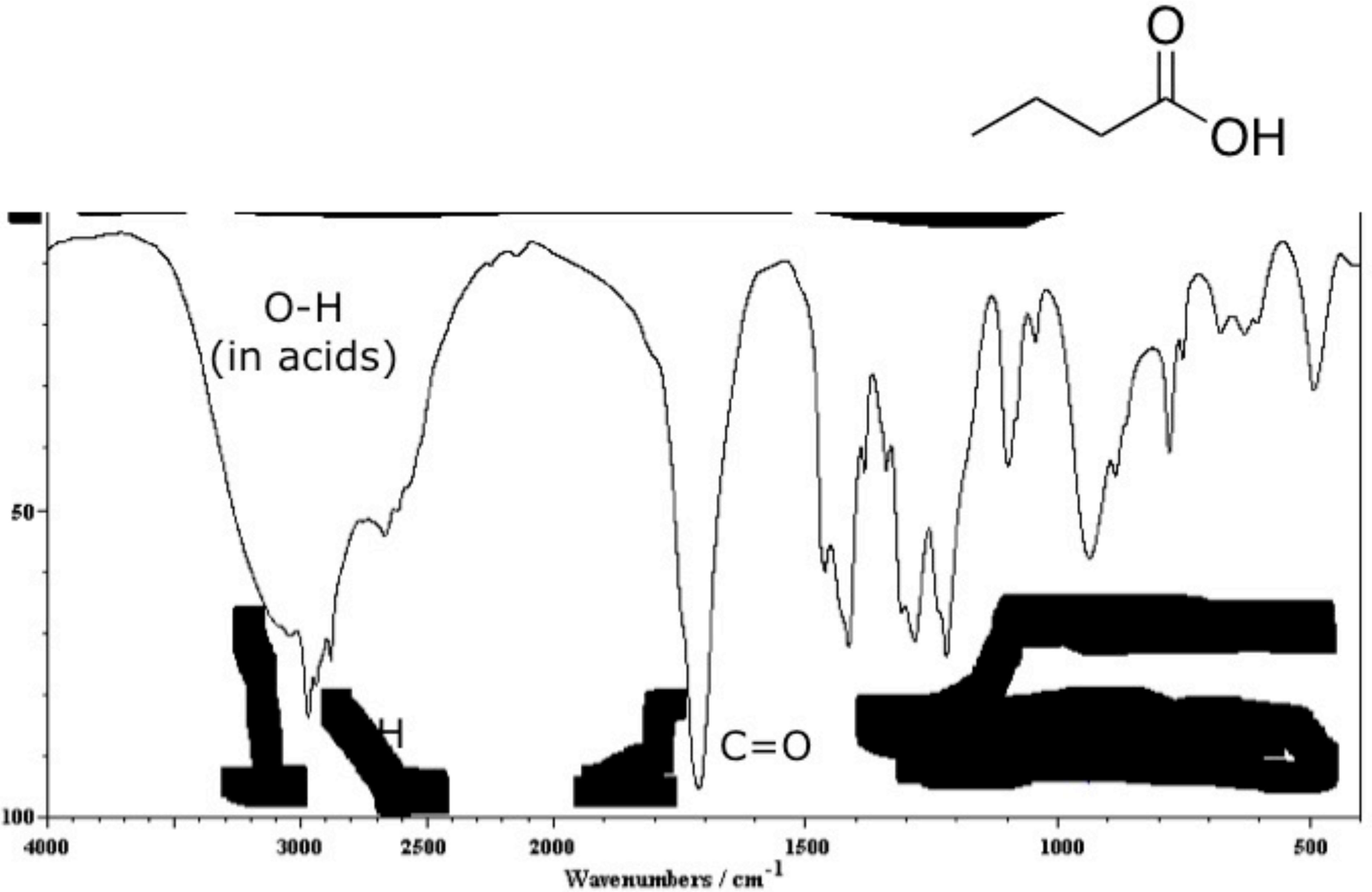
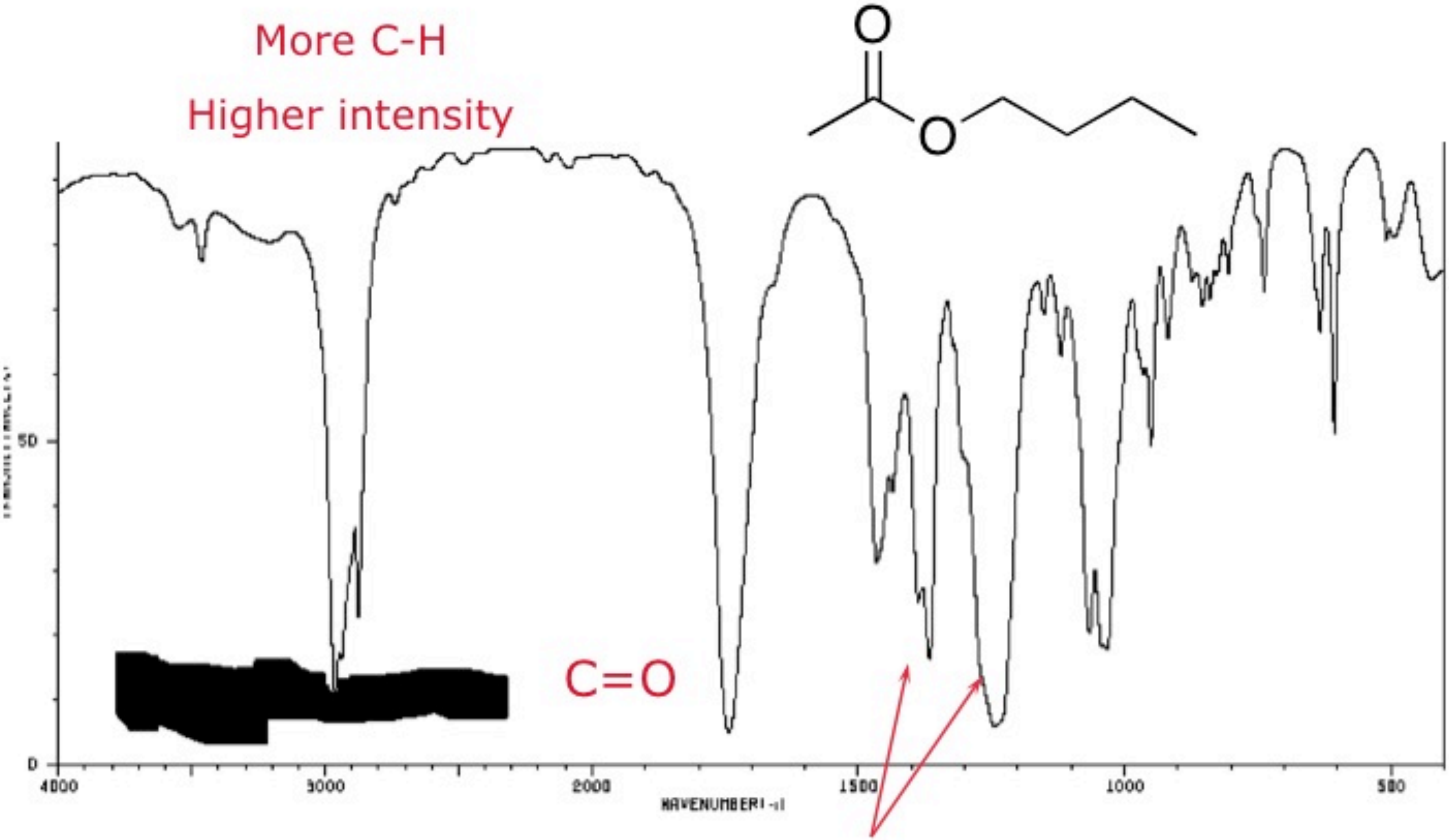


Figure 4.9: IR spectrum of butanoic acid



[redacted]

More C-H

Higher intensity

C=O

C-O

Figure 4.10: IR spectrum of butylacetate

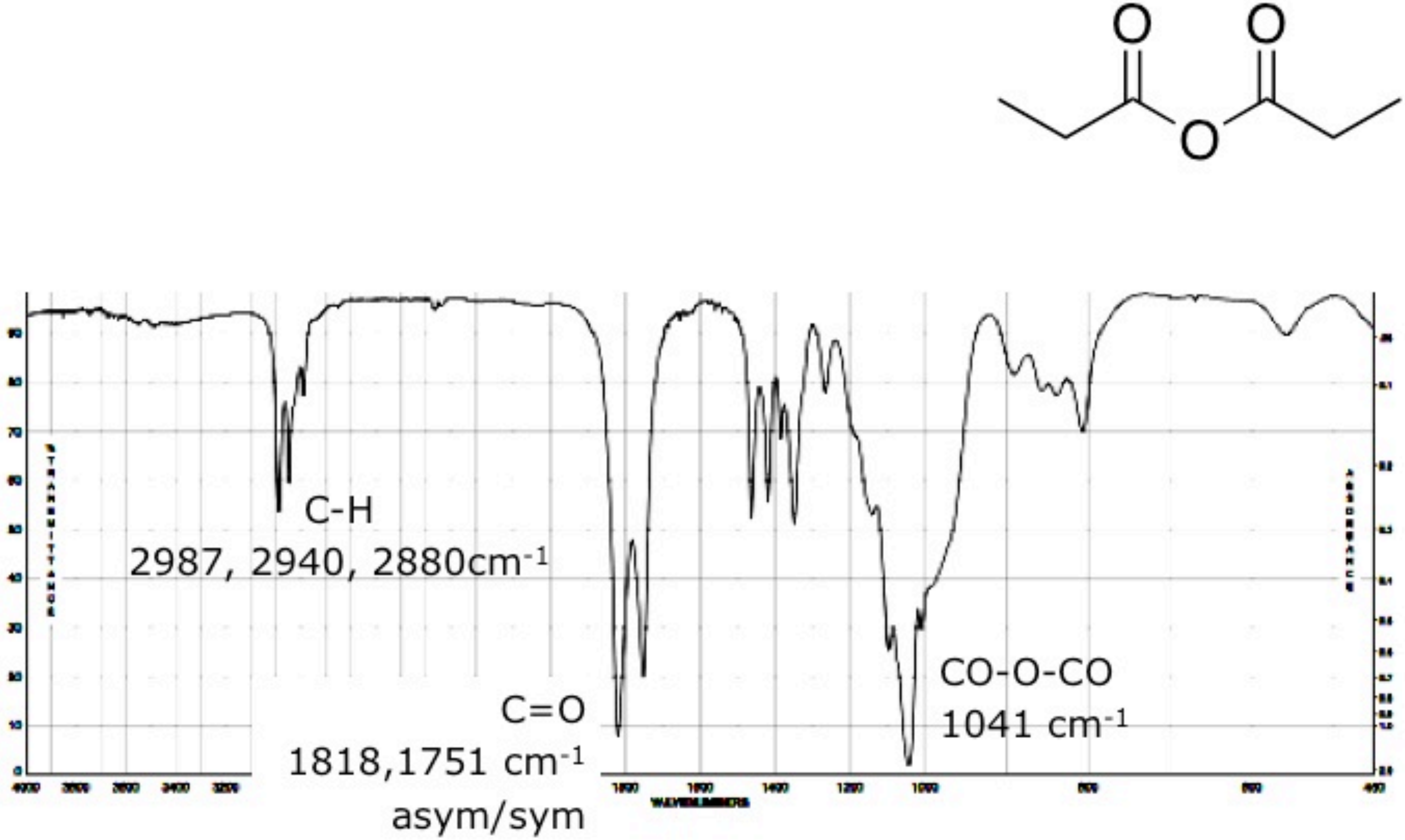
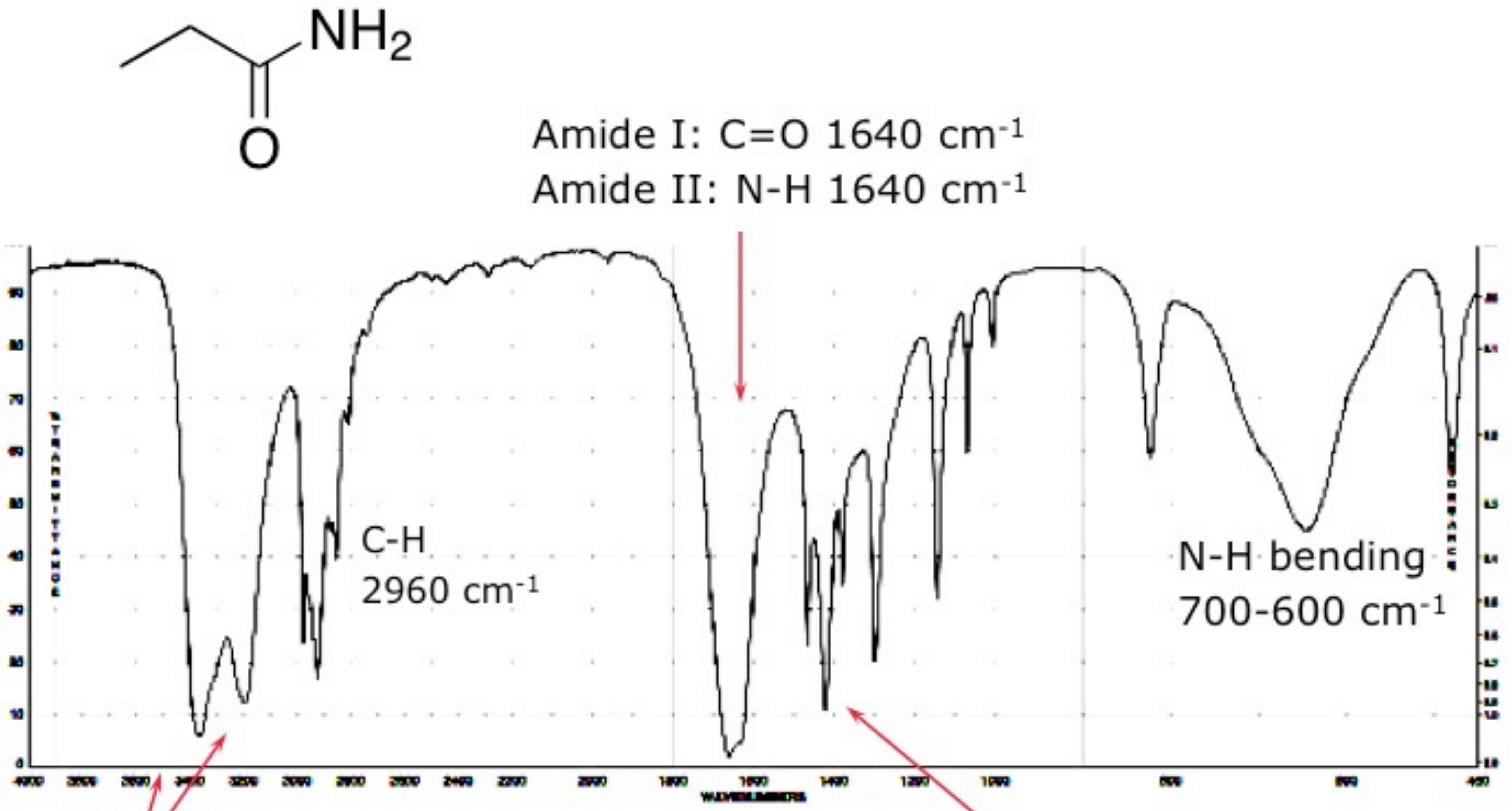


Figure 4.11: IR spectrum of propionic anhydride



Amide I: C=O 1640 cm^{-1}
Amide II: N-H 1640 cm^{-1}

C-H
2960 cm^{-1}

N-H bending
700-600 cm^{-1}

NH$_2$
3350 & 3170cm^{-1}
asym & sym

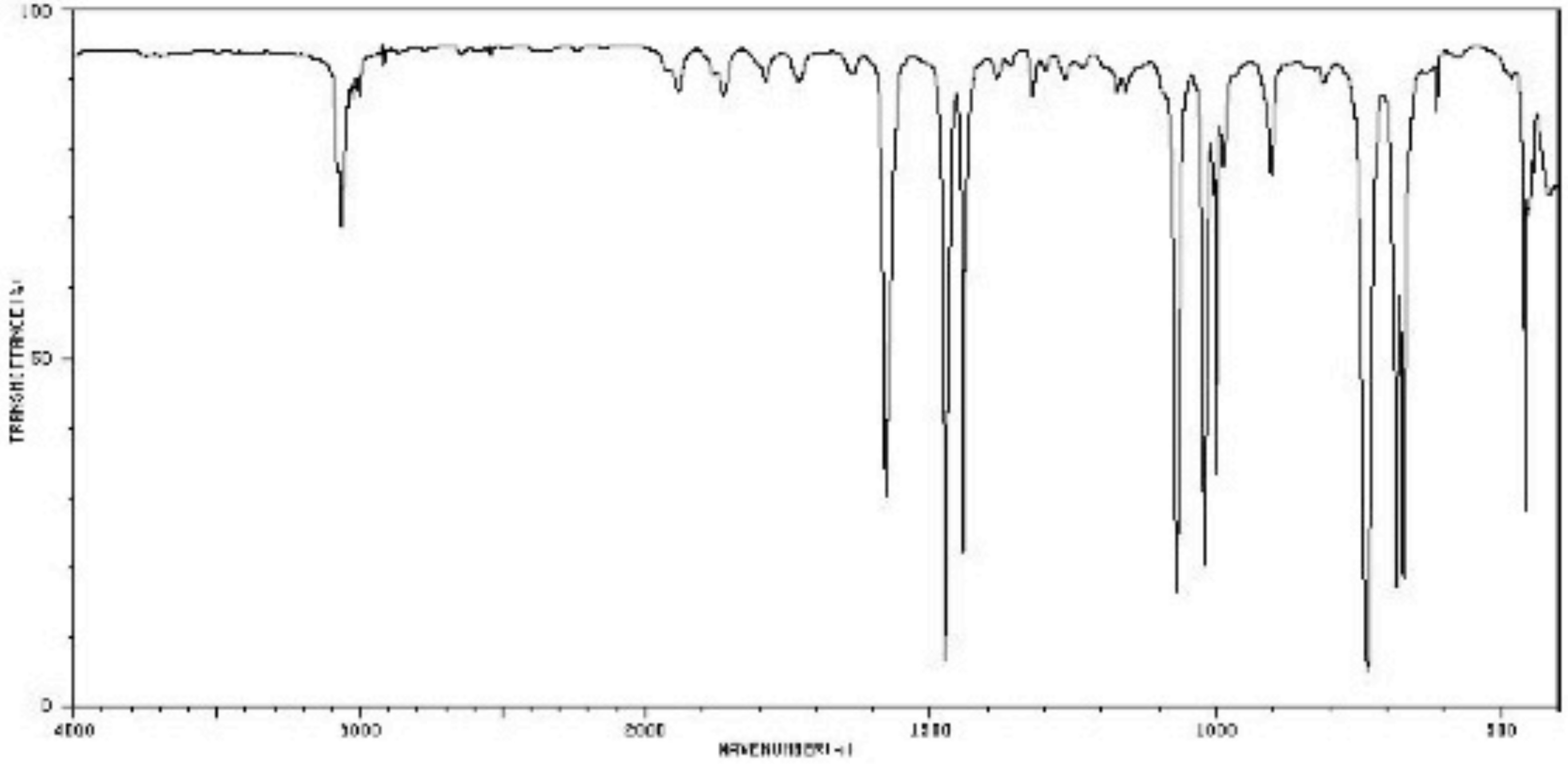
C-N
1425 cm^{-1}

Figure 4.12: IR spectrum of propionamide

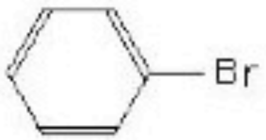
HIT-NO=1058 | SCORE= ( ) | SDBS-NO=660 | IR-NIDA-63553 : LIQUID FILM

BROMOBENZENE

C_6H_5BR



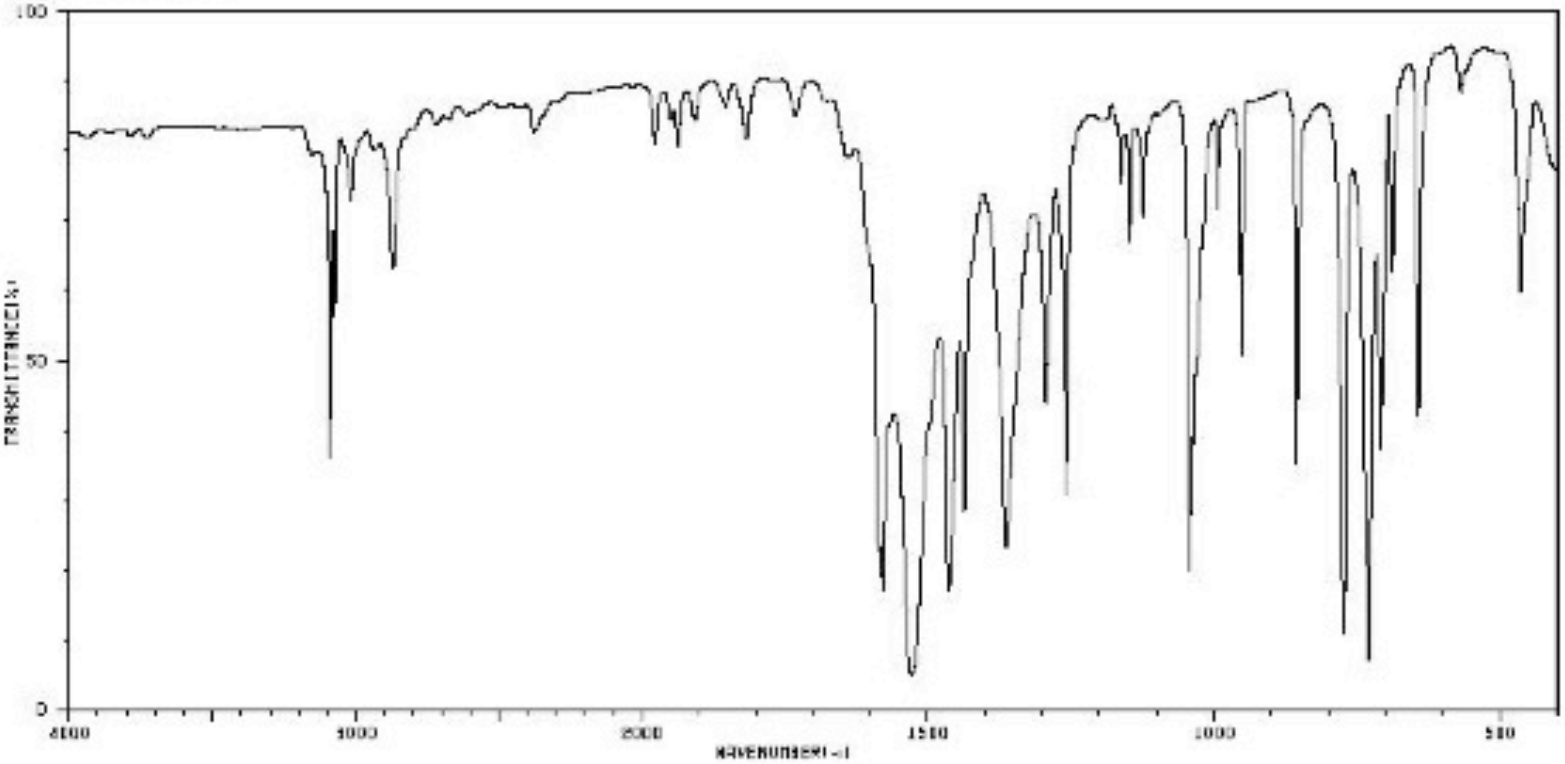
3077	74	1780	86	1158	84	812	85
3066	66	1730	86	1068	15	735	4
3055	72	1579	29	1020	19	684	15
3024	84	1476	6	1006	70	672	17
3003	84	1443	21	1000	32	613	81
1942	84	1322	84	988	74	467	25
1862	84	1174	84	903	72	447	72



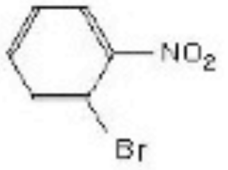
HIT-NO=2081	SCORE= ( )	SDBS-NO=2853	IR-NIDA-07458 : LIQUID FILM

O-BROMONITROBENZENE

$C_6H_4BRNO_2$



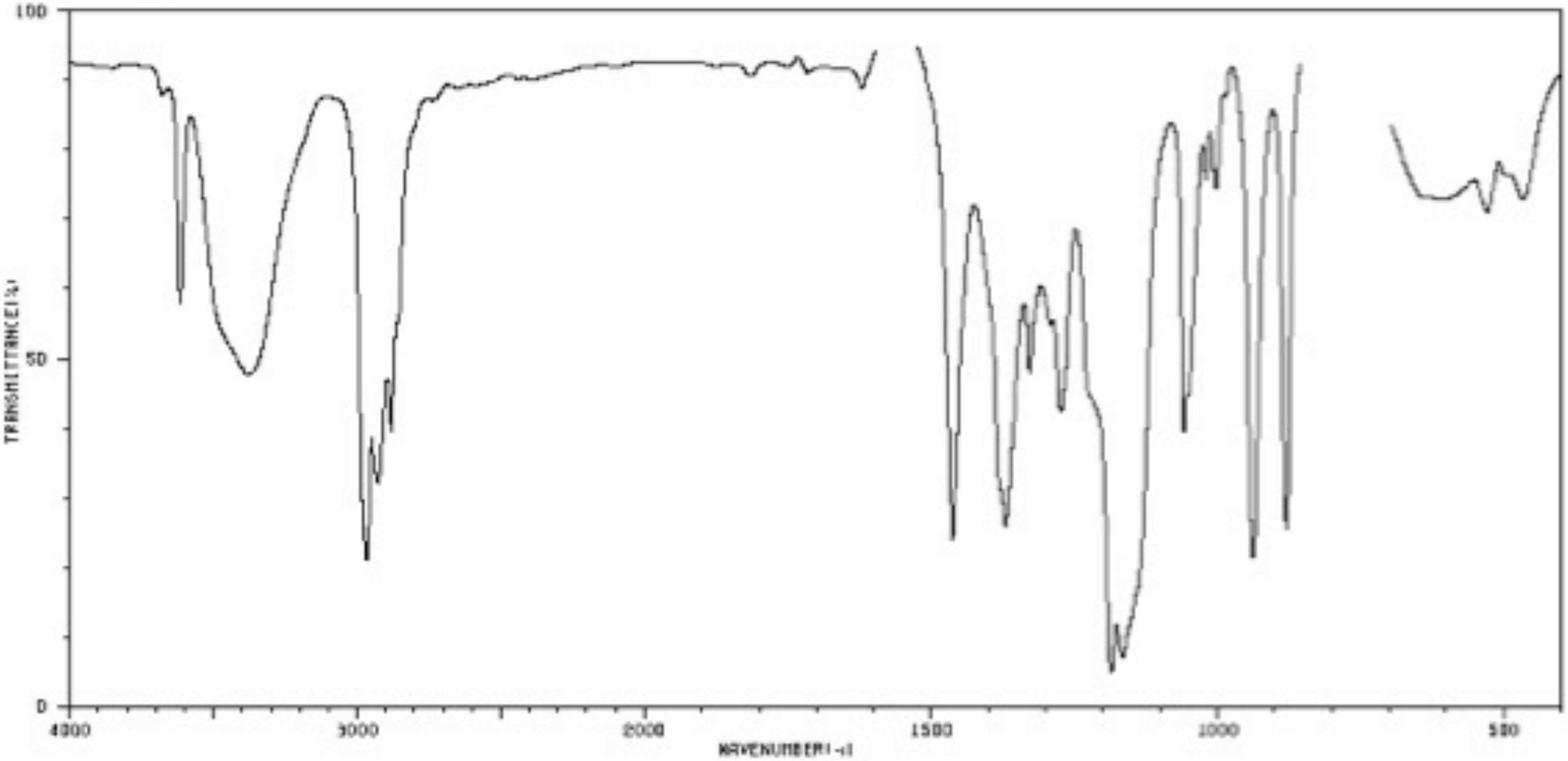
3730	79	1960	81	1529	4	1148	64	856	34
3090	36	1937	77	1464	16	1124	68	773	10
3074	53	1817	78	1436	26	1042	18	729	6
3016	70	1731	81	1364	22	1037	36	708	36
2869	80	1639	77	1295	42	1030	49	689	60
2376	79	1588	21	1259	29	993	68	644	41
1977	79	1579	18	1164	72	962	49	464	67



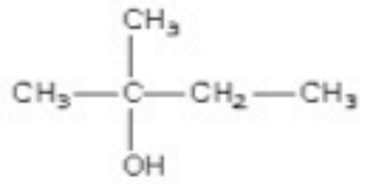
HIT-NO=1407	SCORE= ( )	SDBS-NO=1709	IR-NIDA-06259 : CCL4 SOLUTION

2-METHYL-2-BUTANOL

$C_5H_{12}O$



3616	66	1370	26	1020	72
3376	46	1329	46	1003	72
2967	20	1274	41	938	20
2927	31	1186	4	880	24
2881	38	1167	7	528	68
1621	86	1050	38	466	70
1464	23	1064	43		

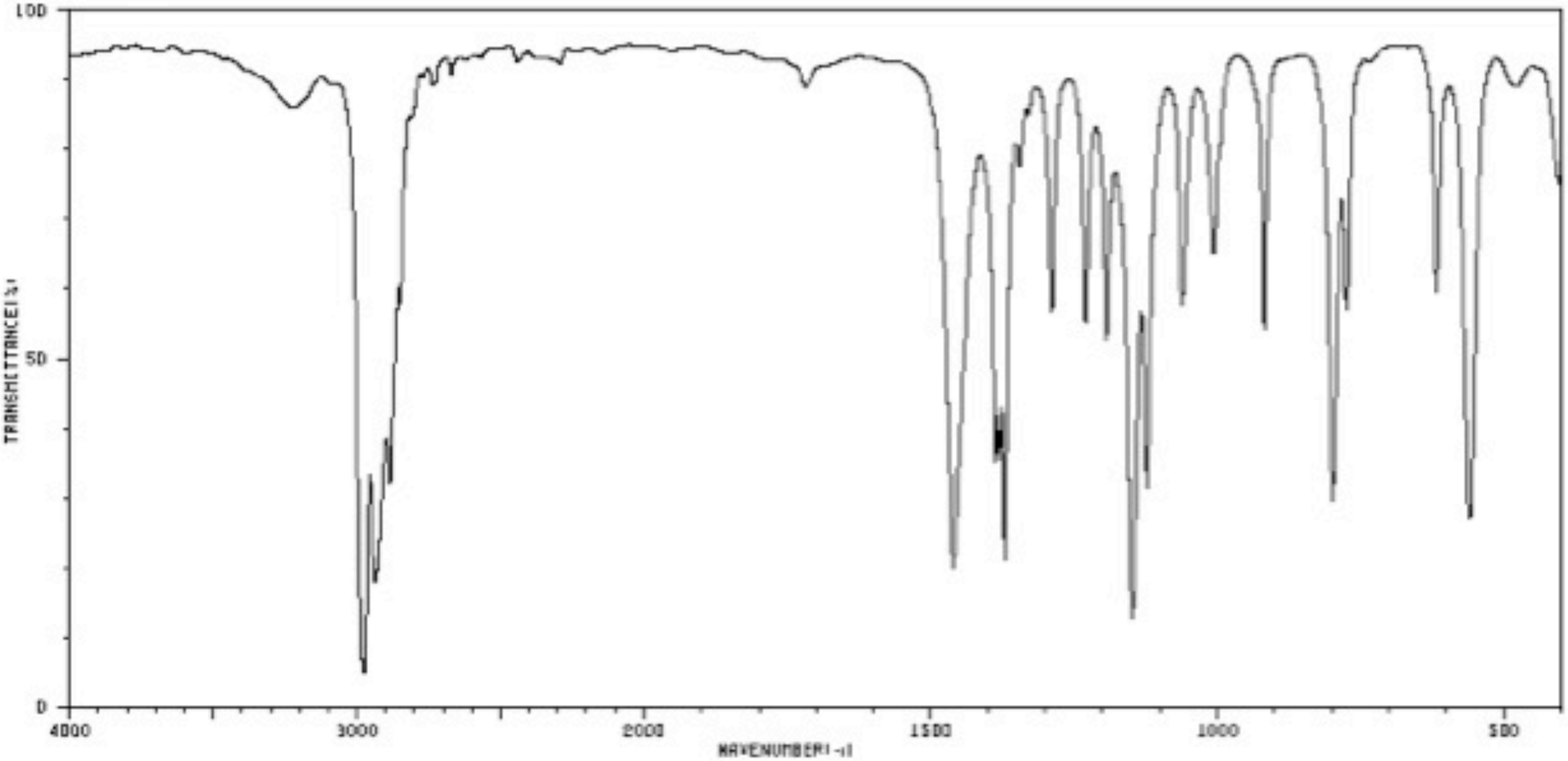


$CH_3-C(CH_3)(OH)-CH_2-CH_3$

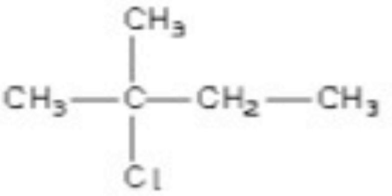
HIT-NO=1050 | SCORE= ( ) | SDBS-NO=534 | IR-NIDA-65783 : LIQUID FILM

2-CHLORO-2-METHYLBUTANE

$C_5H_{11}CL$



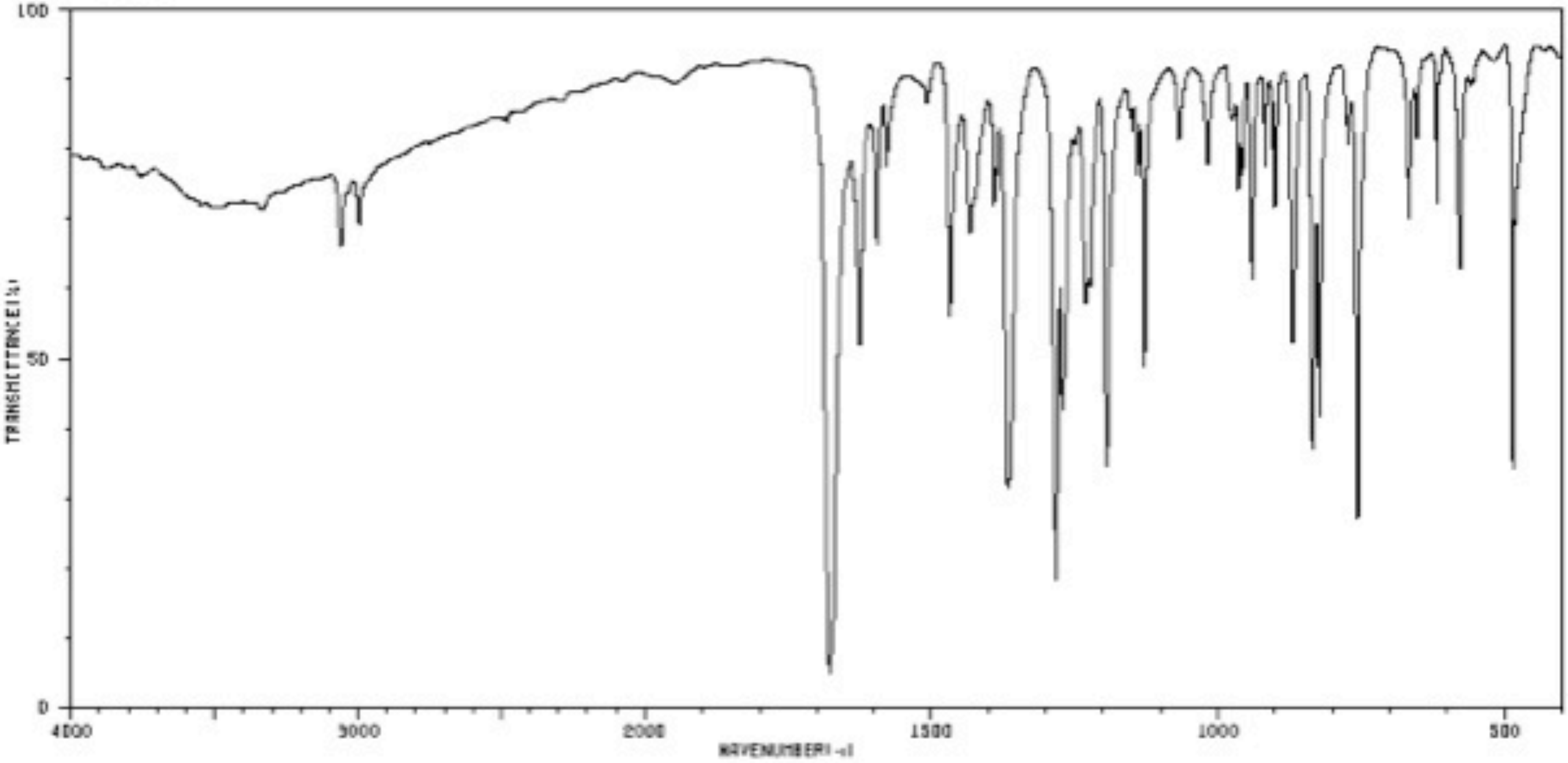
3233	64	1719	86	1230	63	799	28
3222	81	1460	18	1194	50	773	55
2975	4	1387	34	1149	12	617	57
2936	17	1380	34	1123	30	560	26
2884	30	1370	20	1062	55	480	86
2846	55	1344	74	1005	62		
2738	86	1289	66	919	62		



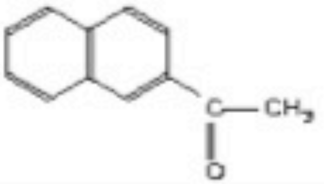
HIT-NO=4385	SCORE= ( )	SDBS-NO=7051	IR-NIDA-19176 : KBR DISC

2'-ACETONAPHTHONE

$C_{12}H_{10}O$



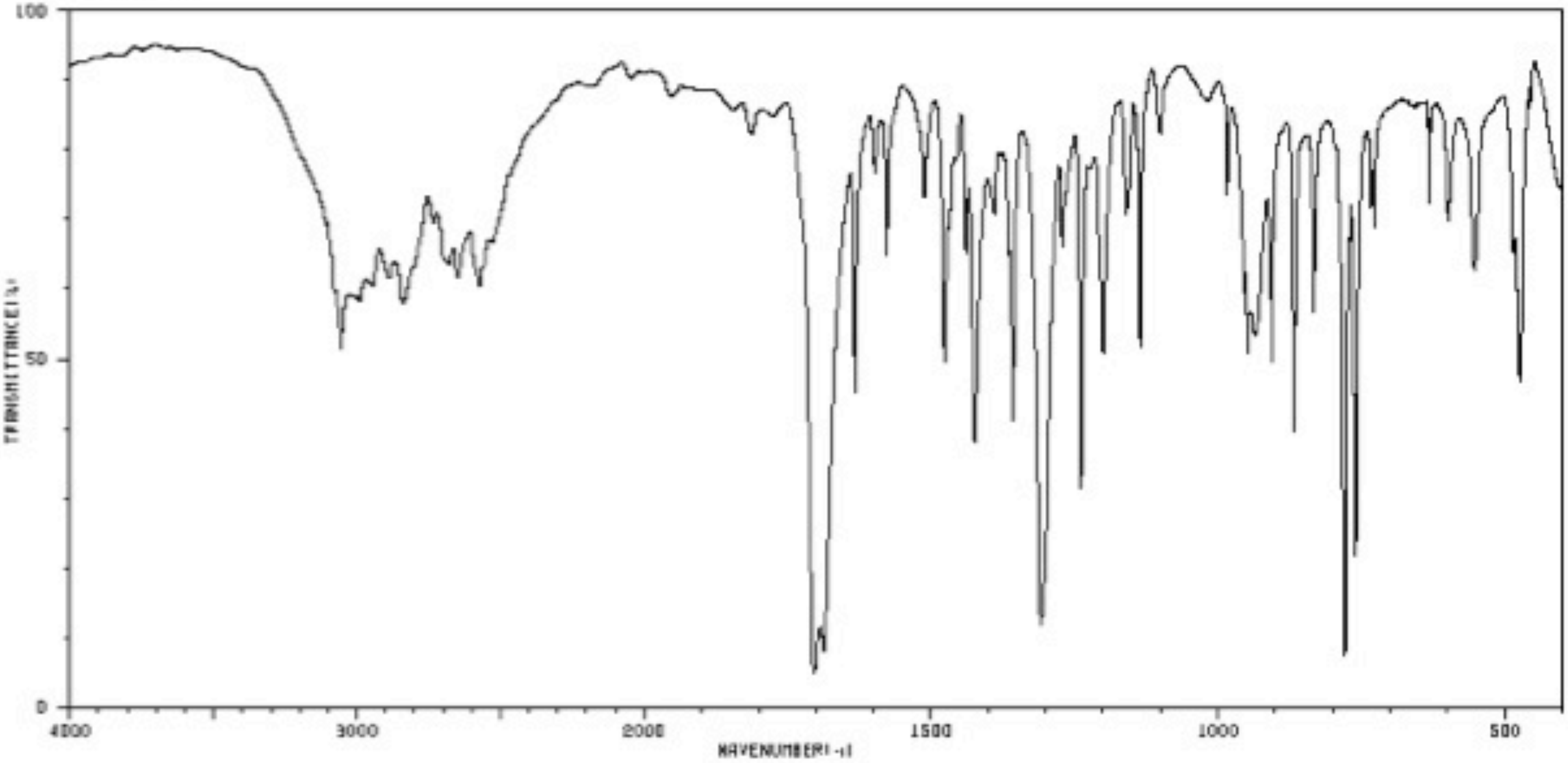
3766	72	1578	74	1282	17	1018	74	823	39
3059	64	1468	53	1270	41	965	72	756	26
3042	70	1433	65	1231	55	958	74	667	68
2996	66	1426	70	1224	68	941	68	619	70
1677	4	1391	70	1194	33	900	68	578	60
1625	50	1388	72	1141	74	870	50	486	33
1596	64	1366	30	1128	47	834	36	479	72



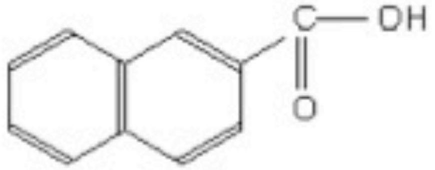
HIT-NO=4294	SCORE= ( )	SDBS-NO=6884	IR-NIDA-63348 : KBR DISC

2-NAPHTHOIC ACID

$C_{11}H_8O_2$



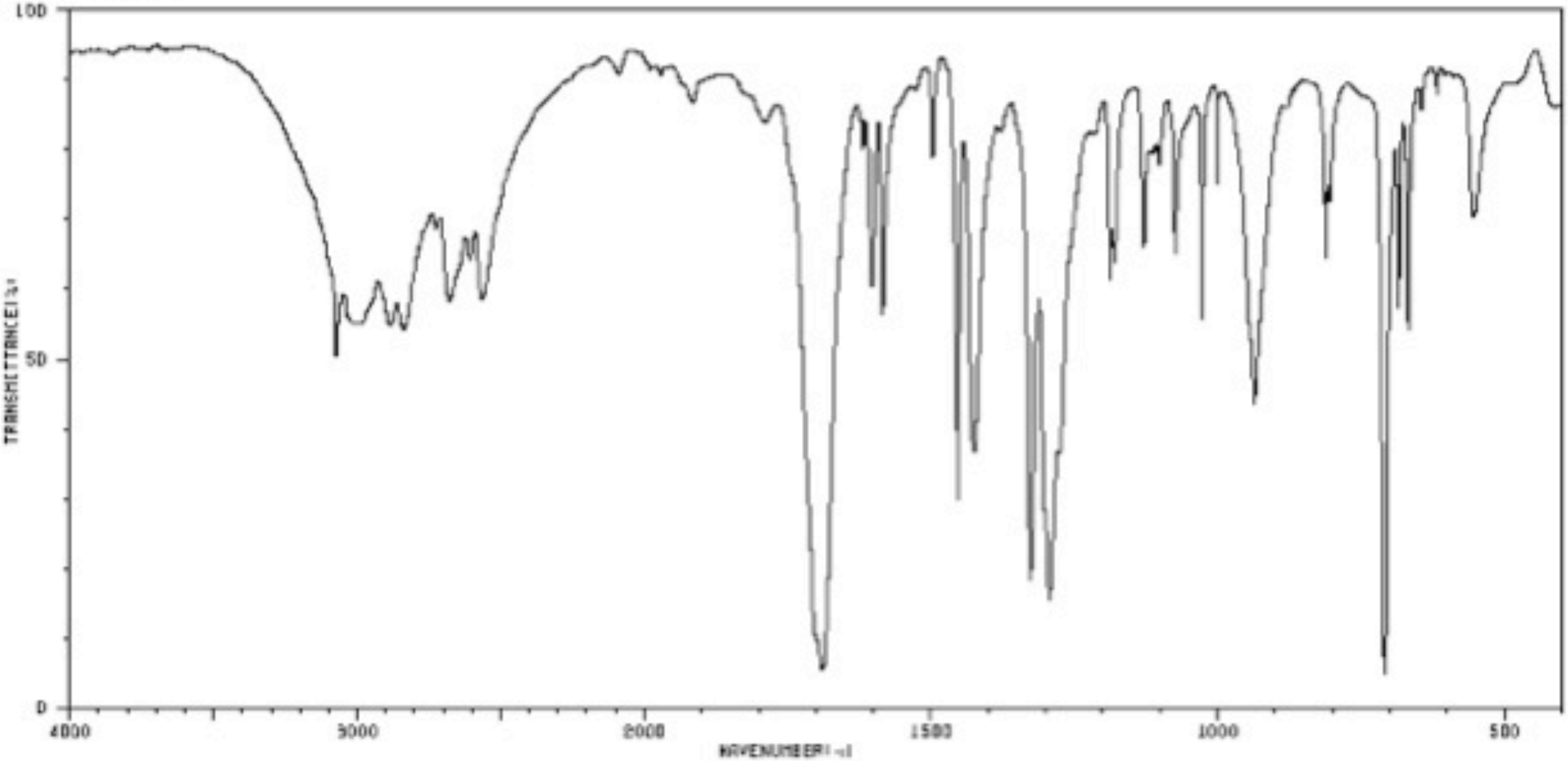
3054	49	2573	58	1439	62	1136	60	779	7
3031	57	2560	60	1424	36	956	57	771	64
2887	58	1703	4	1364	82	948	49	761	21
2837	66	1687	7	1358	39	936	62	664	60
2693	62	1633	43	1309	11	906	47	486	62
2679	82	1577	62	1239	30	858	38	480	58
2647	68	1477	47	1200	49	833	66	474	44



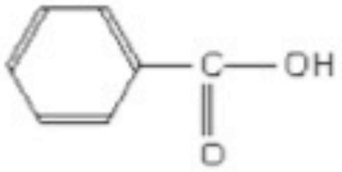
HIT-NO=1081	SCORE= ( )	SDBS-NO=673	IR-NIDA-63340 : KBR DISC

BENZOIC ACID

$C_7H_6O_2$



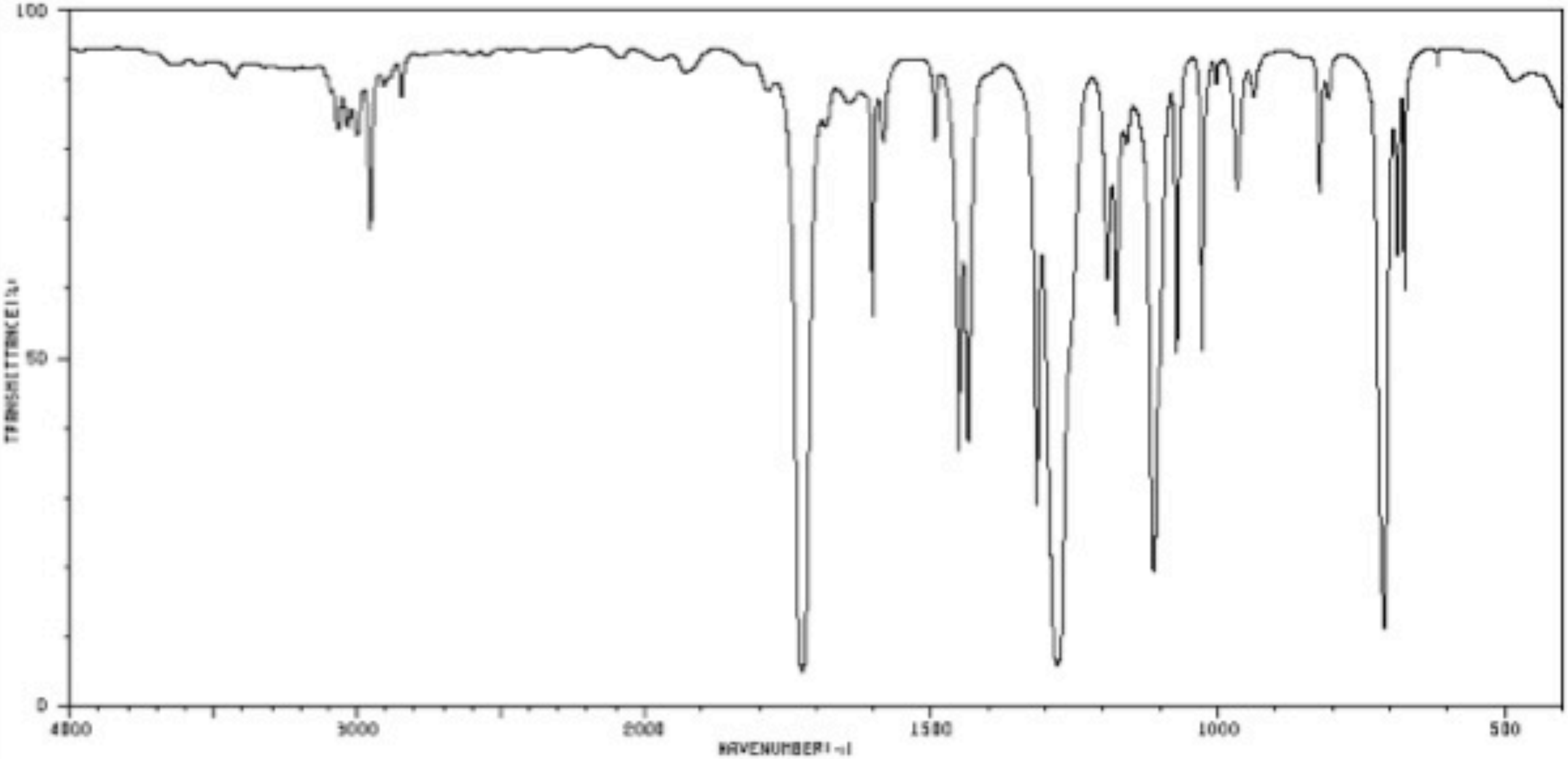
3073	49	2678	67	1426	36	1112	77	936	42
3012	53	2607	62	1327	17	1107	77	812	62
2998	53	2564	57	1294	14	1102	74	805	70
2986	63	1689	6	1187	68	1074	62	708	4
2886	52	1603	58	1180	60	1028	53	685	55
2836	52	1585	59	1129	64	1001	72	667	52
2726	66	1464	28	1118	77	943	50	664	68



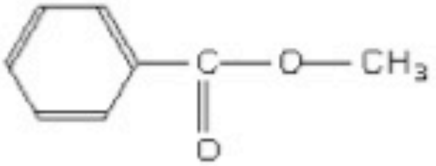
HIT-NO=1155	SCORE= ( )	SDBS-NO=725	IR-NIDA-00428 : LIQUID FILM

METHYL BENZOATE

$C_8H_8O_2$



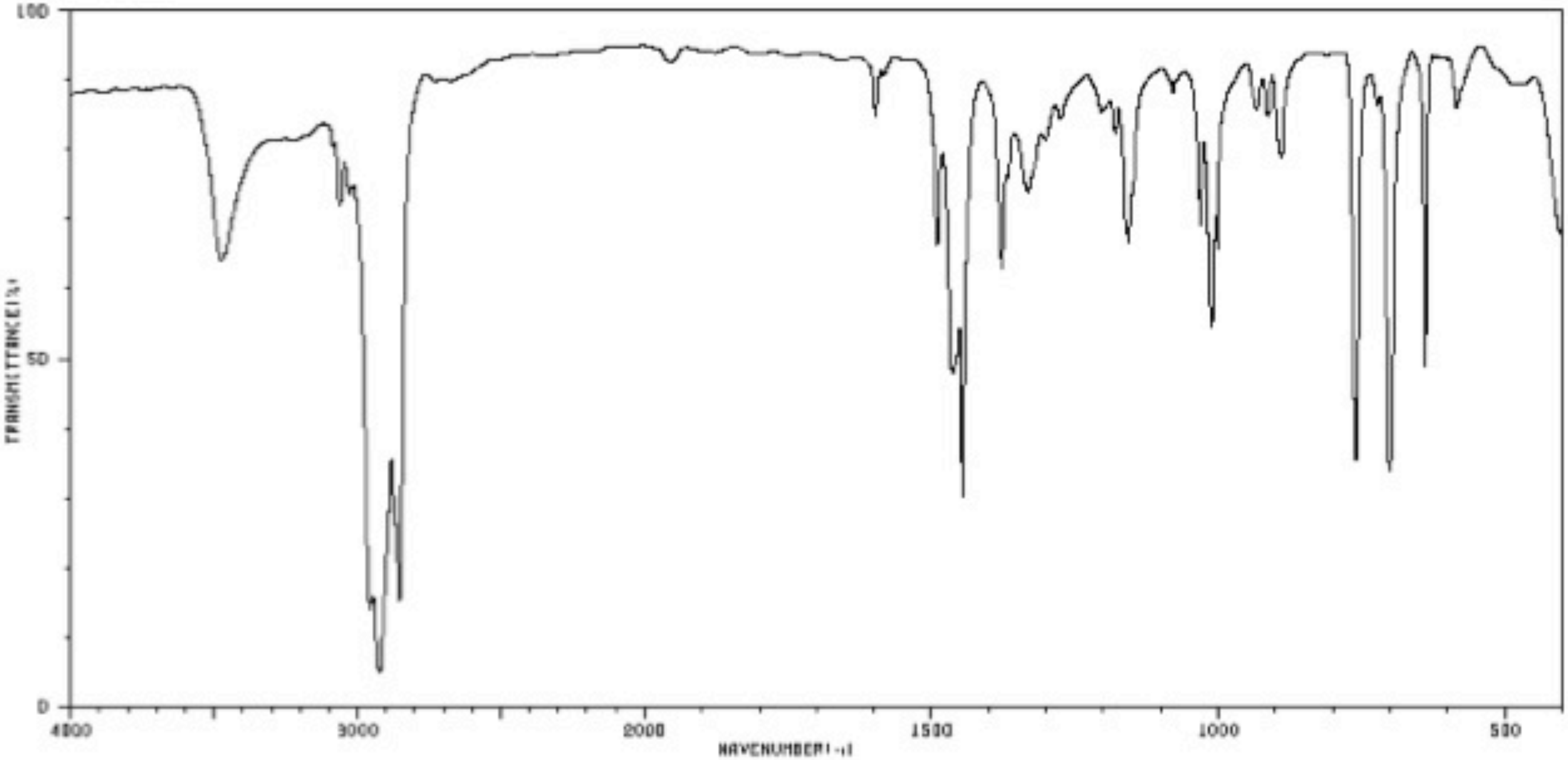
3066	79	1724	4	1316	27	1028	49	688	62
3034	79	1644	84	1279	5	1003	86	676	58
2999	79	1602	55	1193	58	966	72	483	86
2953	66	1582	79	1177	62	937	84		
2907	86	1493	79	1160	77	823	70		
2845	84	1453	35	1112	18	808	84		
1784	84	1436	36	1072	49	710	10		



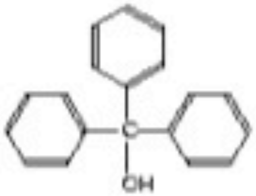
HIT-NO=3027	SCORE= ( )	SDBS-NO=5971	IR-NIDA-64310 : NUJOL MULL

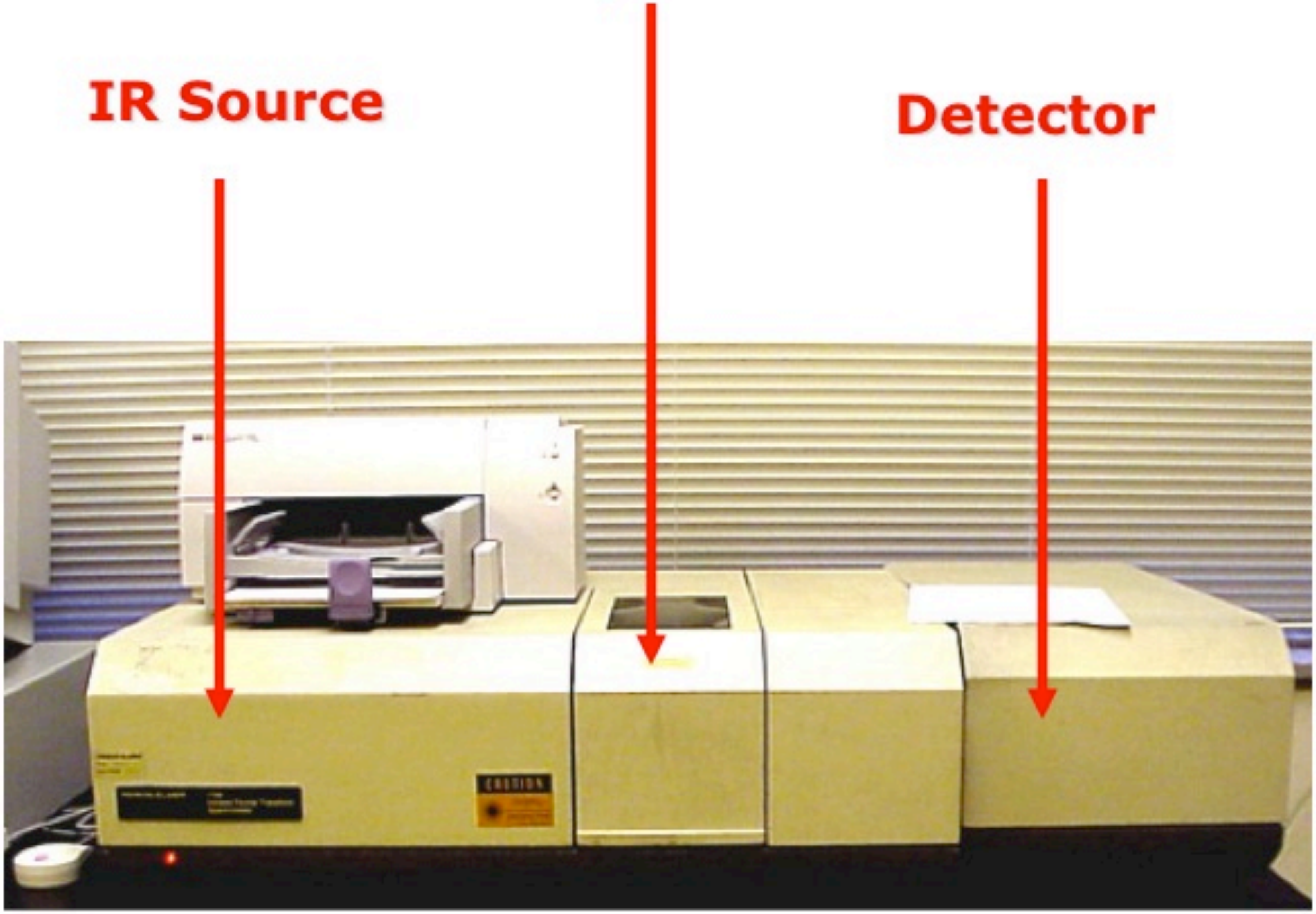
TRIPHENYLMETHANOL

$C_{19}H_{16}O$



3471	62	1491	64	1206	81	1011	62	722	84
3061	68	1463	46	1180	79	1002	62	702	33
3024	70	1448	28	1156	84	940	84	640	47
2956	13	1378	60	1150	70	932	81	592	86
2924	4	1367	72	1084	86	913	81	585	84
2854	14	1332	70	1079	84	890	77	580	84
1598	81	1276	81	1031	66	760	34	476	86



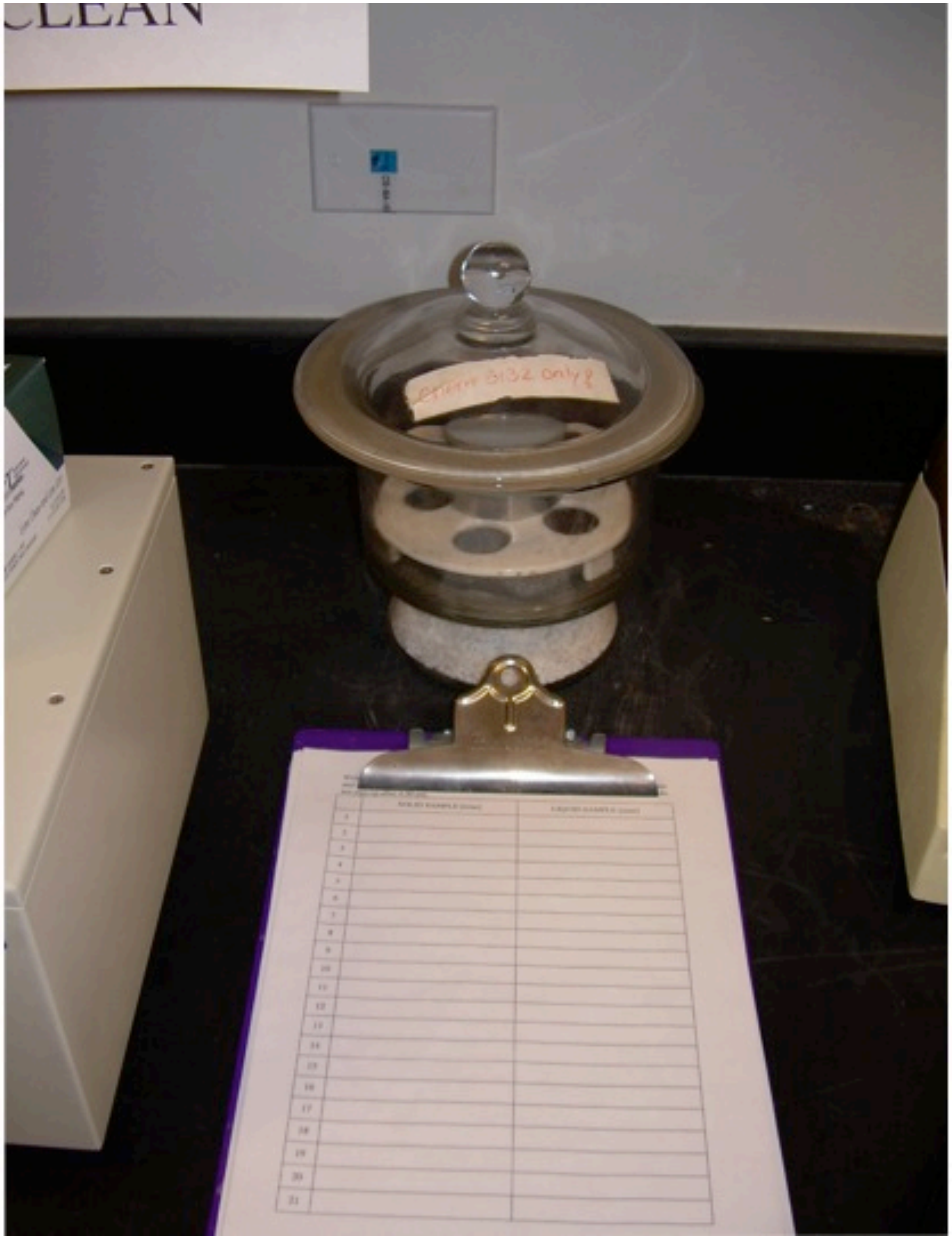


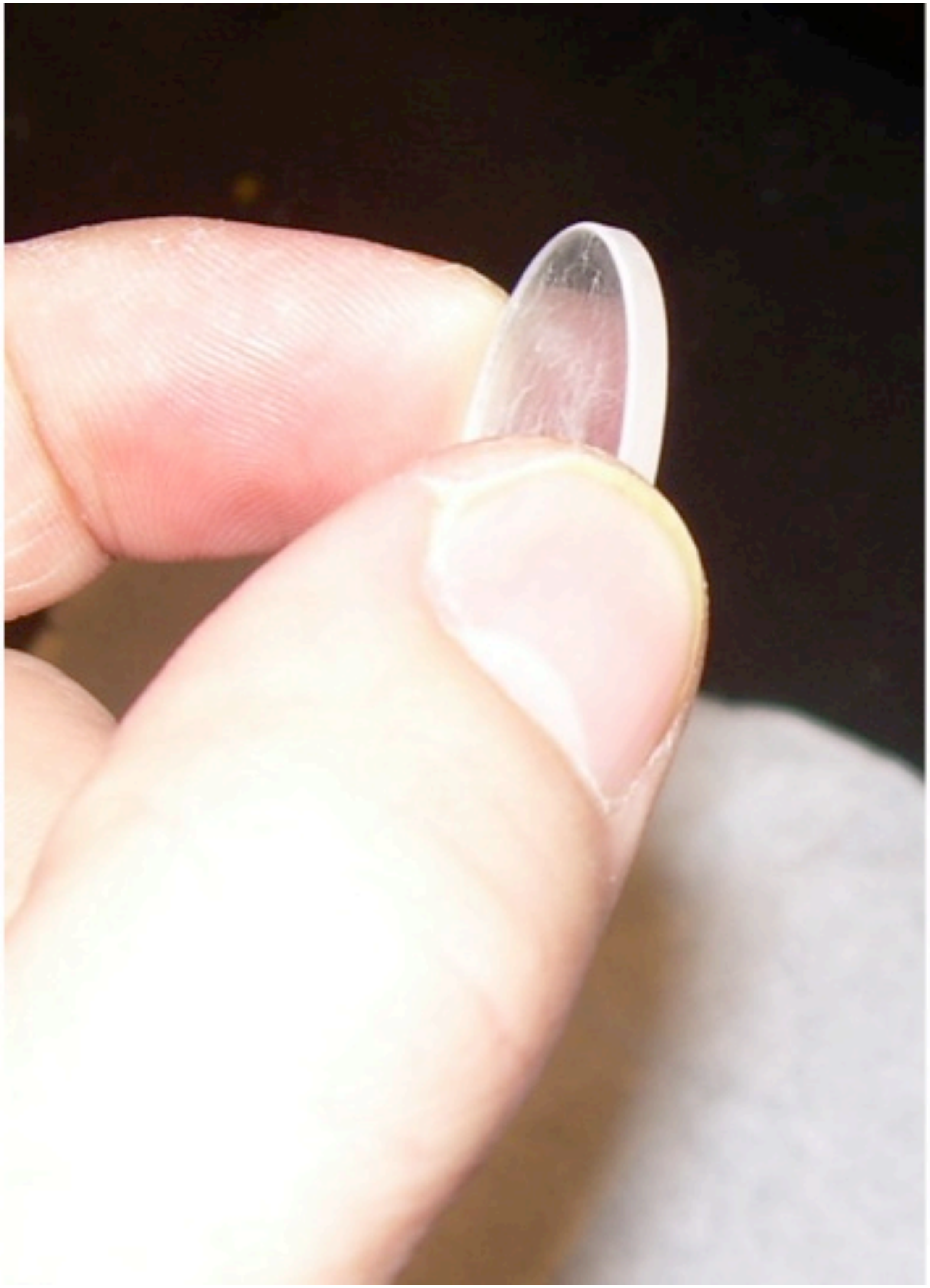
Sample Compartment

IR Source

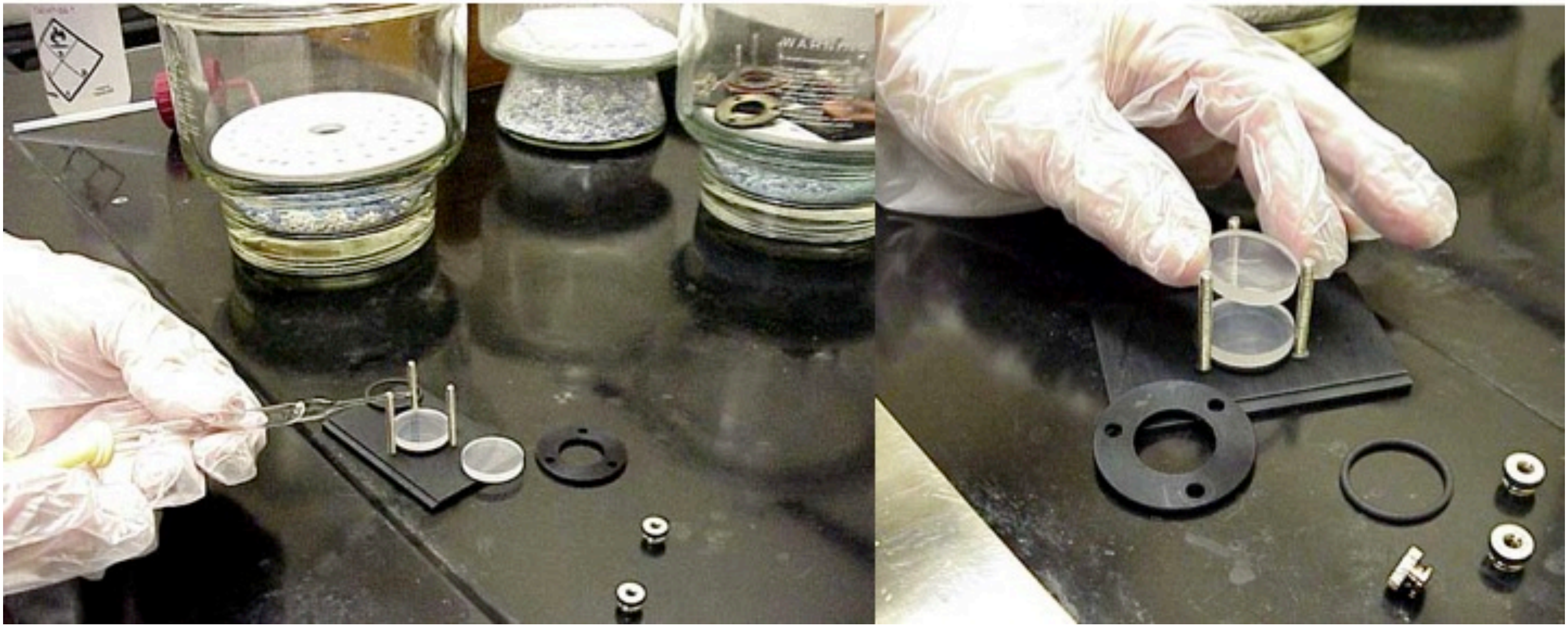
Detector

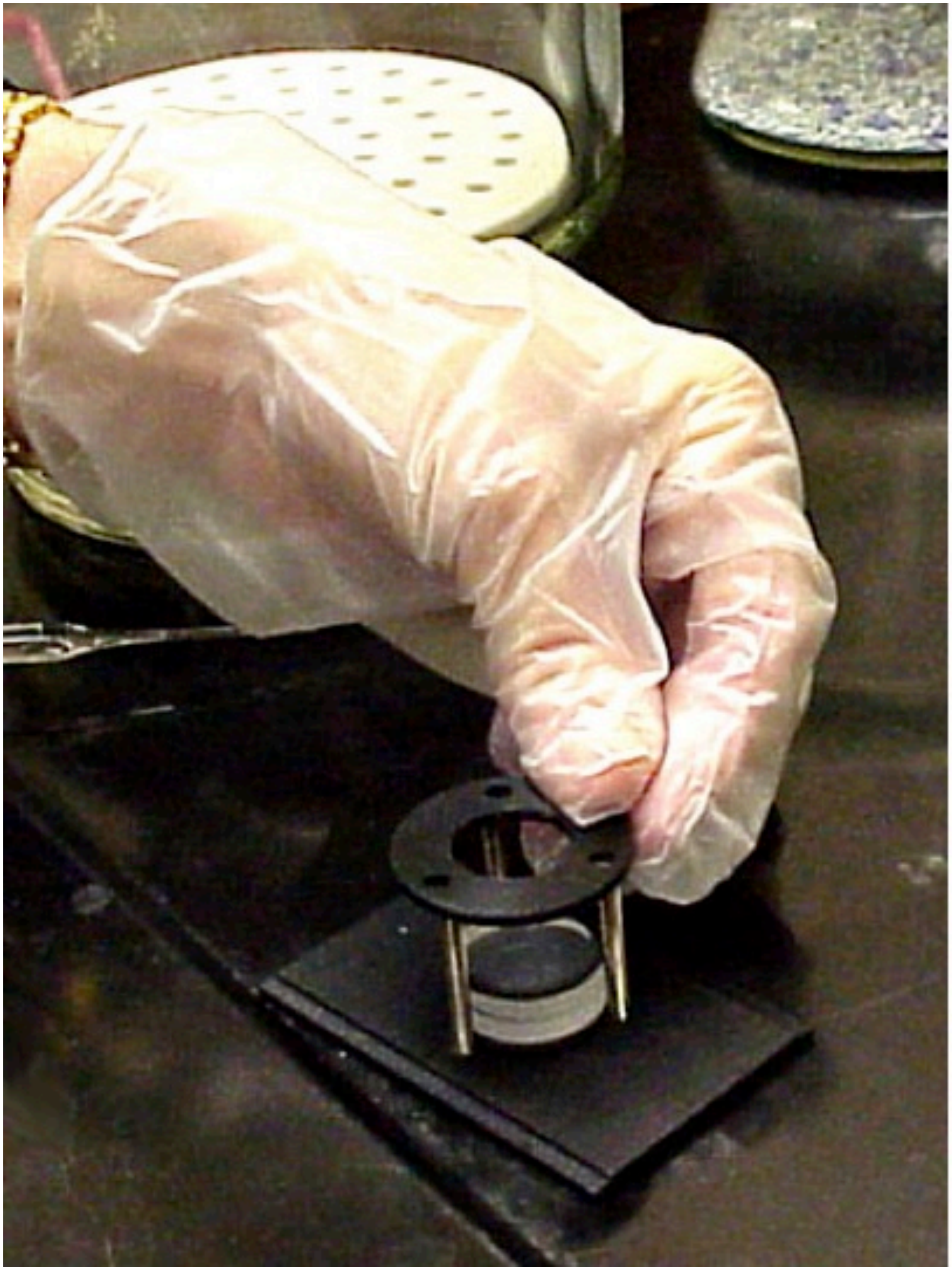

PLEASE KEEP THIS AREA CLEAN
CAUTION
FIRST AID KIT
VWR SAFETY

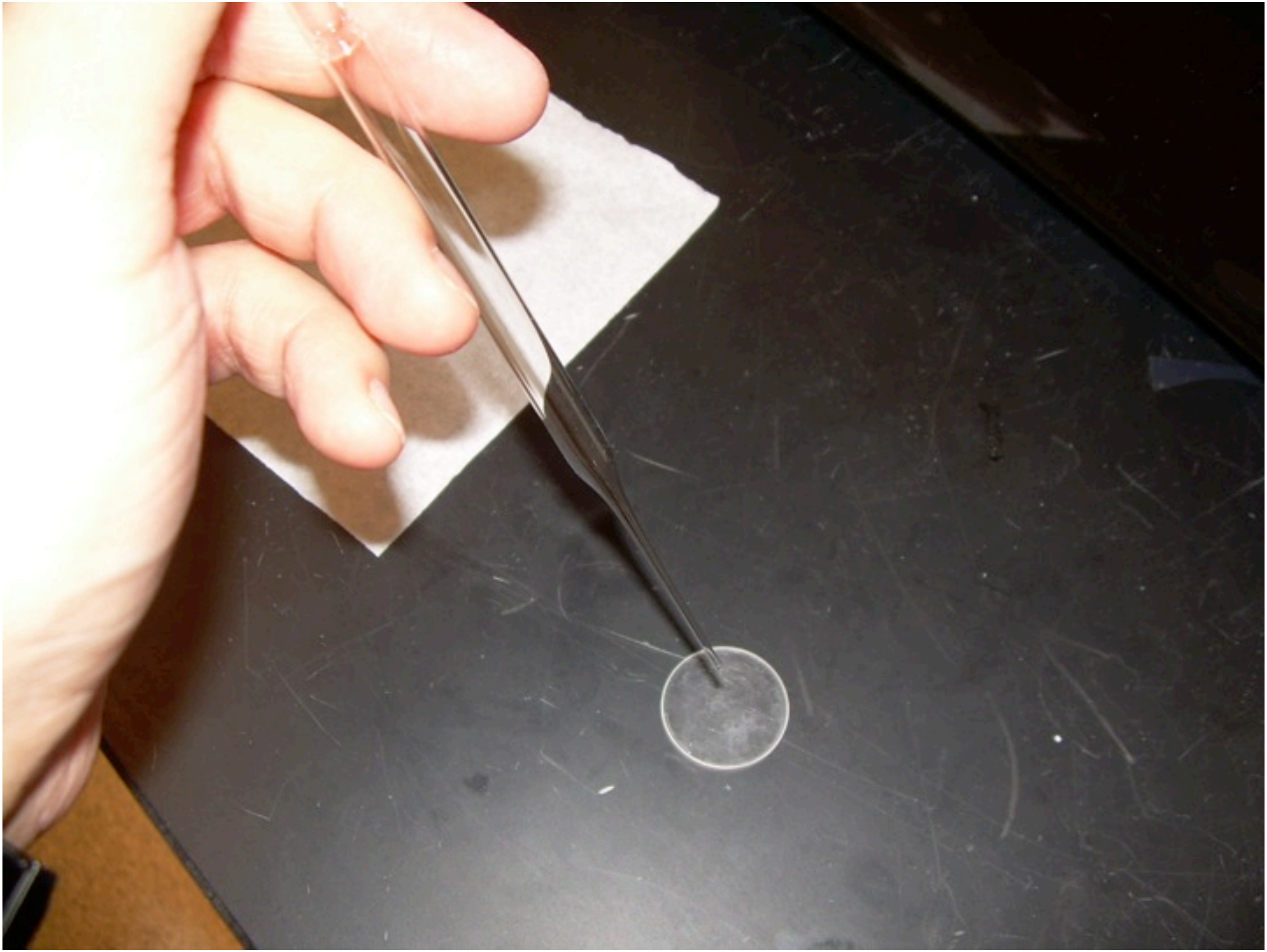

CLEAN
3132 only

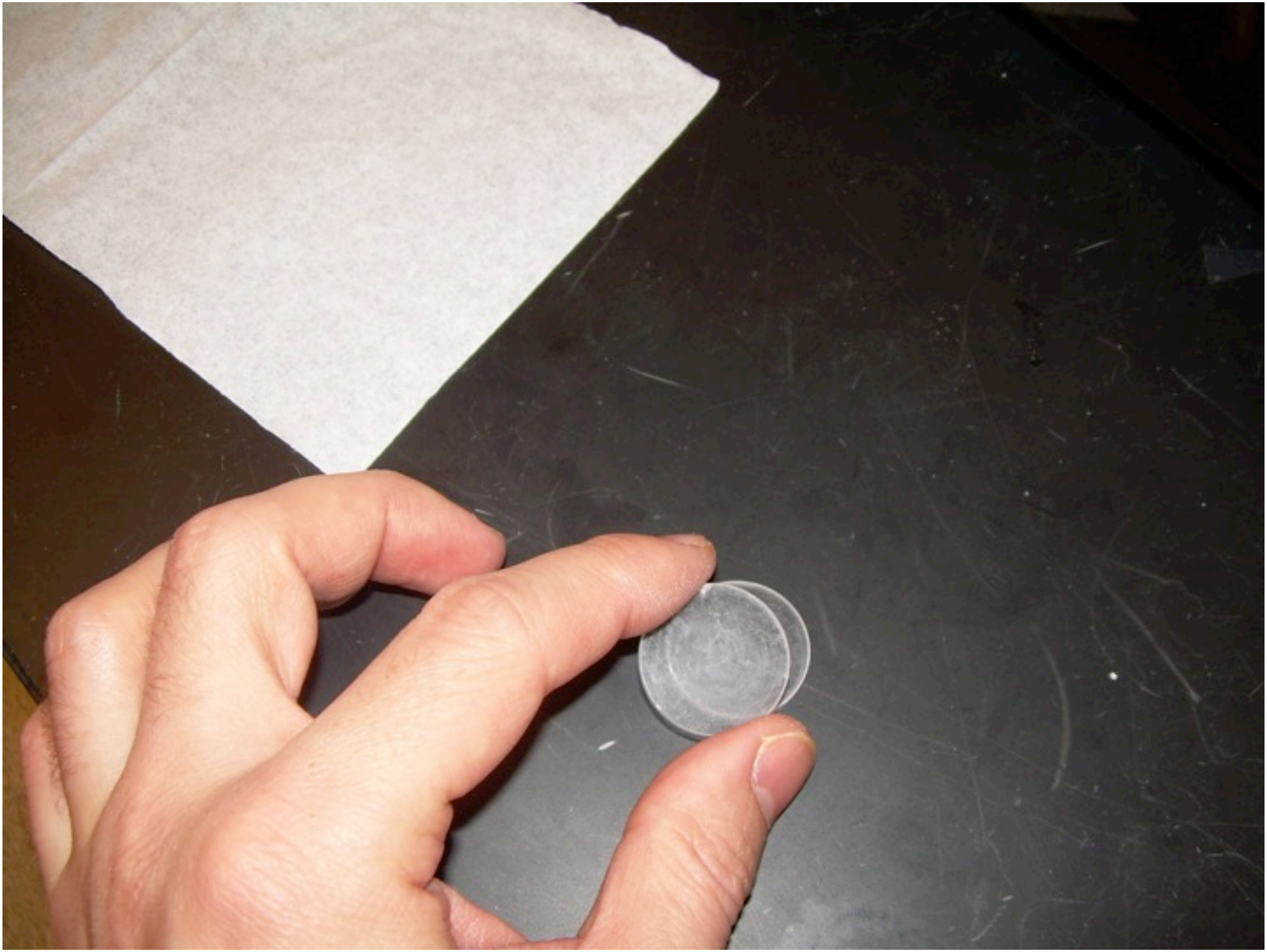


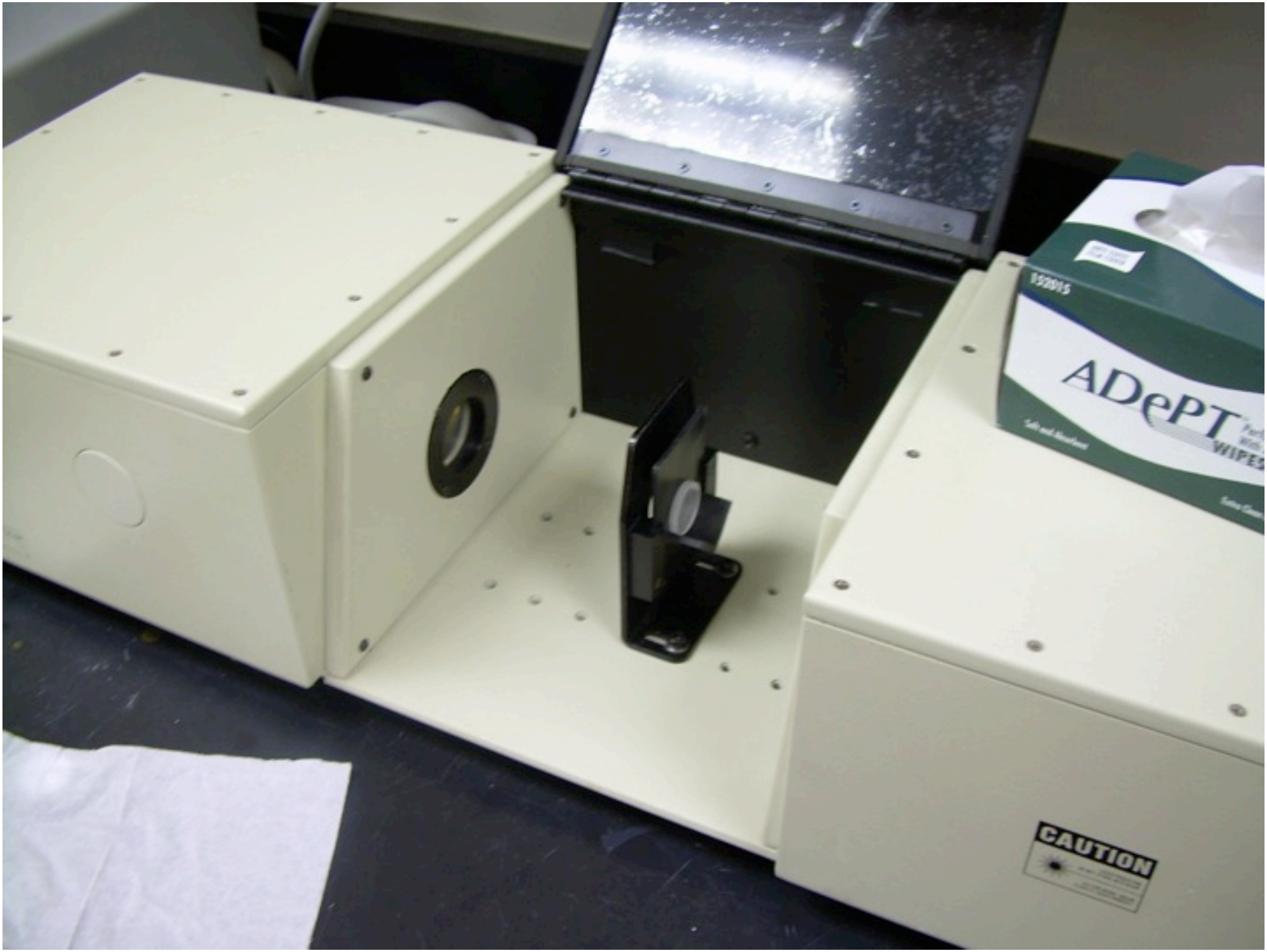
To run an IR spectrum of a liquid sample, a drop or two of the liquid sample is applied to a salt plate (NaCl)

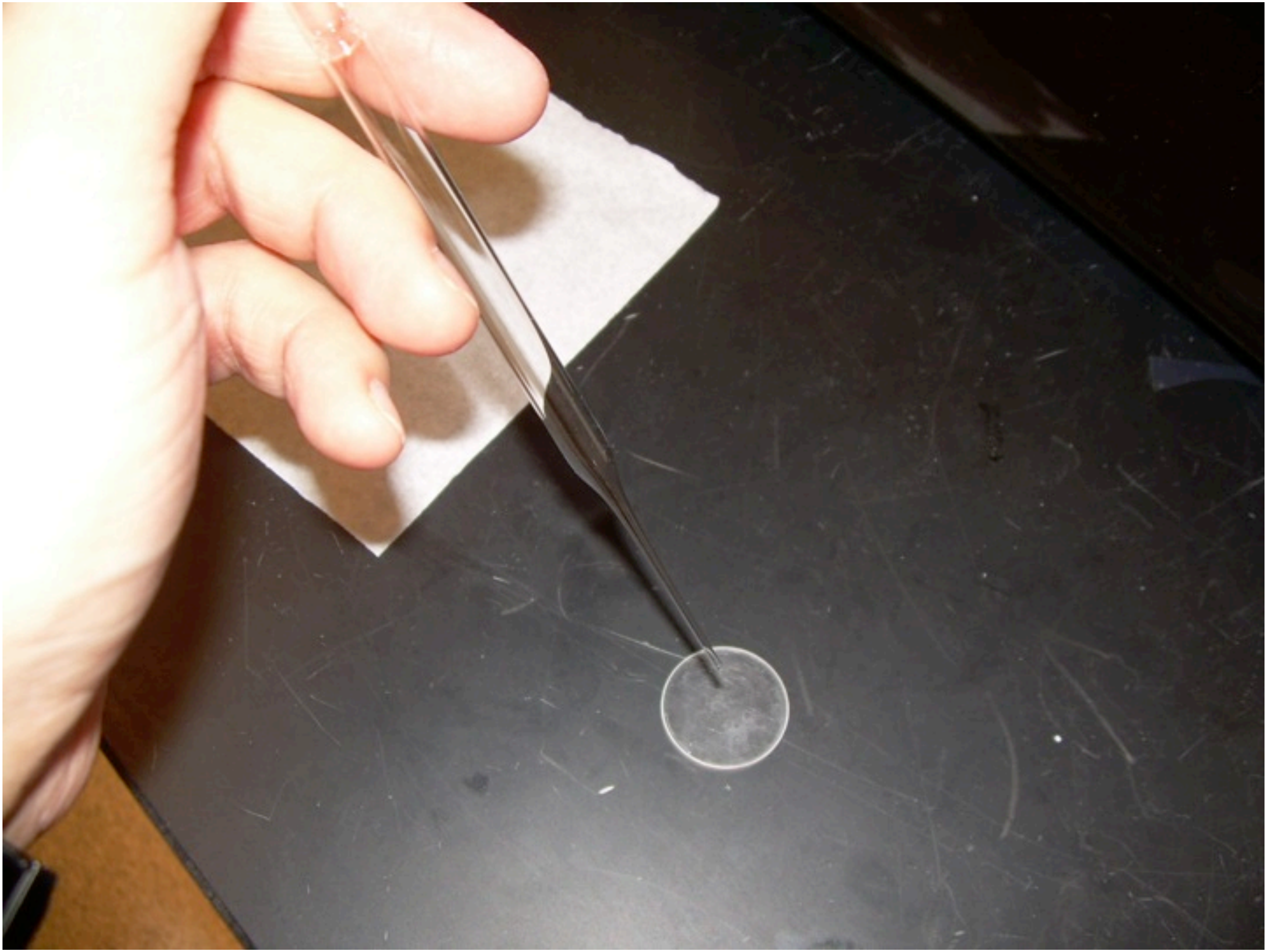


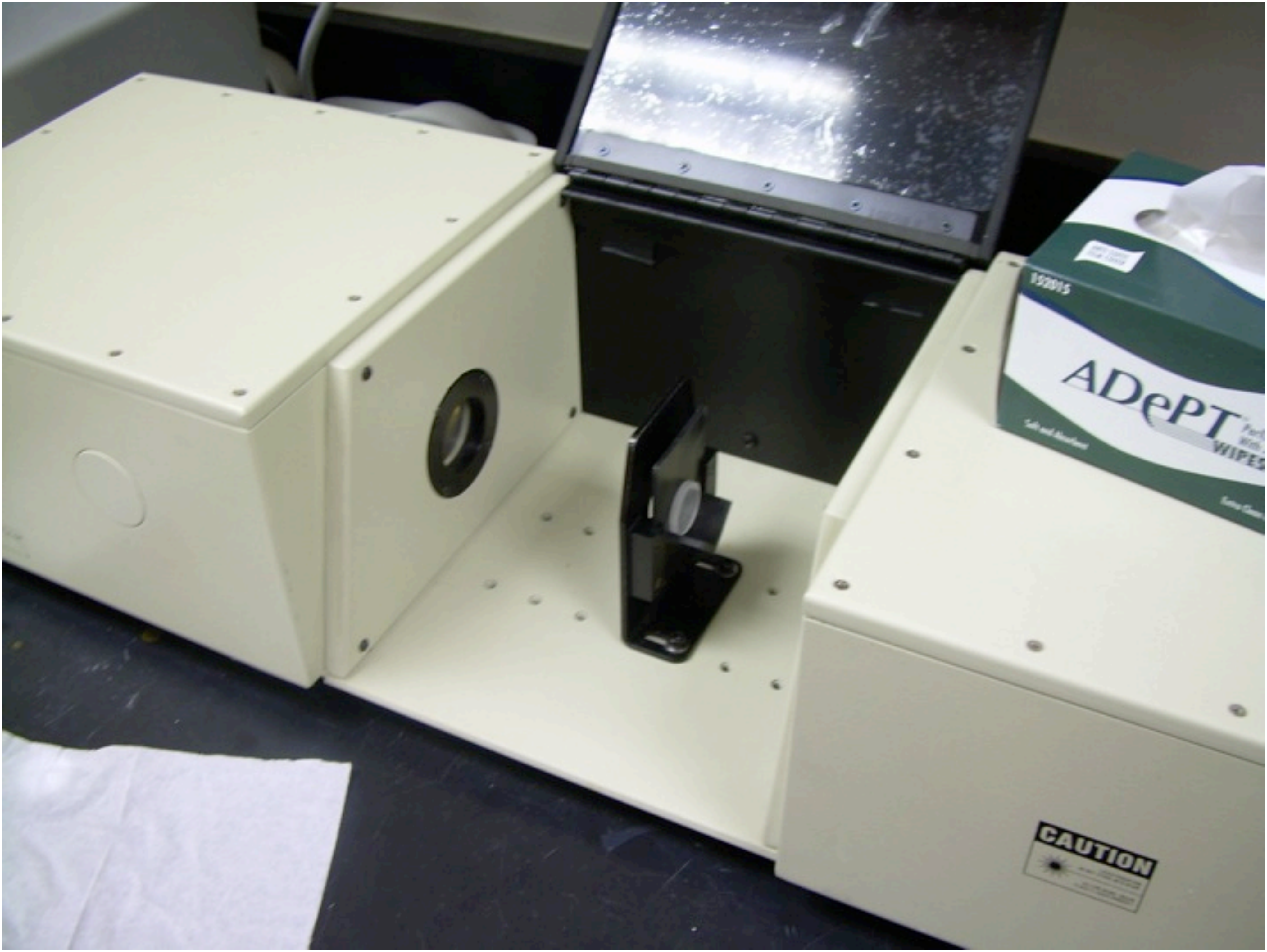


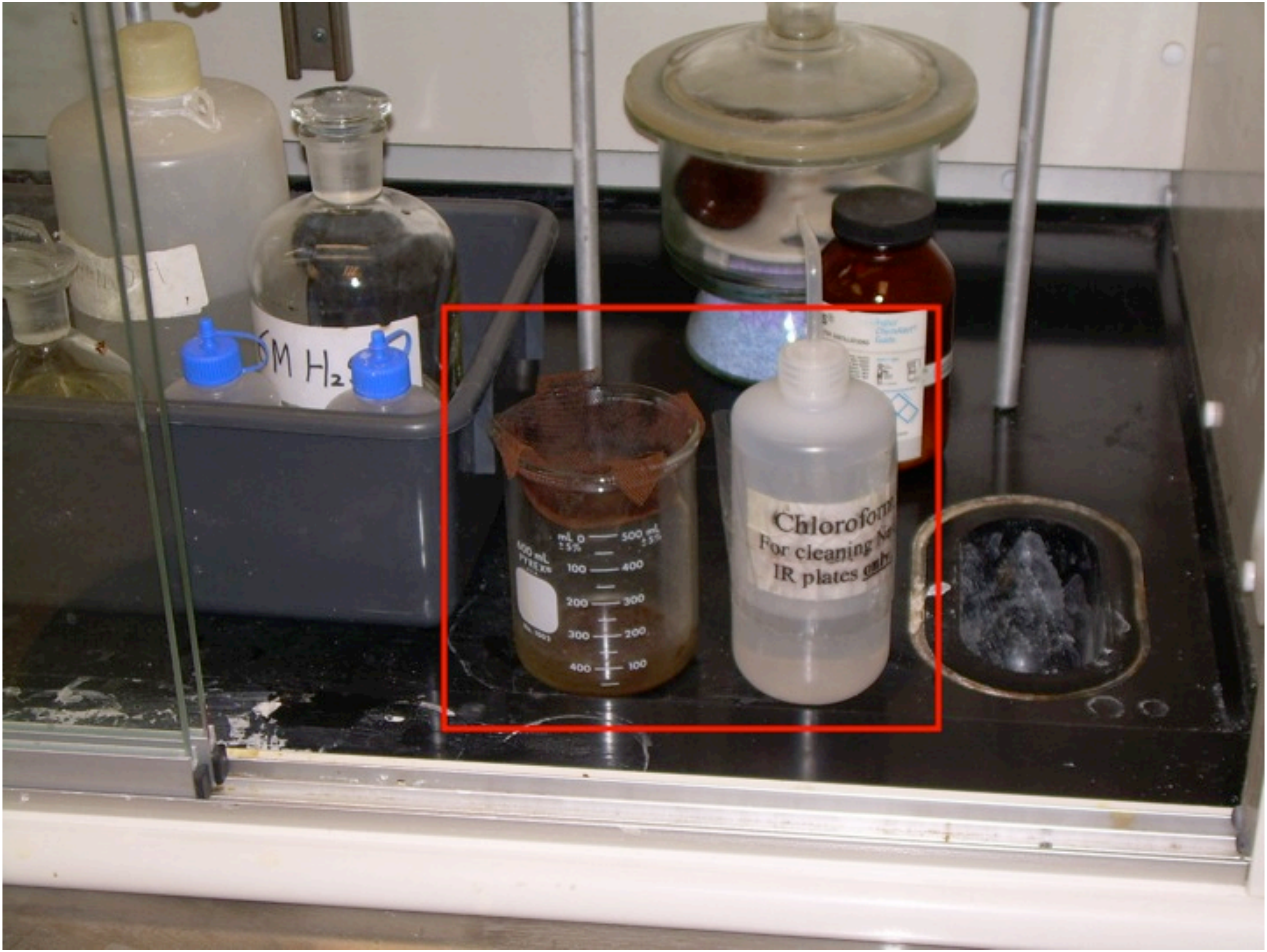





ADePT
WIPES
CAUTION

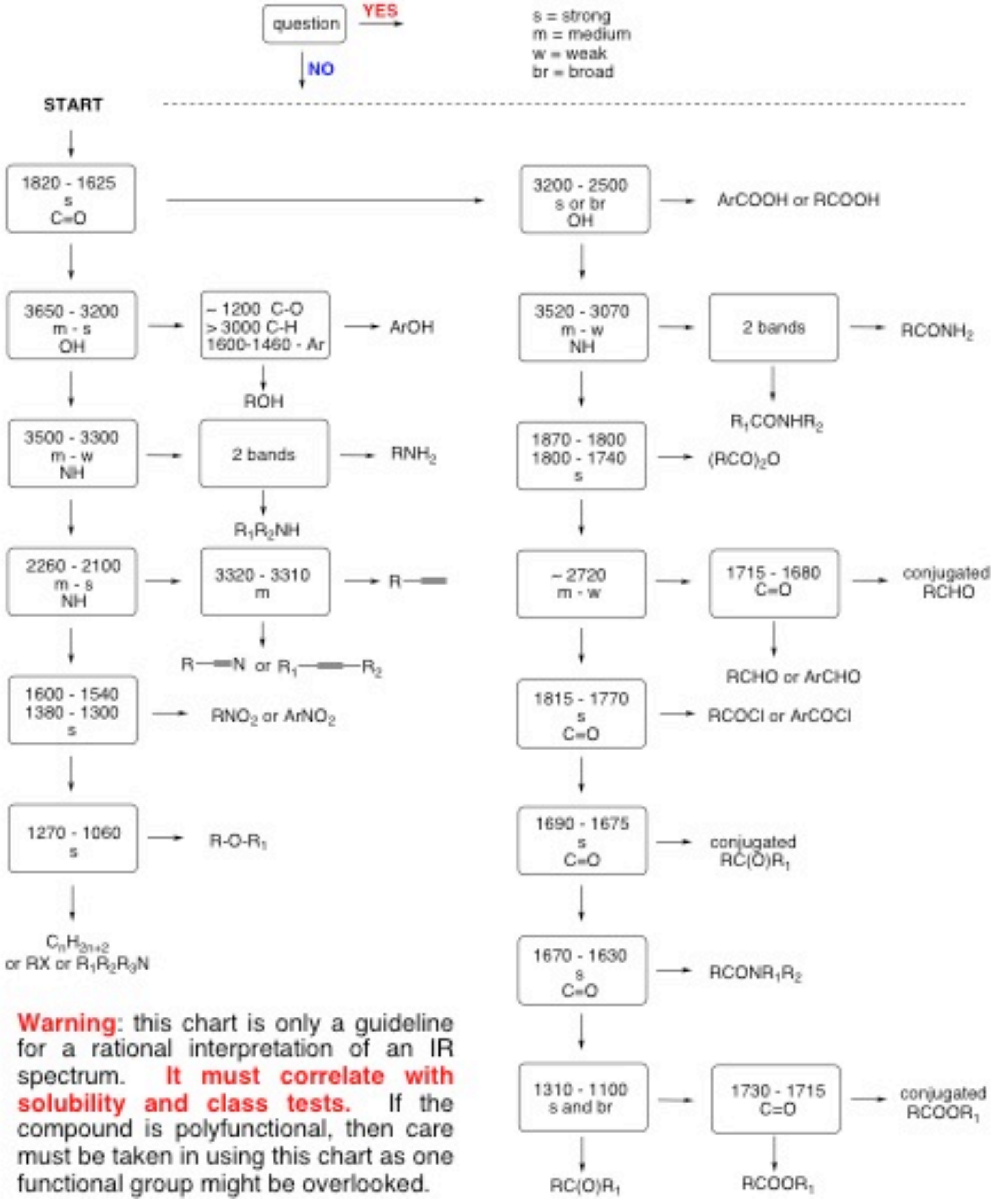



ADePT
WIPES
CAUTION

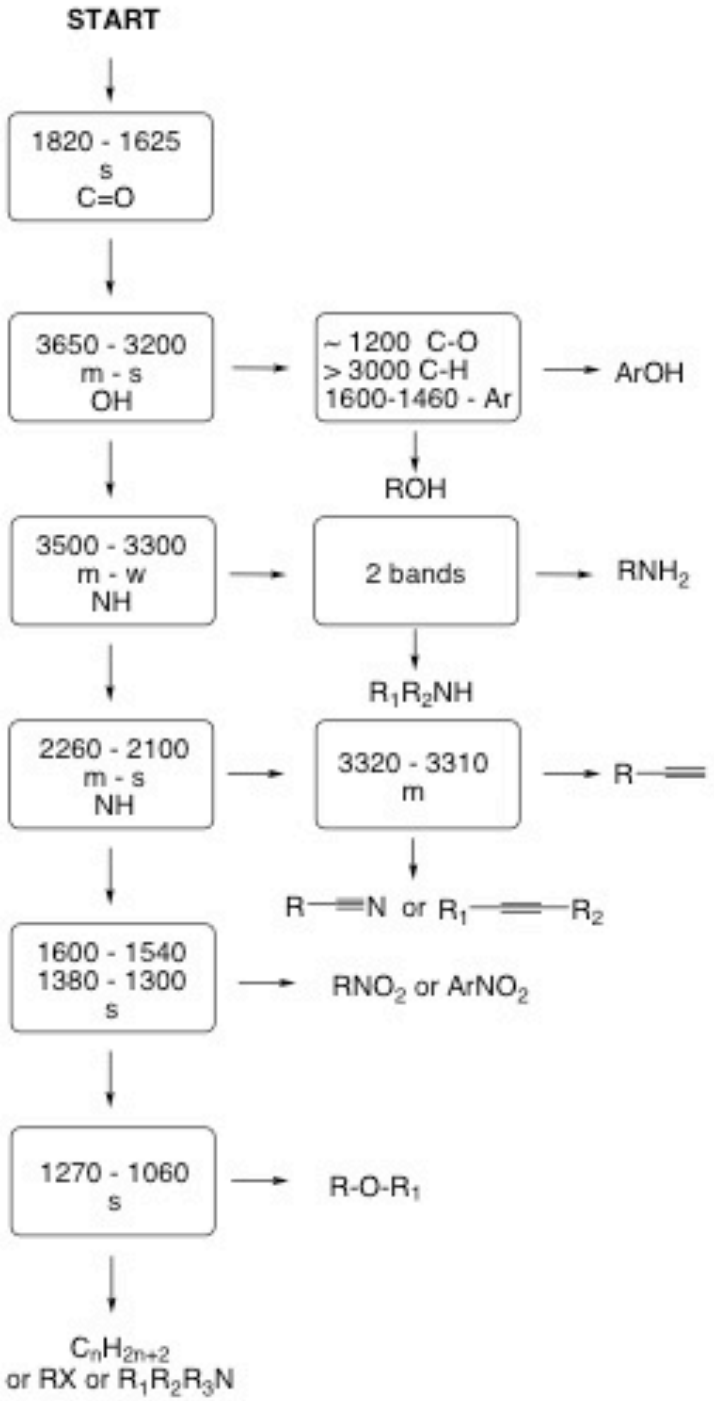

M H₂
Chloroform
For cleaning Na
IR plates only
600 mL
PYREX
mL 0
±5%
500 mL
±5%
100
400
200
300
300
200
400
100

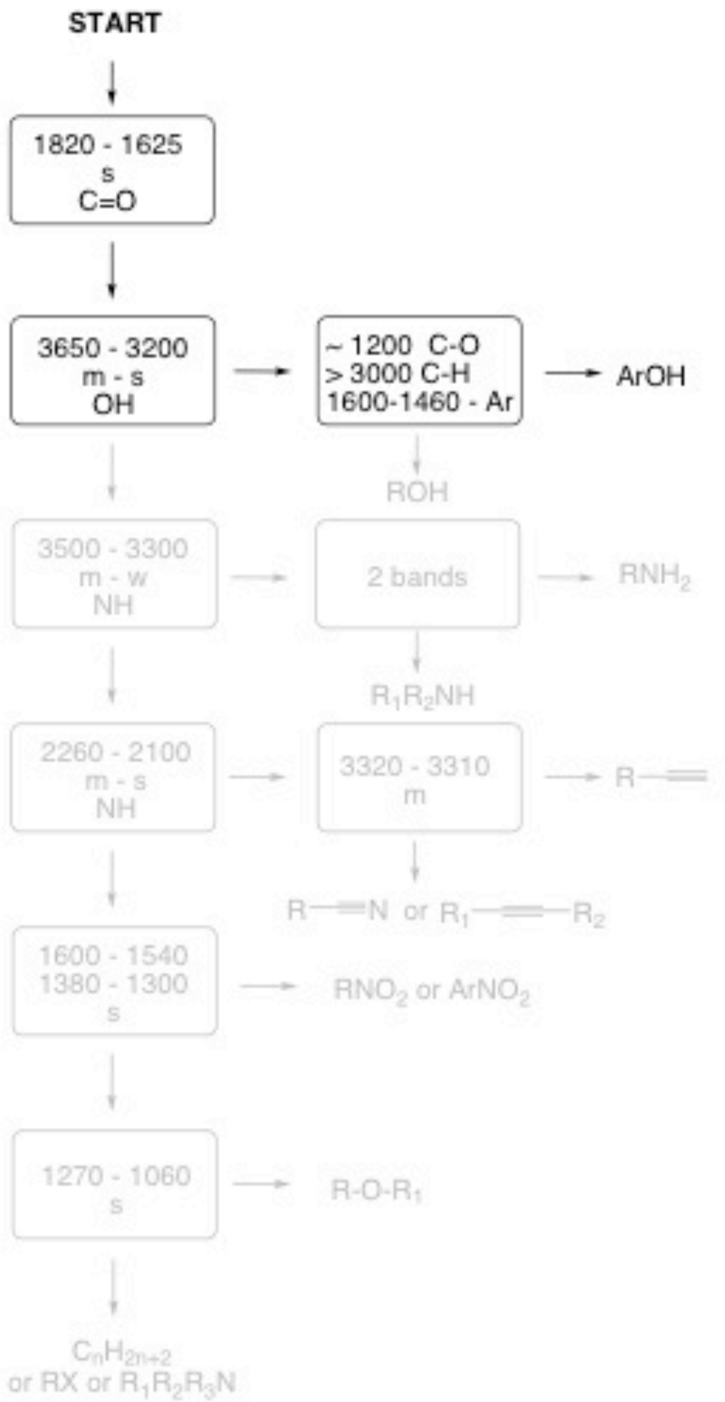

SO4

INTERPRETATION OF INFRARED SPECTRUM



Warning: this chart is only a guideline for a rational interpretation of an IR spectrum. **It must correlate with solubility and class tests.** If the compound is polyfunctional, then care must be taken in using this chart as one functional group might be overlooked.


START
1820 - 1625
s
C=O
3650 - 3200
m - s
OH
~ 1200 C-O
> 3000 C-H
1600-1460 - Ar
ArOH
ROH
3500 - 3300
m - w
NH
2 bands
RNH_2
R_1R_2NH
2260 - 2100
m - s
NH
3320 - 3310
m
R—≡
R—≡N or R_1—≡—R_2
1600 - 1540
1380 - 1300
s
RNO_2 or $ArNO_2$
1270 - 1060
s
R-O-R_1
C_nH_{2n+2}
or RX or $R_1R_2R_3N$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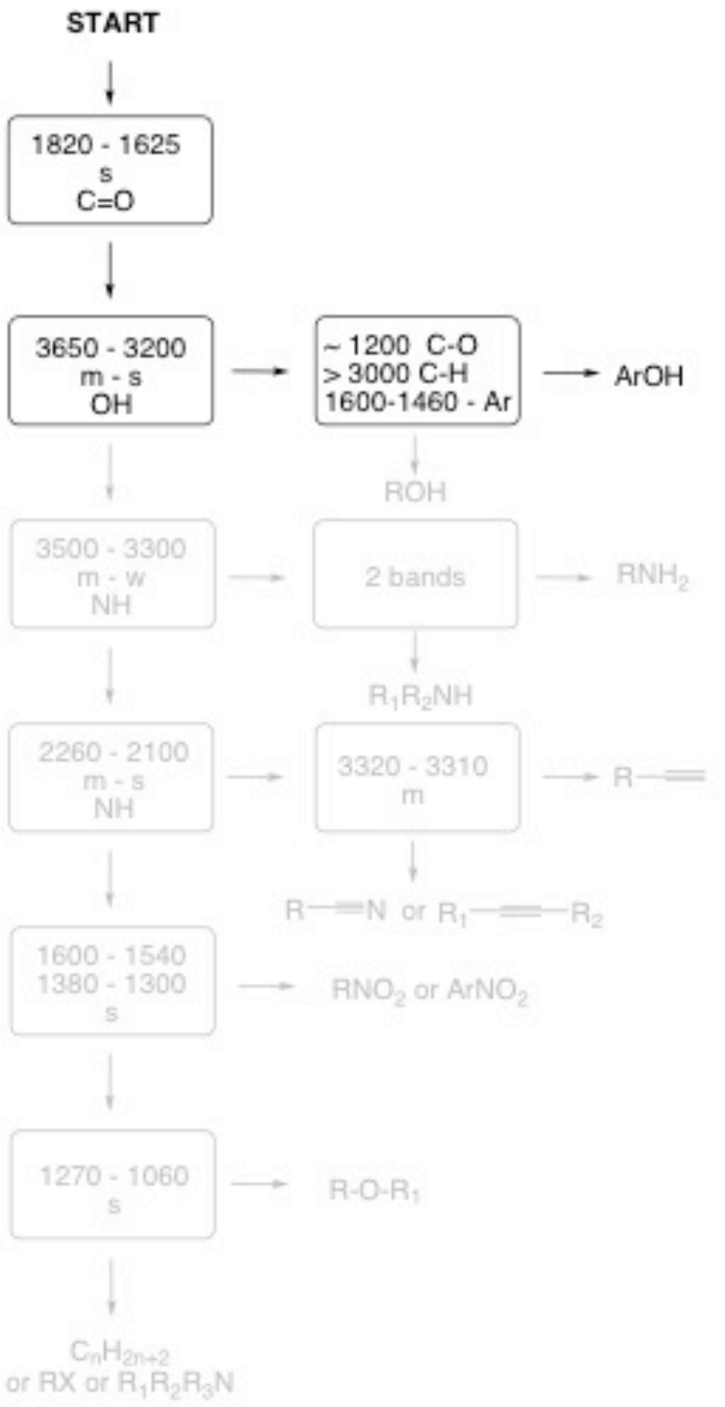
m - w
NH
2 bands
RNH_2
R_1R_2NH
2260 - 2100
m - s
NH
3320 - 3310
m
R—≡
R—≡N or R_1—≡—R_2
1600 - 1540
1380 - 1300
s
RNO_2 or $ArNO_2$
1270 - 1060
s
R-O-R_1
C_nH_{2n+2}
or RX or $R_1R_2R_3N$



START

1820 - 1625
s
C=O

3650 - 3200
m - s
OH

~ 1200 C-O
> 3000 C-H
1600-1460 - Ar

ArOH

ROH

3500 - 3300
m - w
NH

2 bands

RNH_2

R_1R_2NH

2260 - 2100
m - s
NH

3320 - 3310
m

R—≡

R—≡N or R_1—≡—R_2

1600 - 1540
1380 - 1300
s

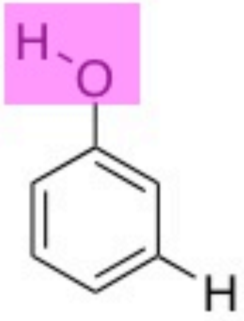
RNO_2 or $ArNO_2$

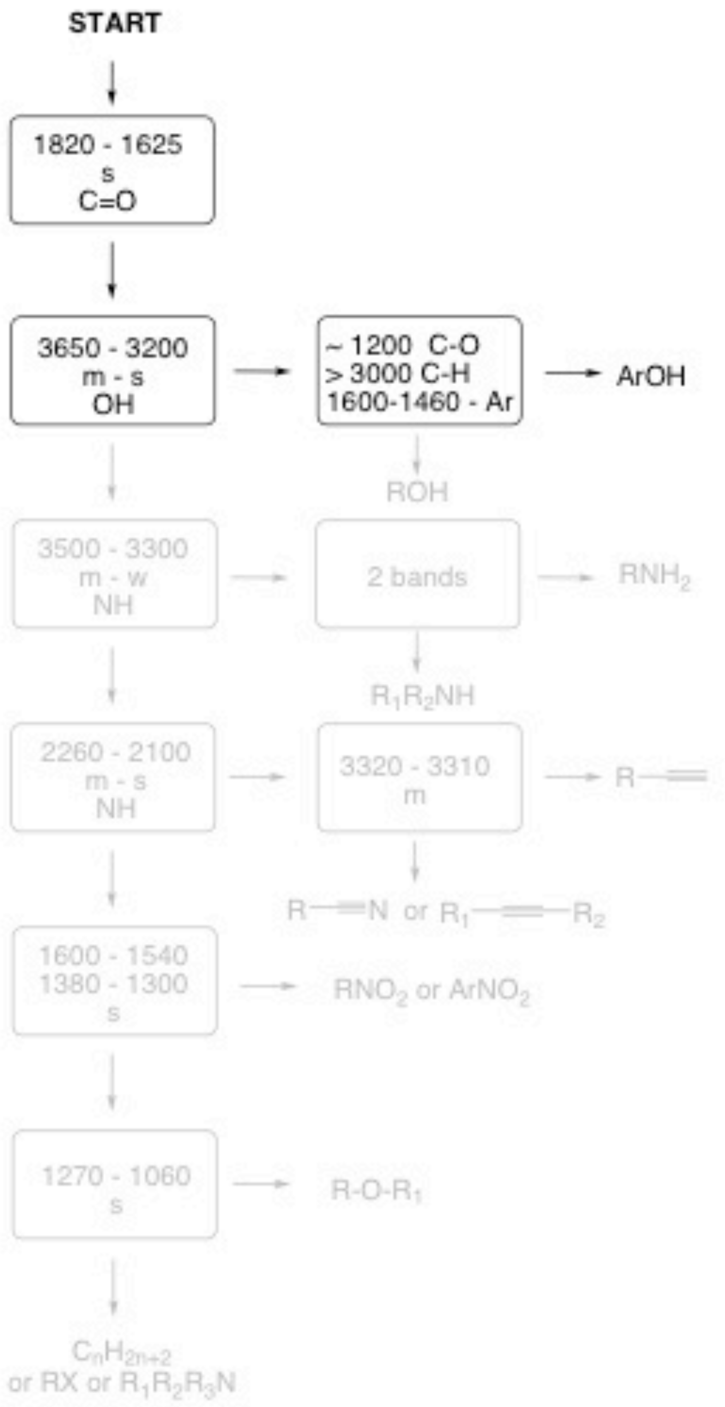
1270 - 1060
s

R-O-R_1

C_nH_{2n+2}
or RX or $R_1R_2R_3N$

3650 - 3200





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C=O

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OH

~ 1200 C-O
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1380 - 1300
s

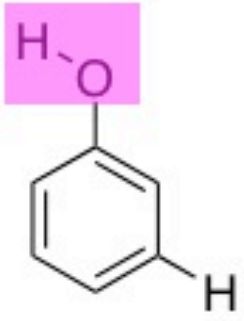
RNO_2 or $ArNO_2$

1270 - 1060
s

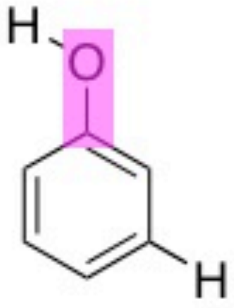
$R\text{-}O\text{-}R_1$

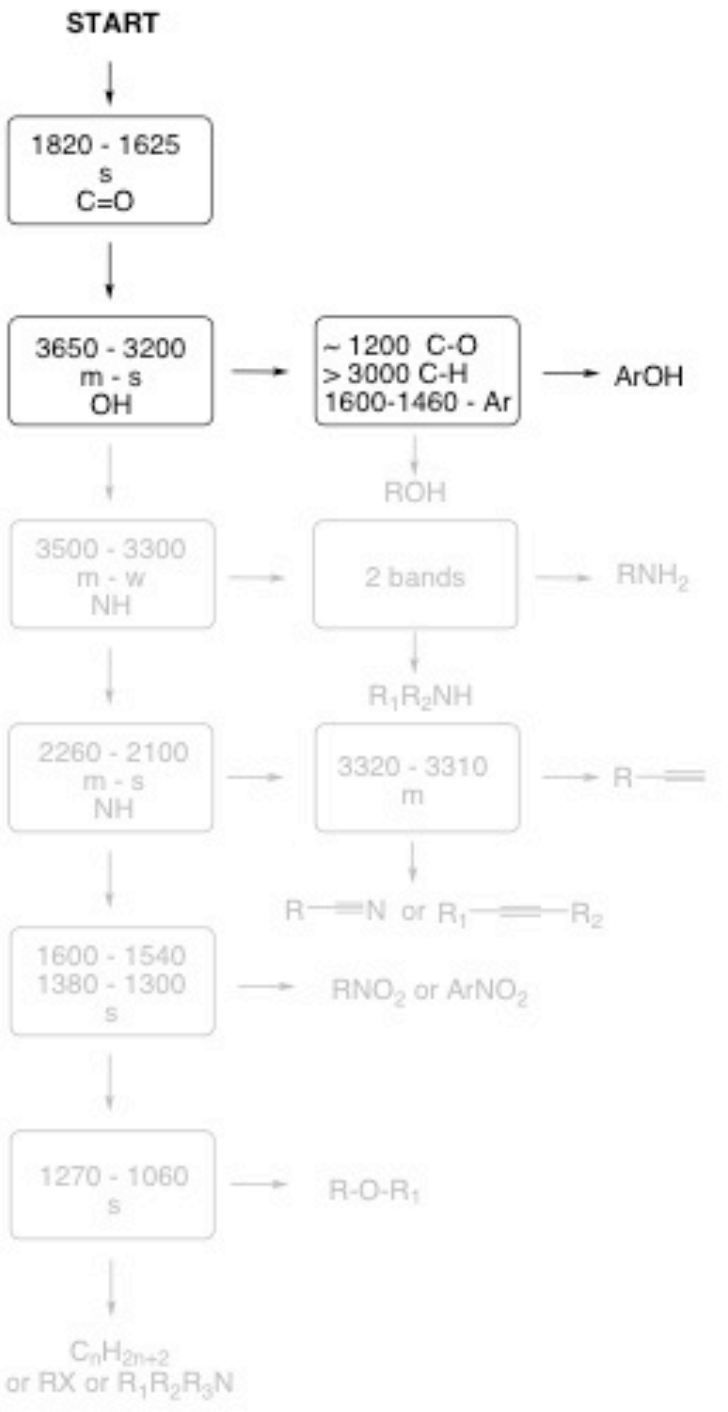
C_nH_{2n+2}
or RX or $R_1R_2R_3N$

3650 - 3200



1200-1000





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1600 - 1540
1380 - 1300
s

RNO_2 or $ArNO_2$

1270 - 1060
s

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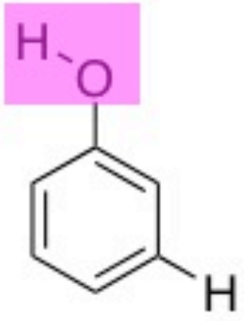
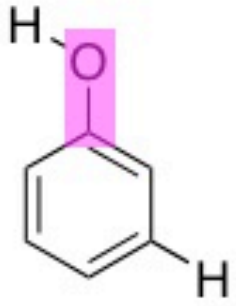
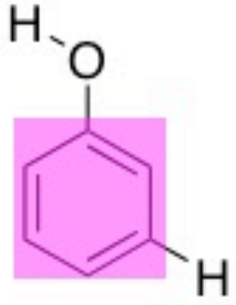
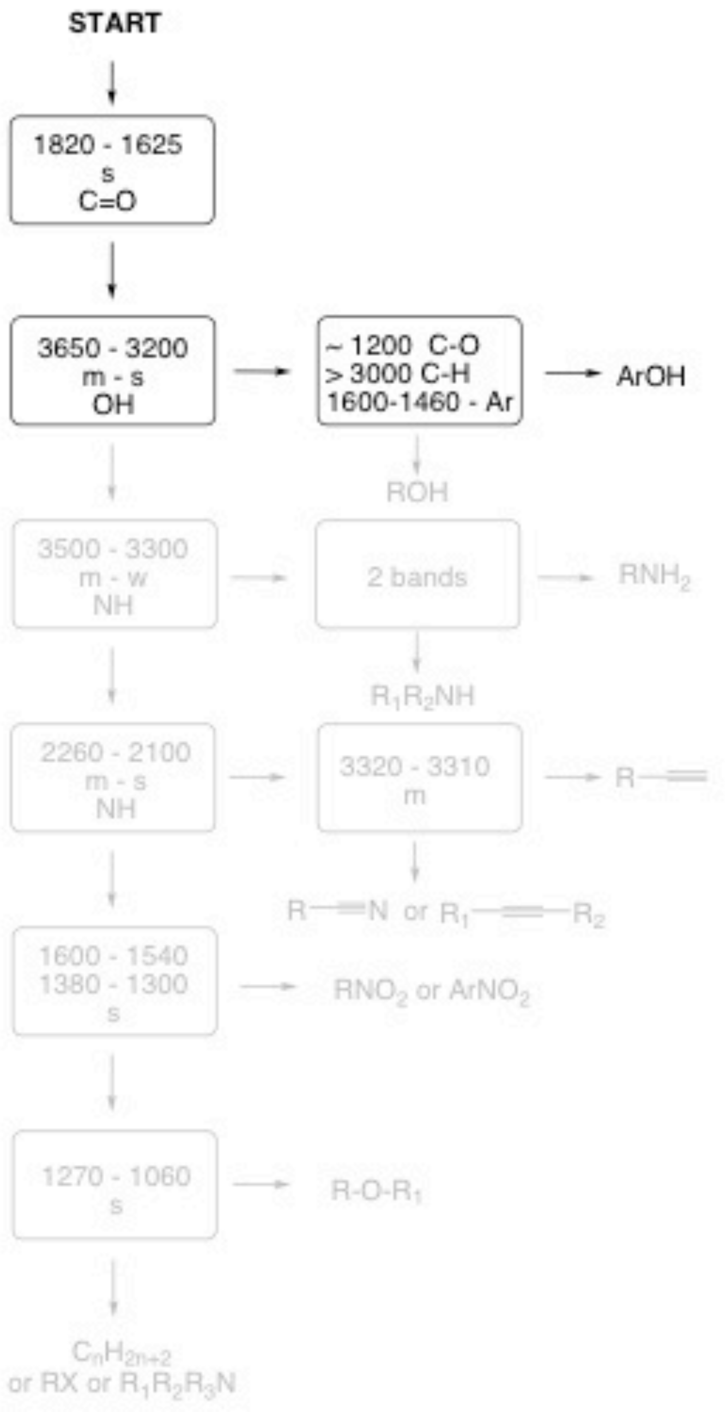


1200-1000





1600-1460
+overtones



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ROH

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m - w
NH

2 bands

RNH_2

R_1R_2NH

2260 - 2100
m - s
NH

3320 - 3310
m

R—≡

R—≡N or R_1—≡—R_2

1600 - 1540
1380 - 1300
s

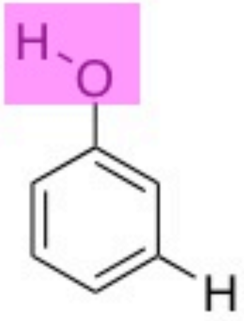
RNO_2 or $ArNO_2$

1270 - 1060
s

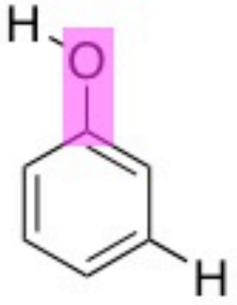
$R\text{-}O\text{-}R_1$

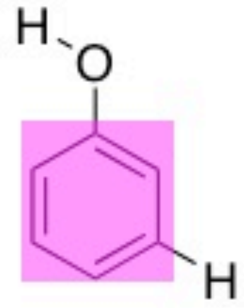
C_nH_{2n+2}
or RX or $R_1R_2R_3N$

3650 - 3200

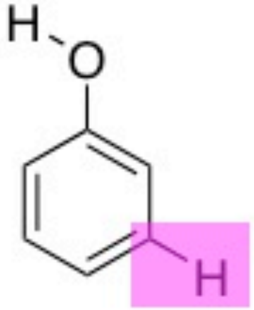


1200-1000

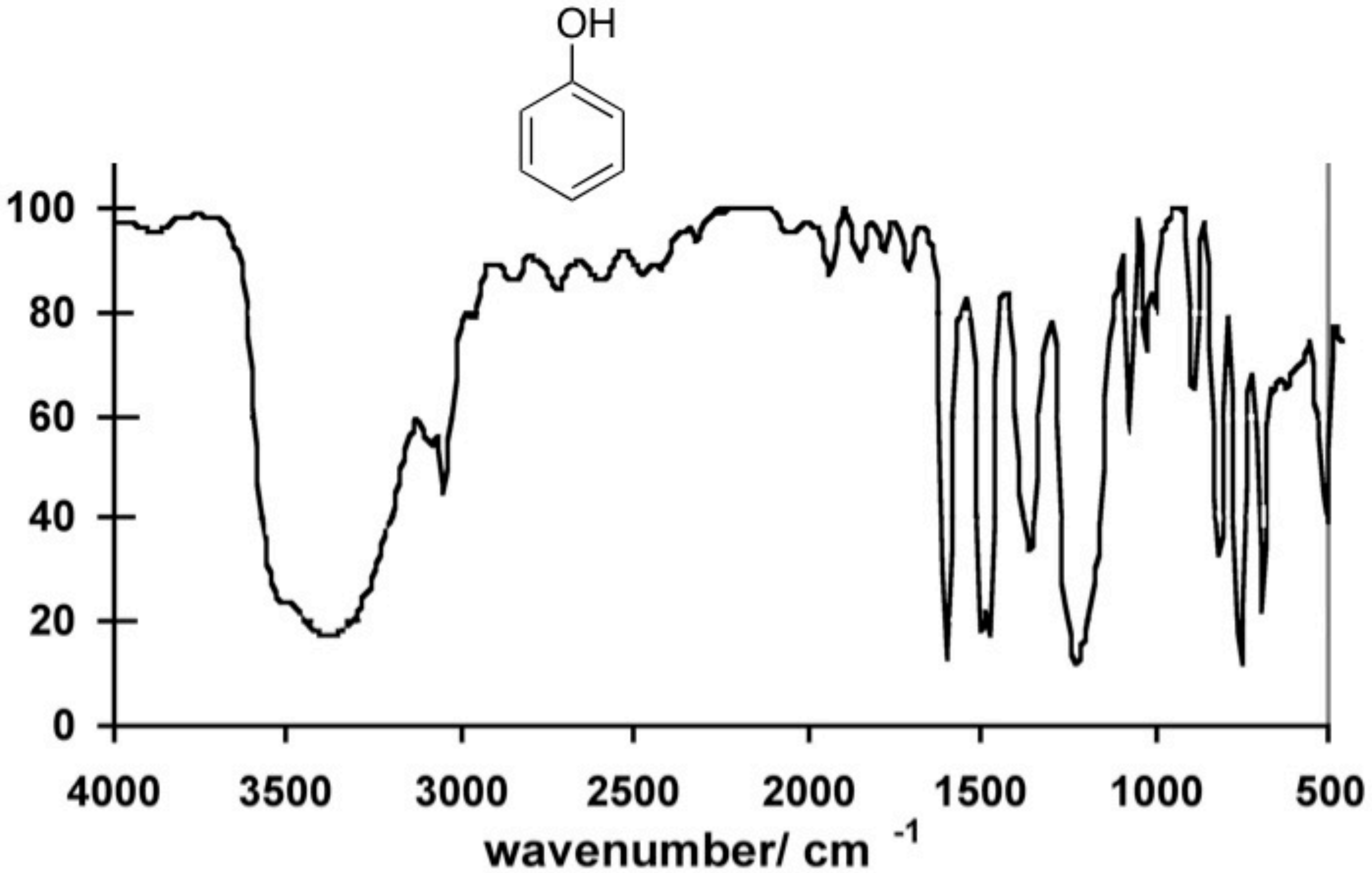


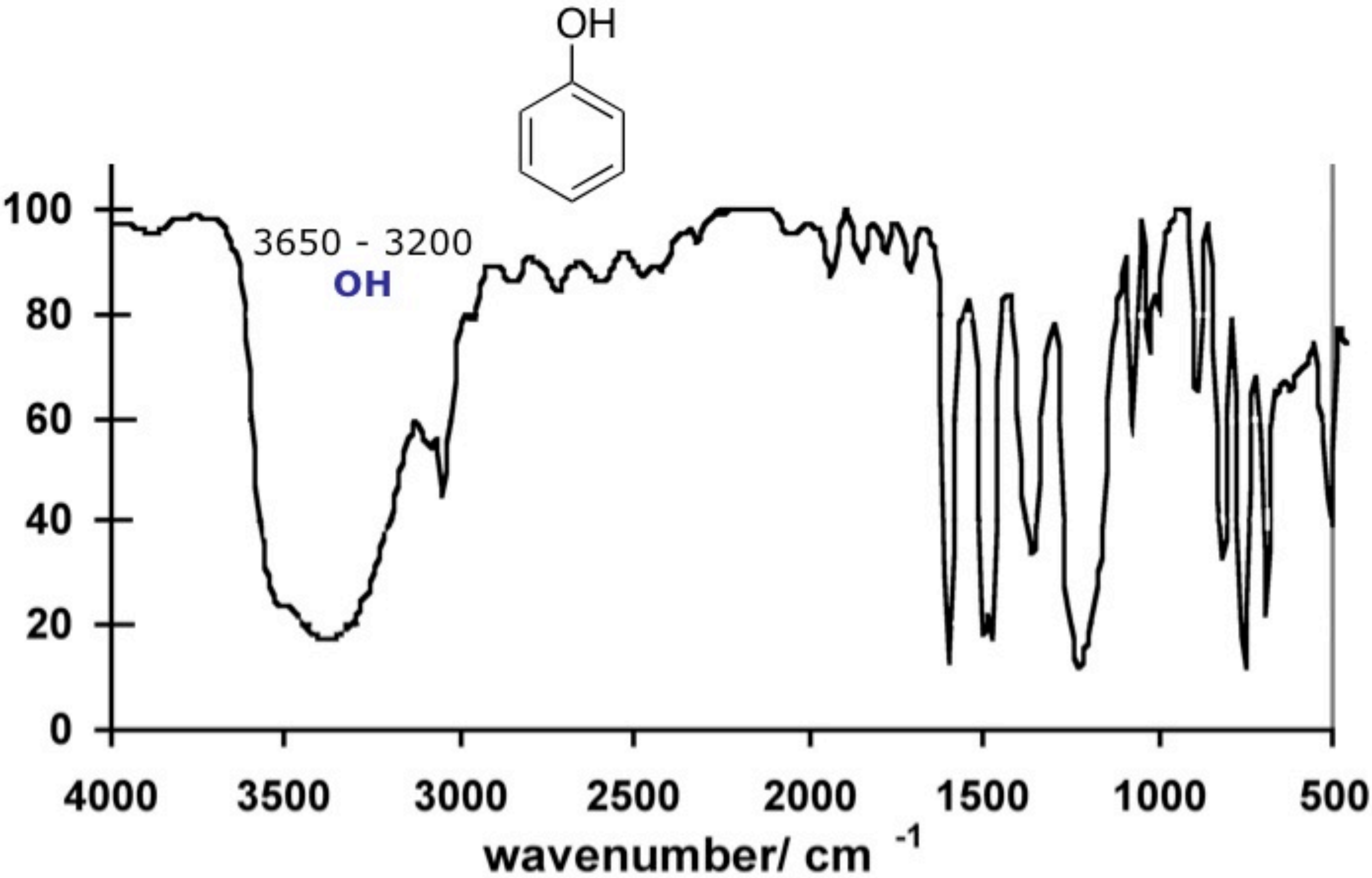


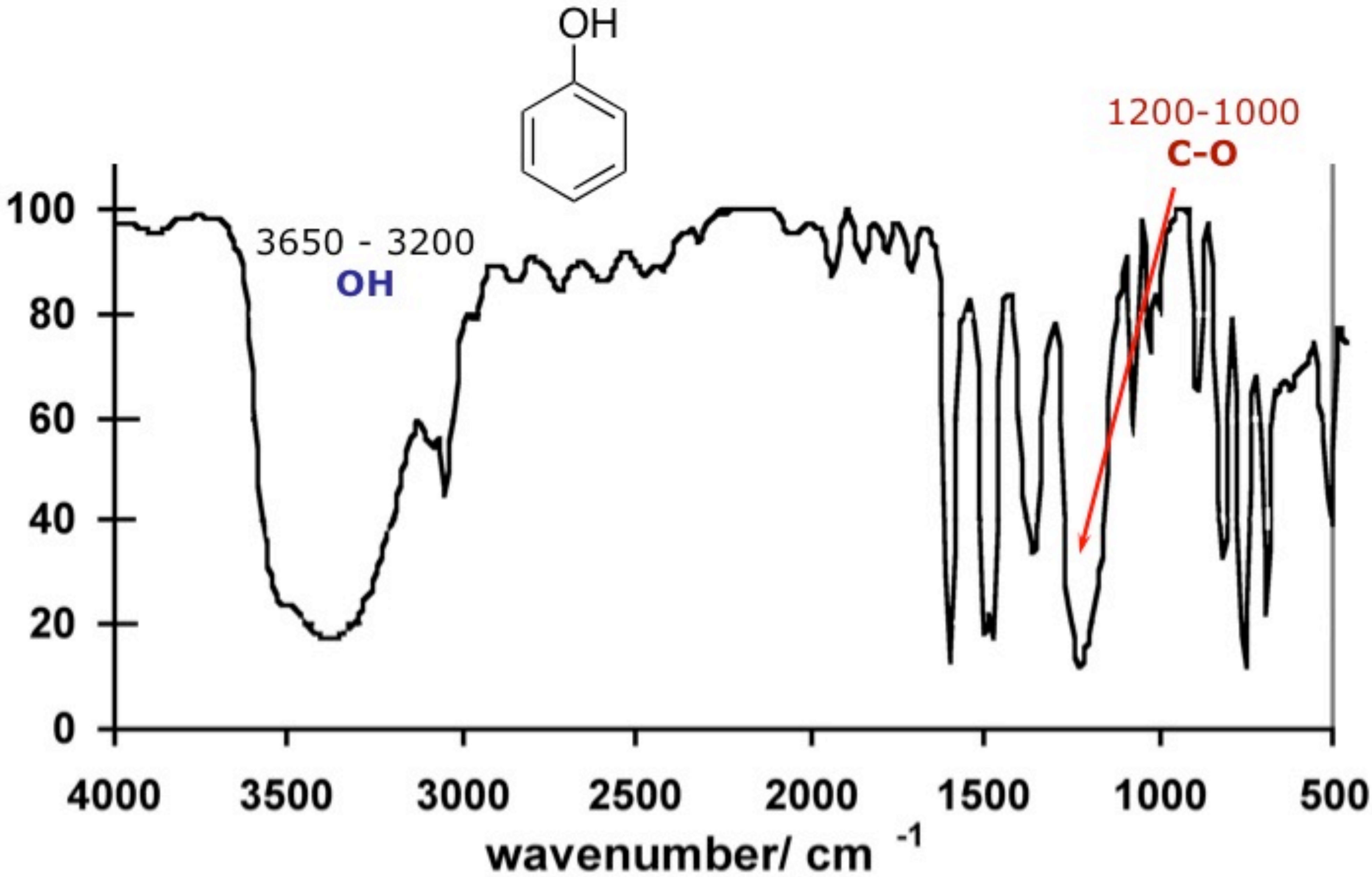
1600-1460
+overtones

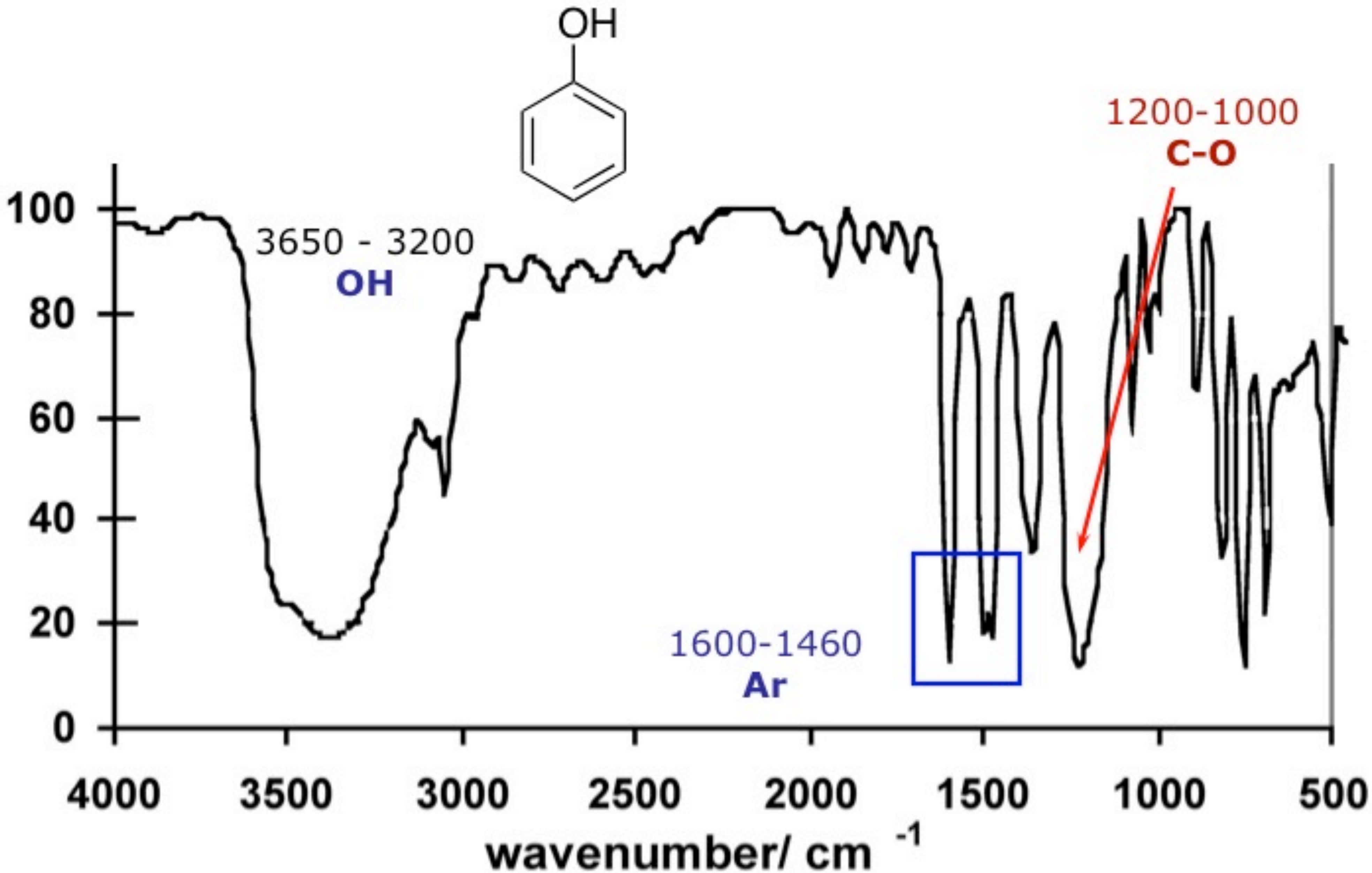


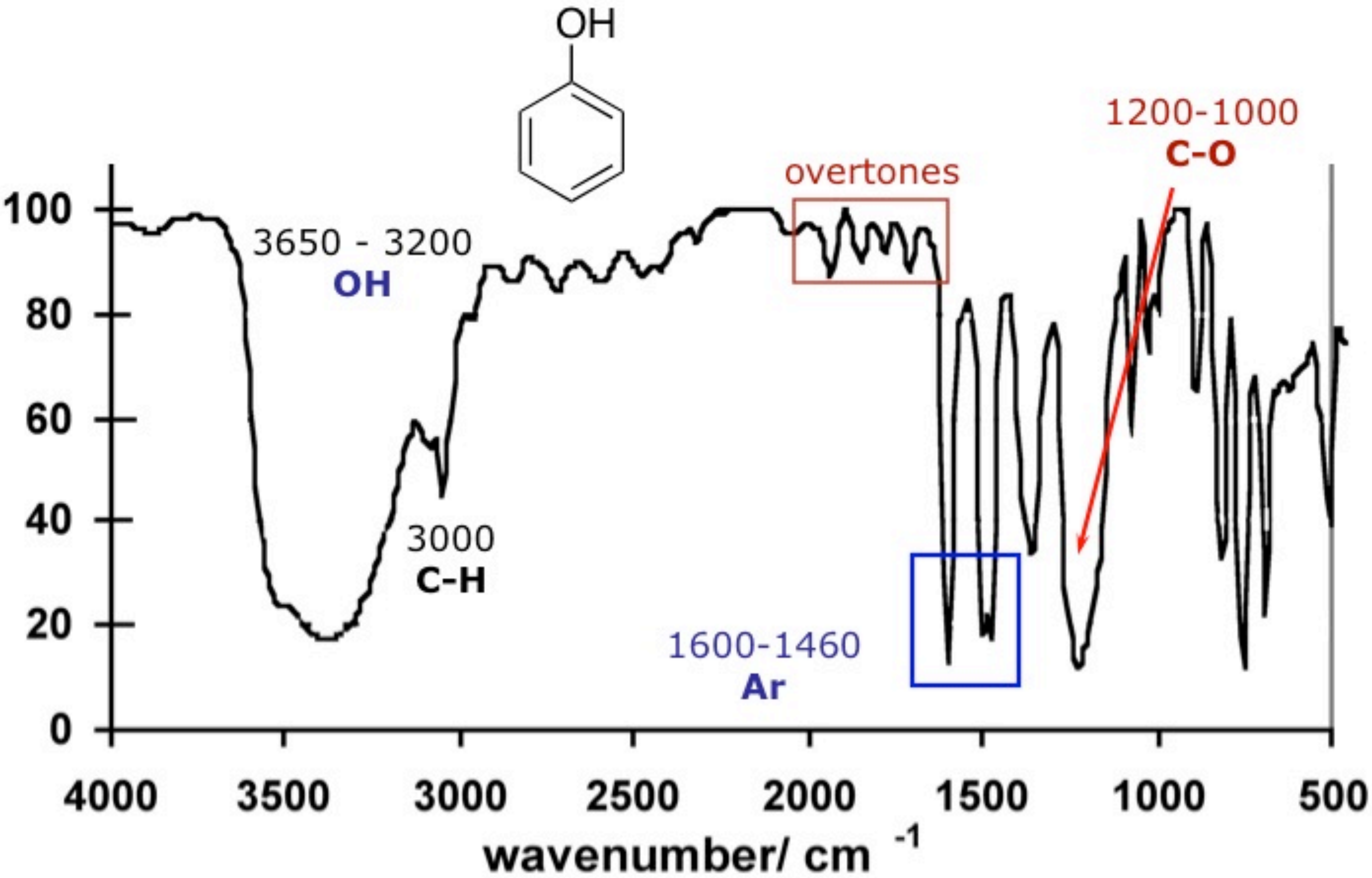
3000


OH
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
wavenumber/ cm -1

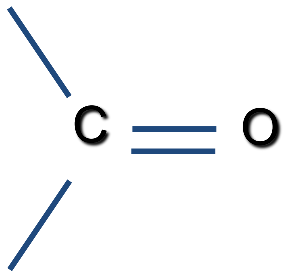

OH
3650 - 3200
OH
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
wavenumber/ cm $^{-1}$


OH
3650 - 3200
OH
1200-1000
C-O
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
wavenumber/ cm -1


OH
3650 - 3200
OH
1200-1000
C-O
1600-1460
Ar
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
wavenumber/ cm -1

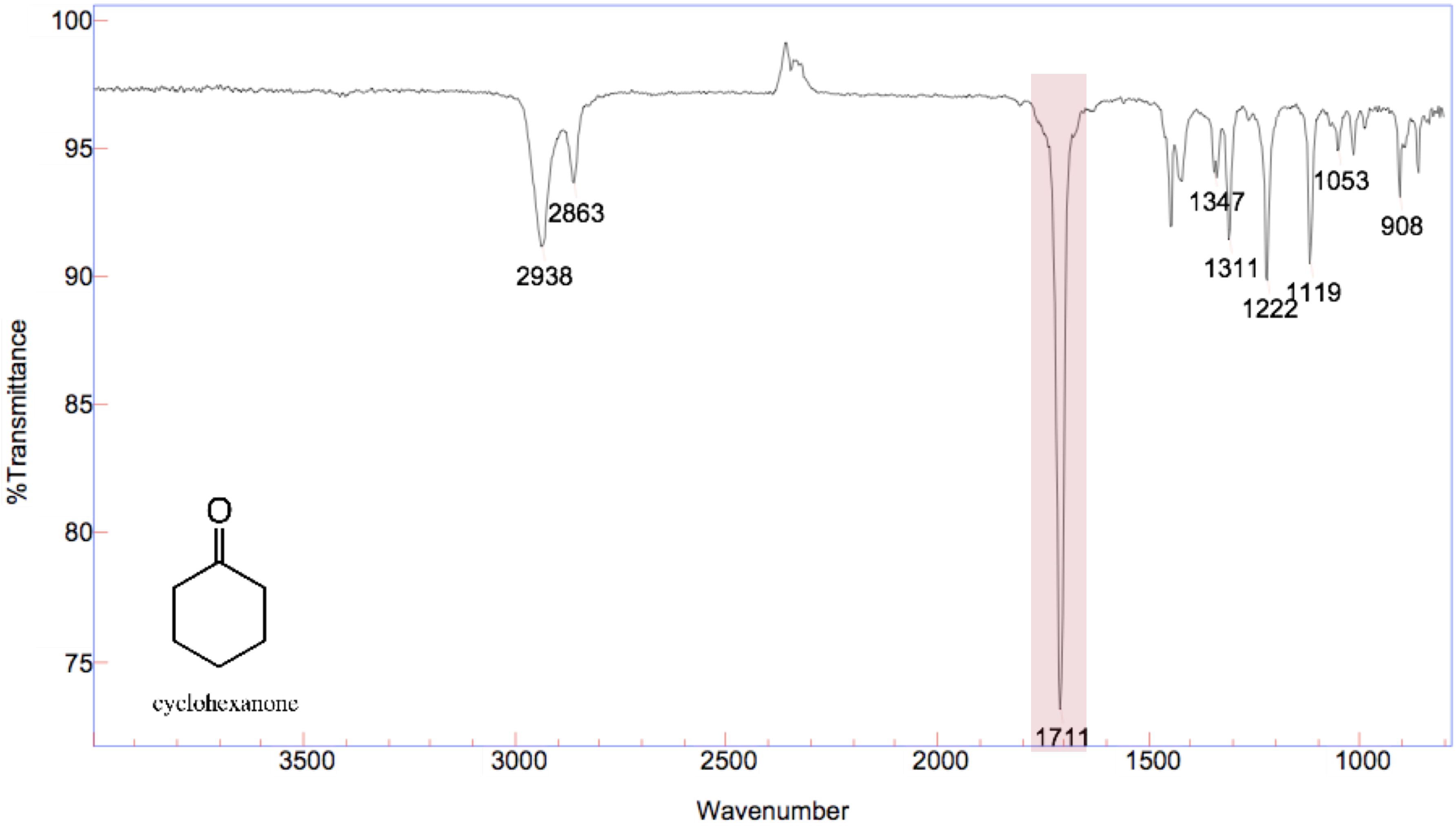

OH
3650 - 3200
OH
3000
C-H
overtones
1200-1000
C-O
1600-1460
Ar
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
wavenumber/ cm -1

Infrared Absorption Frequencies

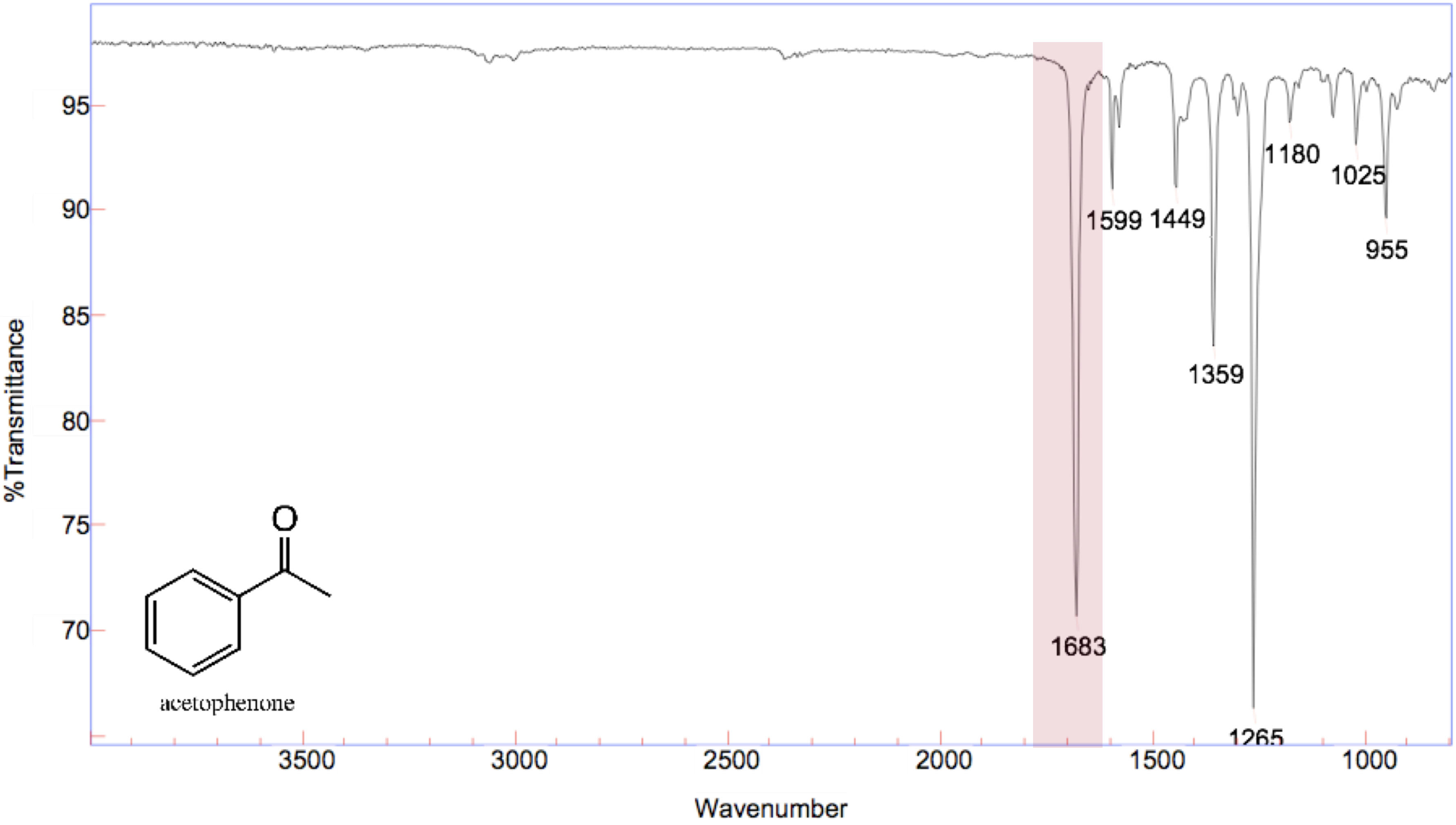


Structural unit	Frequency, cm^{-1}
Stretching vibrations (carbonyl groups)	
Aldehydes and ketones	1710-1750
Carboxylic acids	1700-1725
Acid anhydrides	1800-1850 and 1740-1790
Esters	1730-1750
Amides	1680-1700

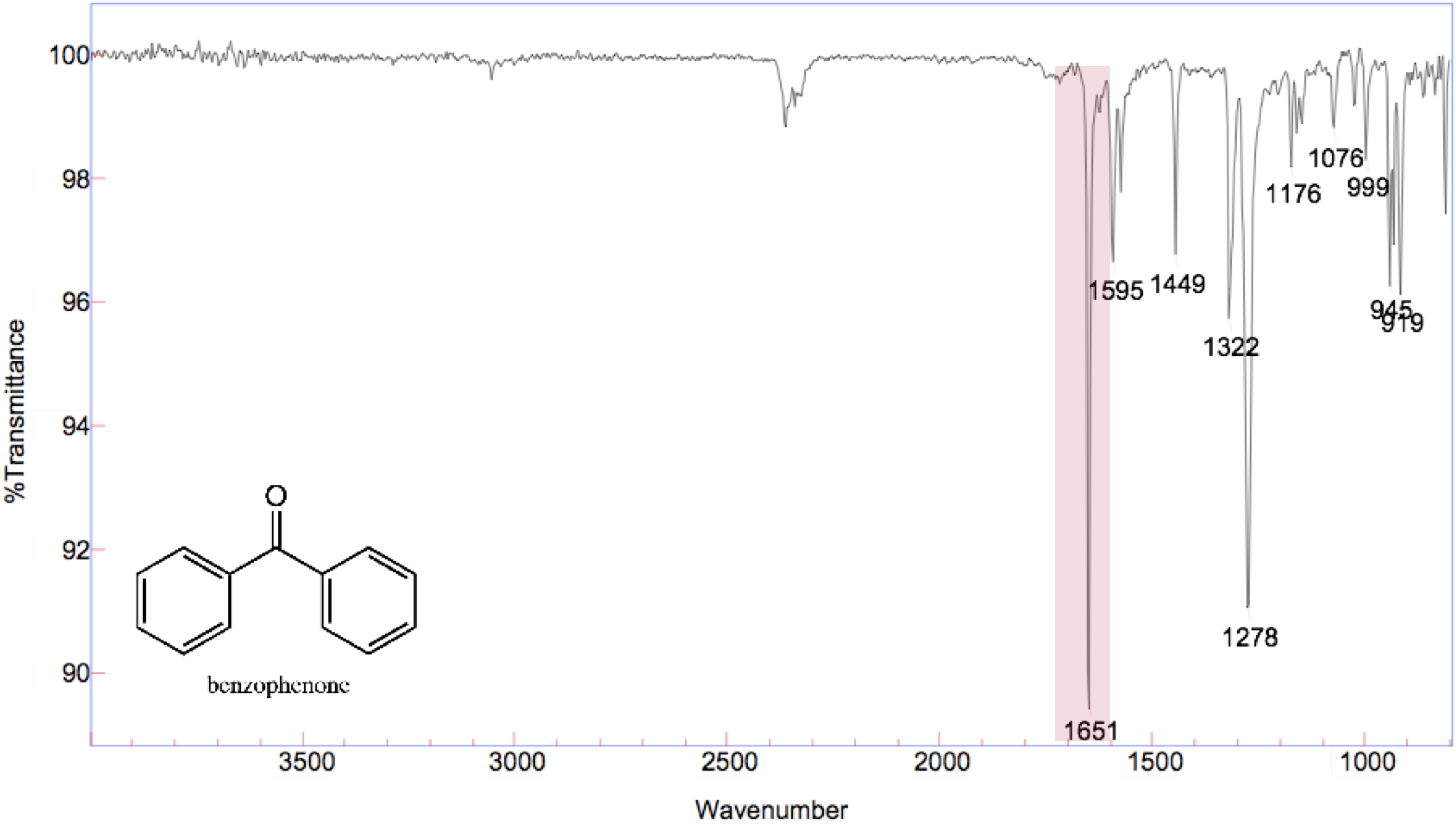
Cyclic aliphatic ketone



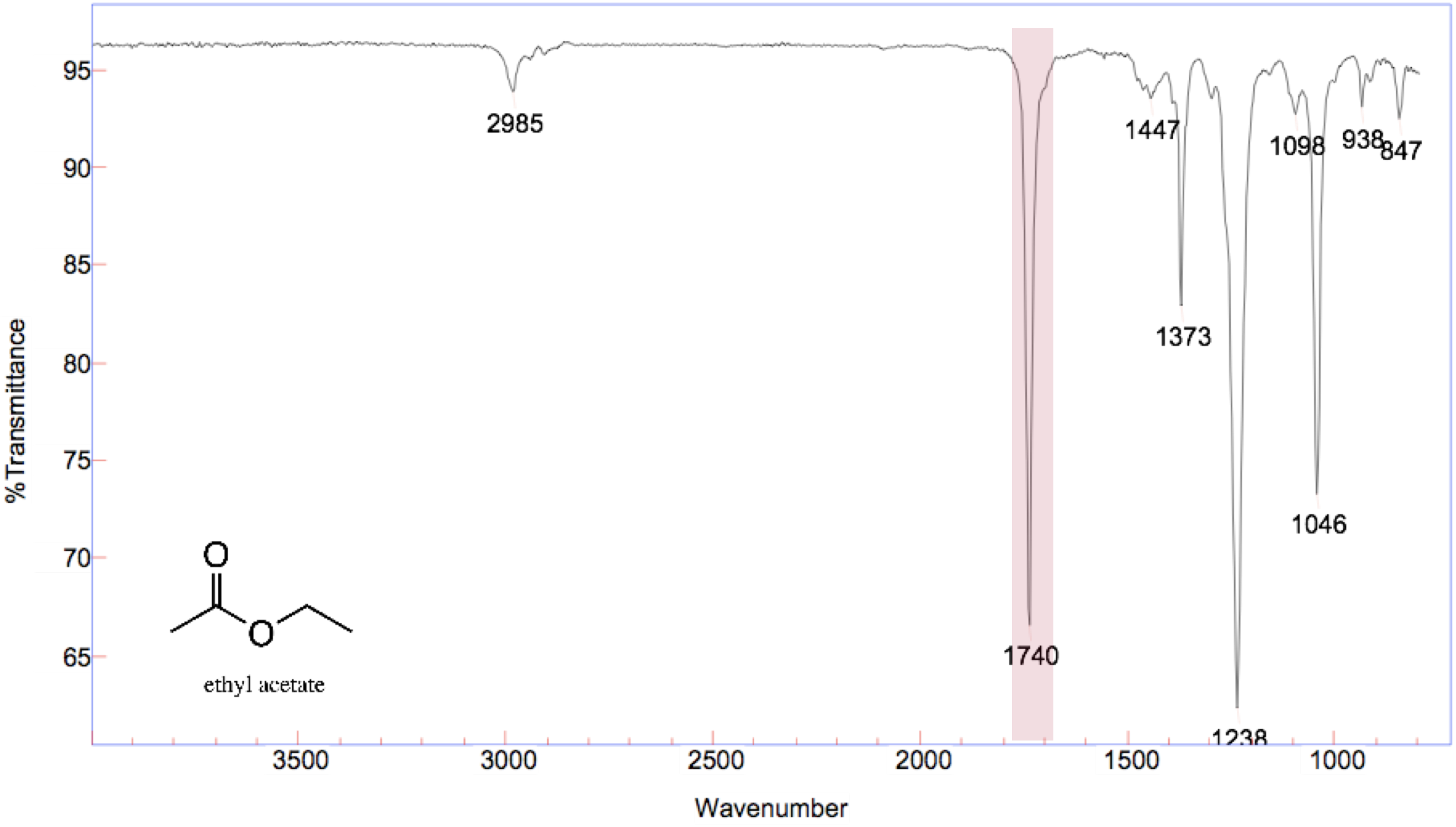
Mono substituted aromatic methyl ketone



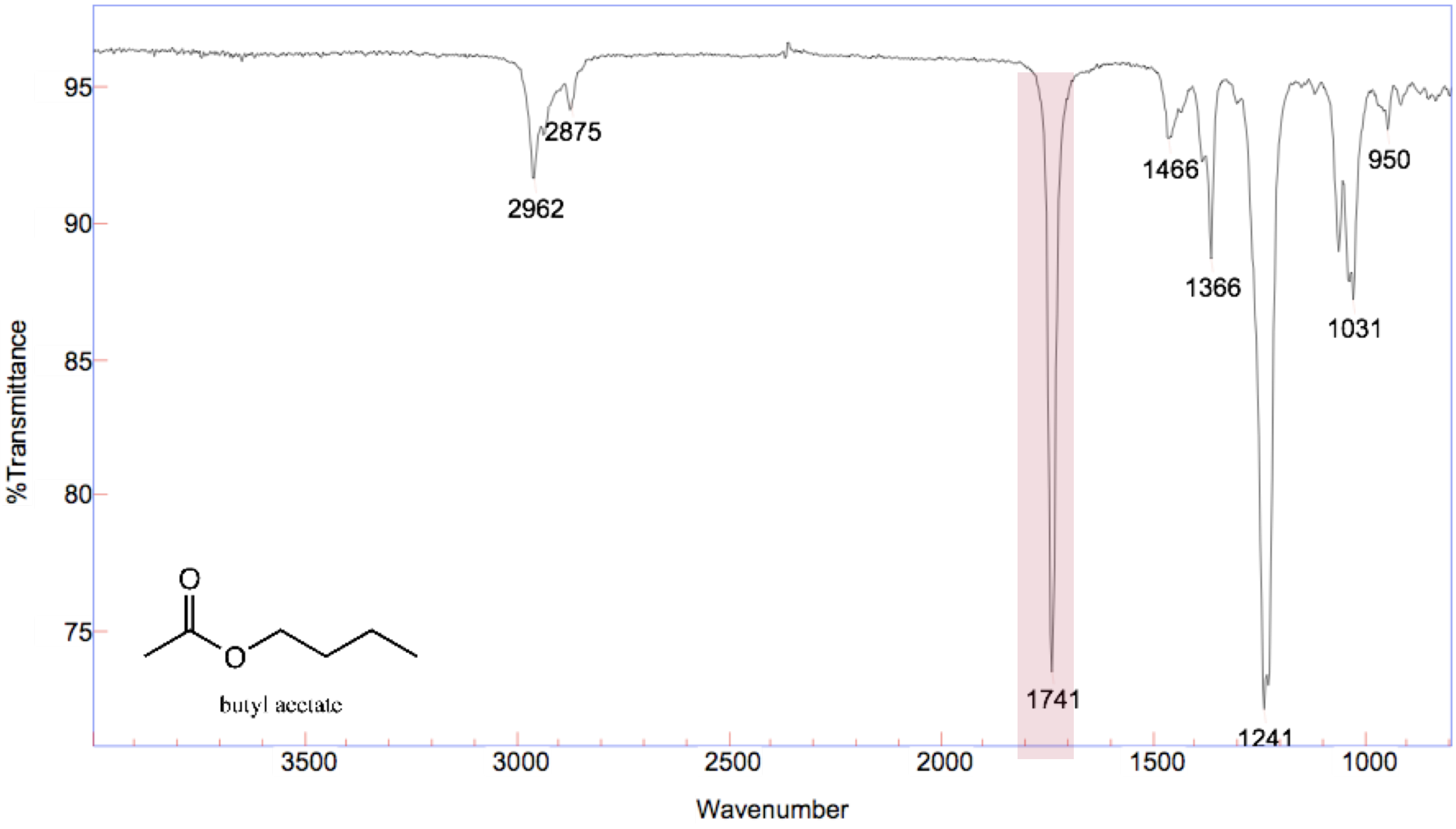
Mono substituted aromatic ketone



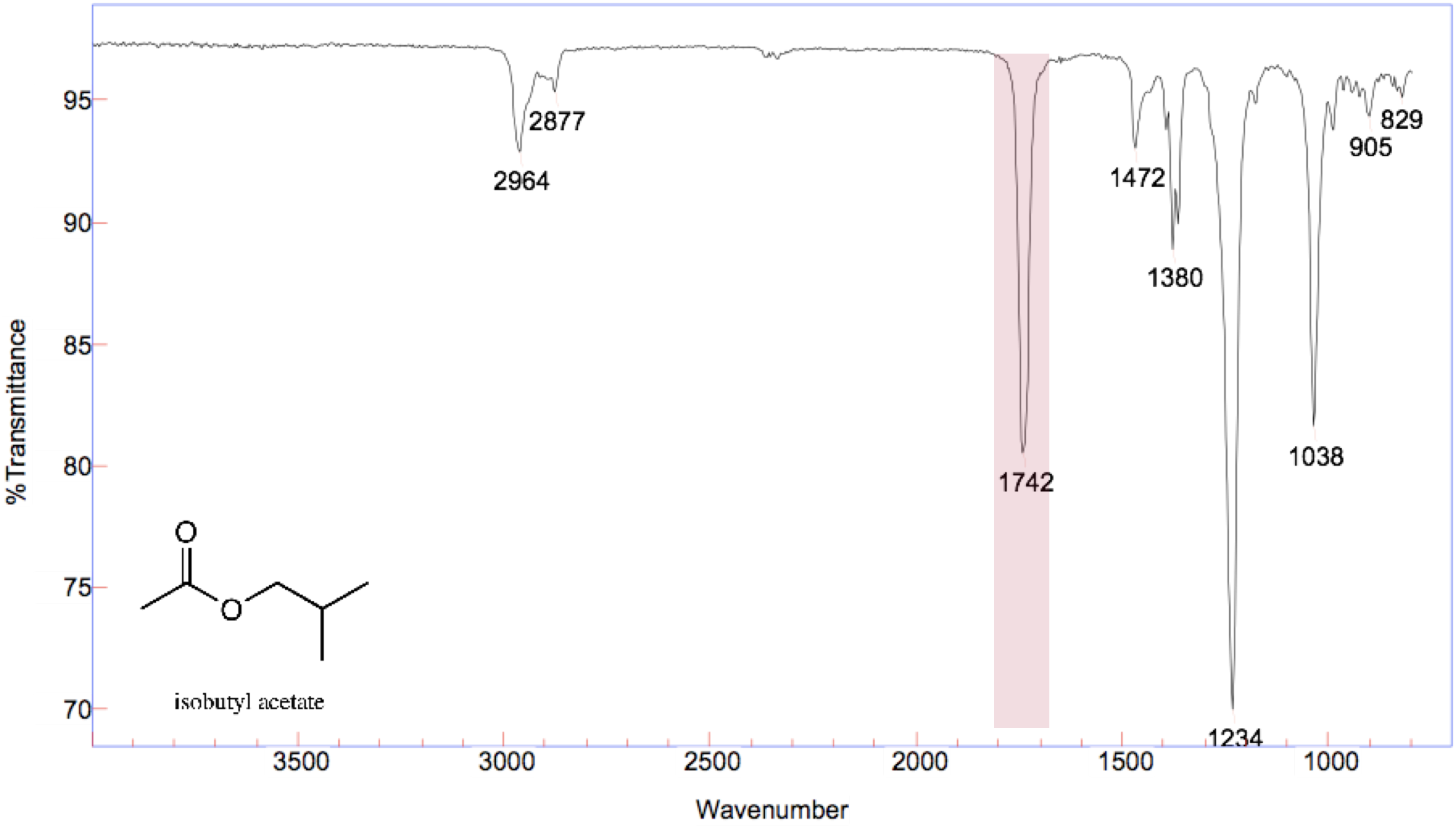
Aliphatic ester I



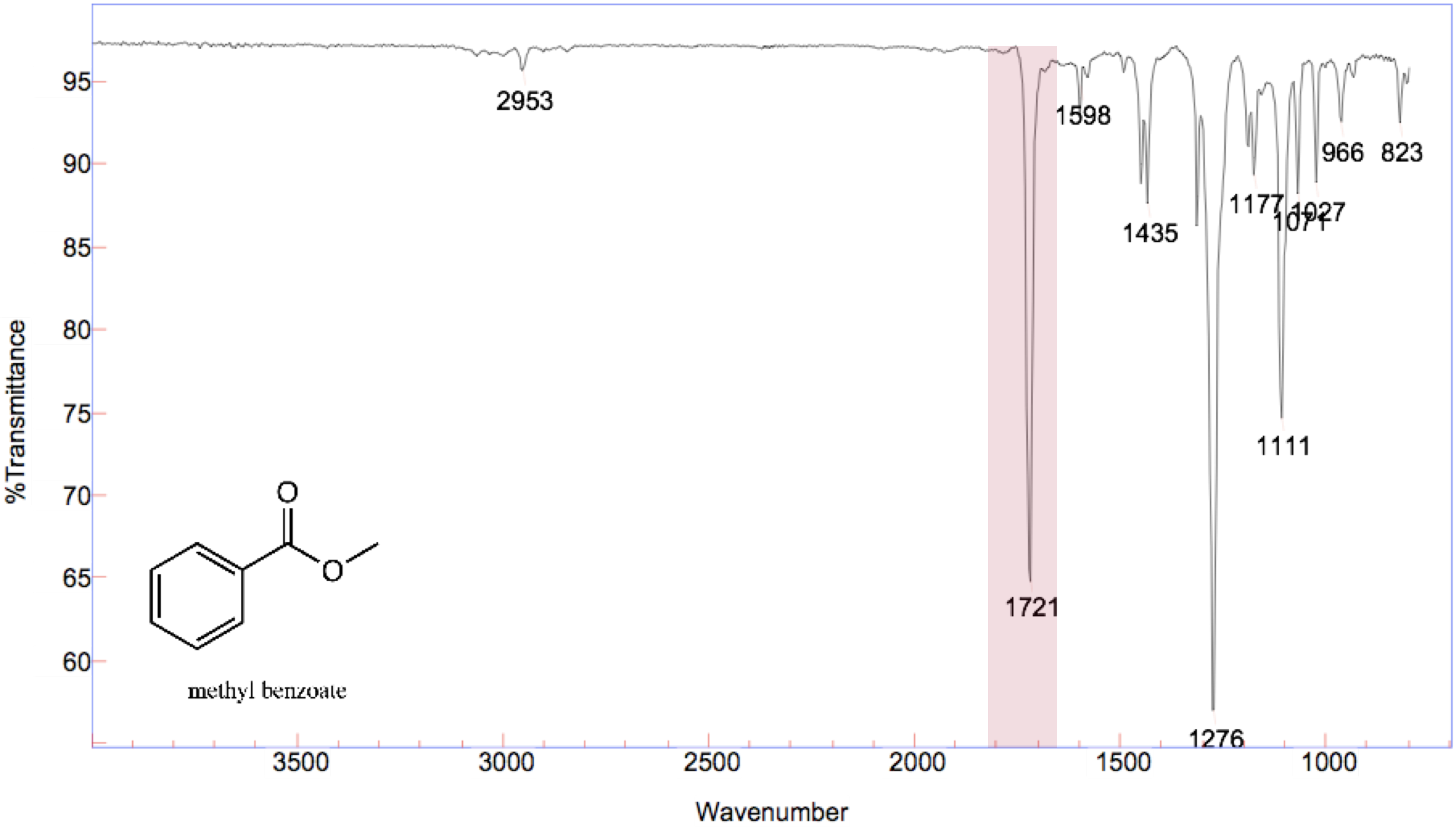
Aliphatic ester II



Aliphatic ester III



Mono substituted aromatic ester



Mono substituted aromatic conjugated ester