Spectra 1

For 3rd Year Chemistry/Zoology Students

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Spectroscopy
Spectra 1

Introduction

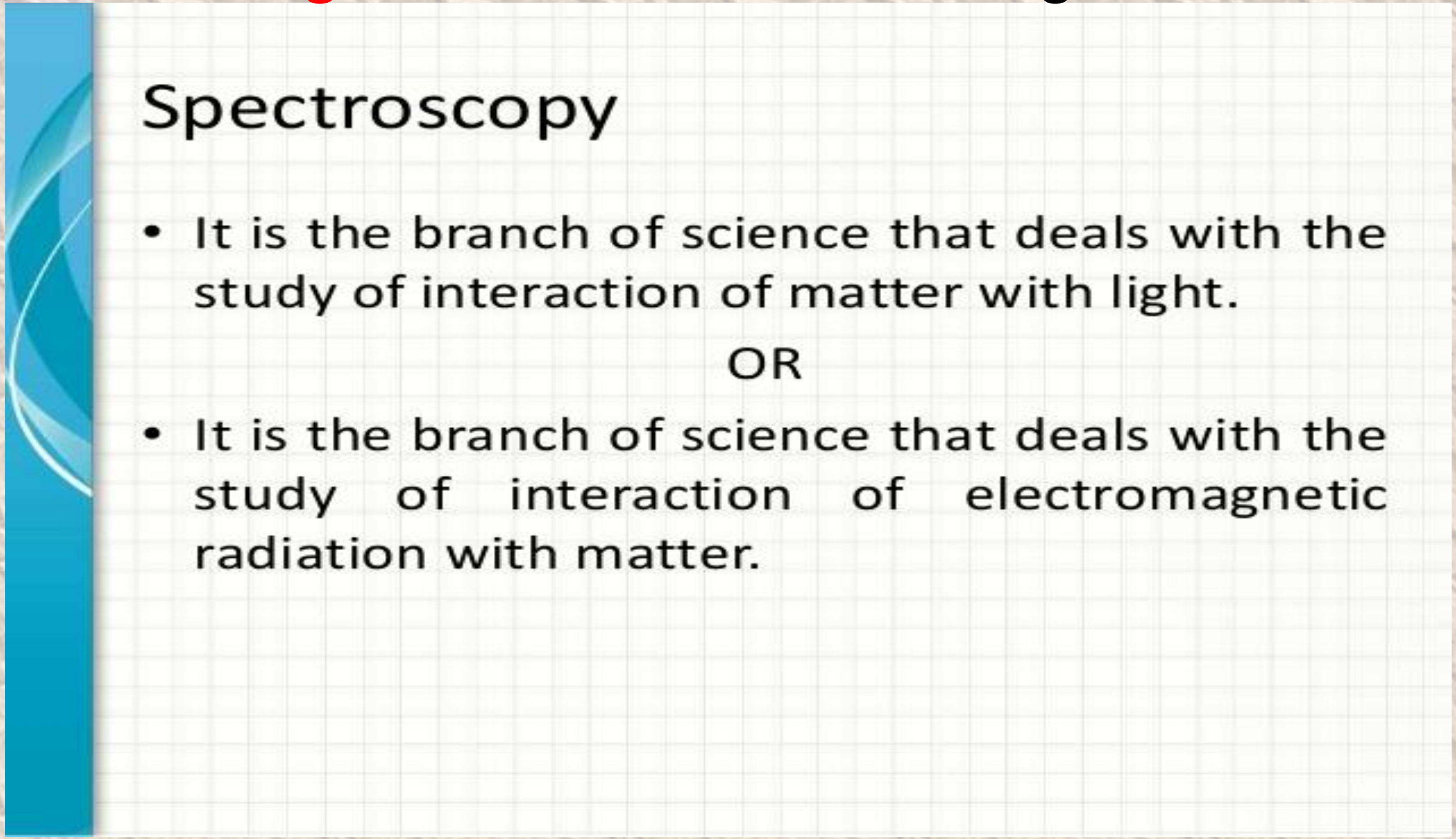
- For synthesis of new compound we use "4" methods of spectral method to make identification for the structure of the compound.

➧ These four methods are:

- **(1)** Ultra Violet (U.V) **(2)** Infrared (I.R)
- **(3)** Mass spectrometry (M.S)
- **(4)** Nuclear Magnetic Resonance (N.M.R)

Spectroscopy

The light is a beams of electromagnetic waves



Spectroscopy

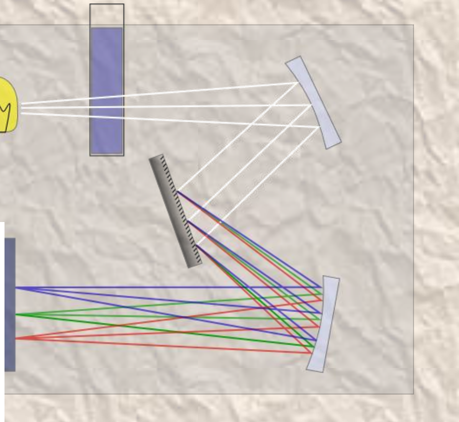
- It is the branch of science that deals with the study of interaction of matter with light.

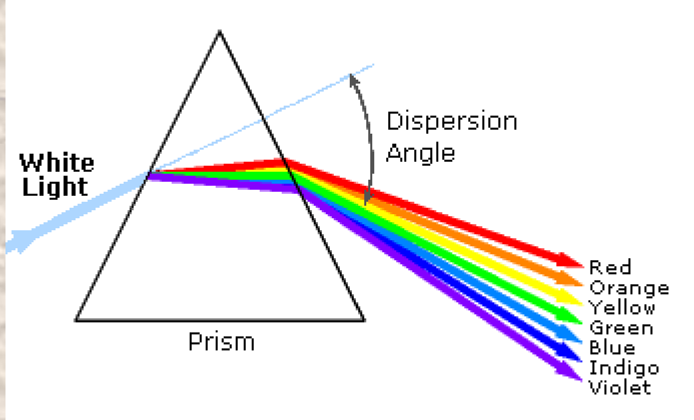
OR

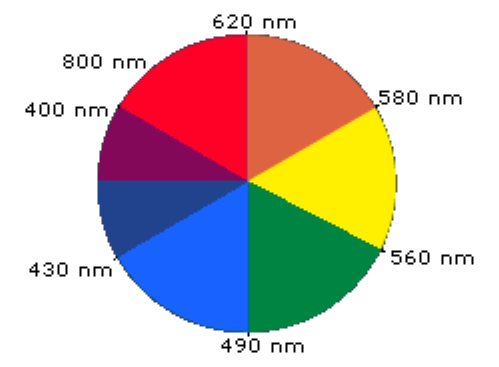
- It is the branch of science that deals with the study of interaction of electromagnetic radiation with matter.

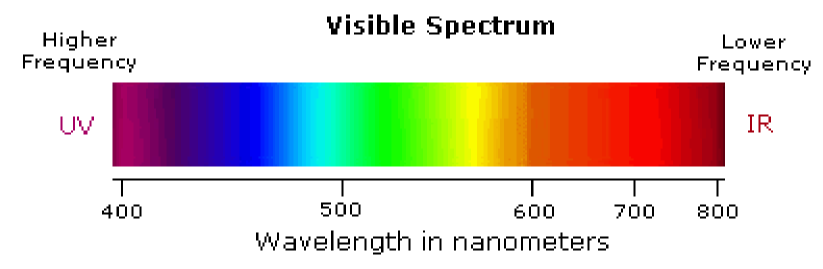
- **Idea**:
  - Compound which we want to identify absorb an energy with a certain wave length causes excitation and then it will emit this energy which pass to detector and pass to plotter to plot a chart. .
-

UV-Vis spectroscopy
Electronic absorption spectroscopy

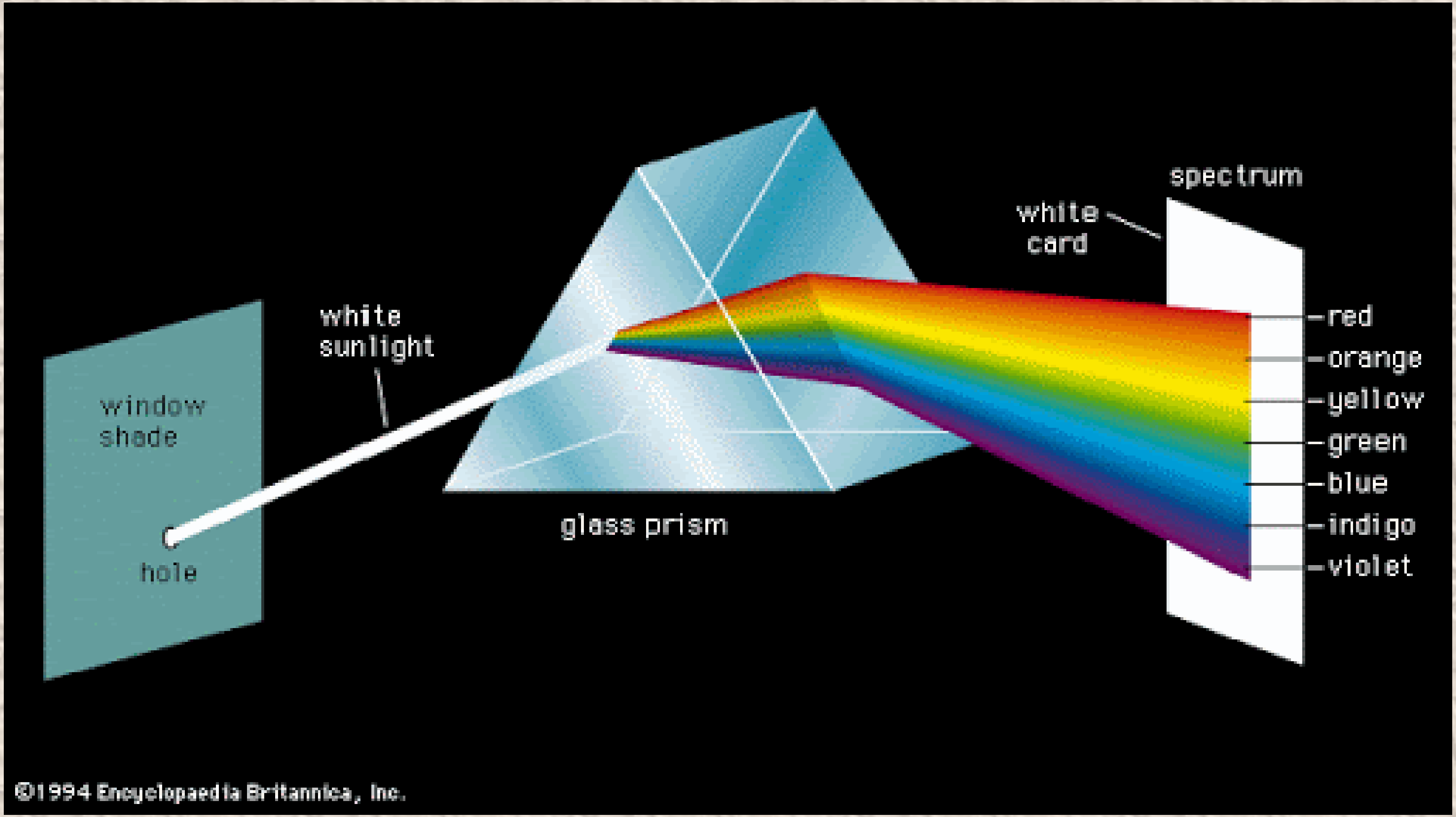




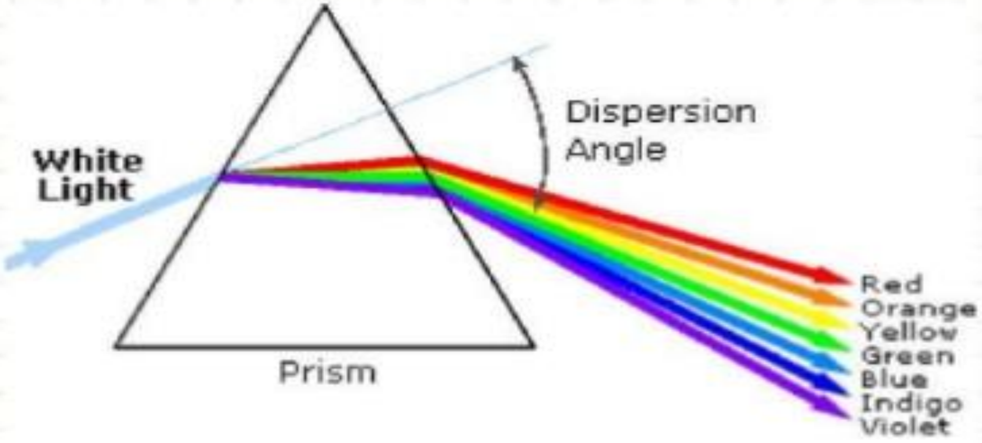




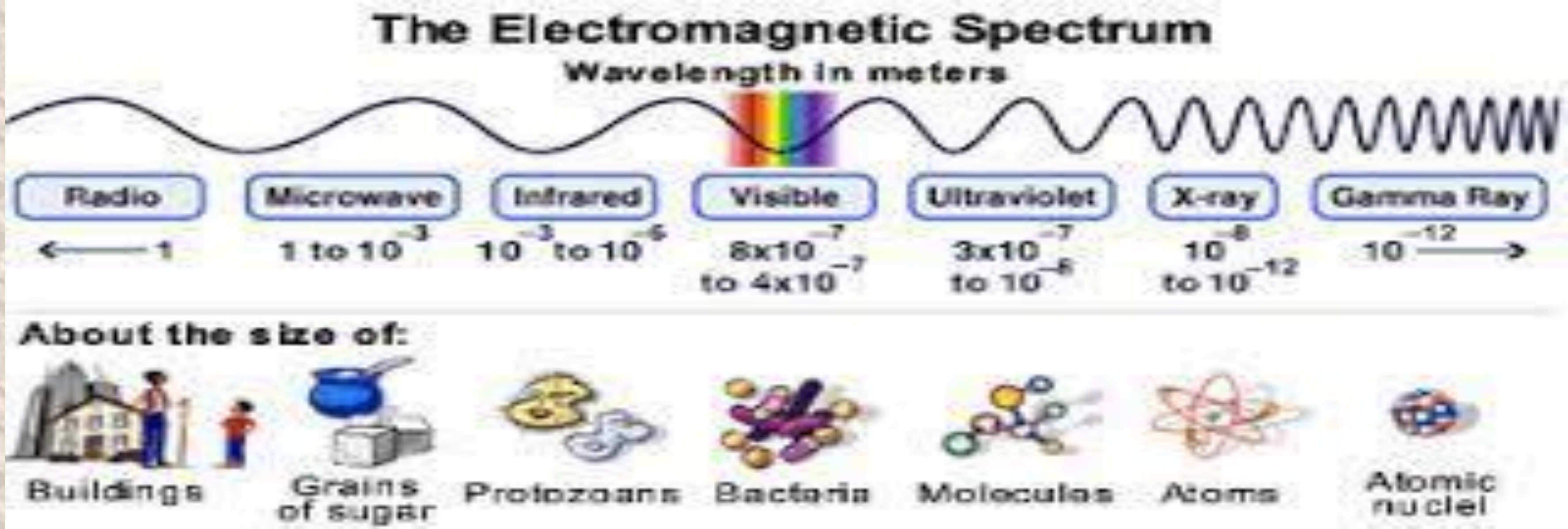
- **Violet:** 400 - 420 nm
- **Indigo:** 420 - 440 nm
- **Blue:** 440 - 490 nm
- **Green:** 490 - 570 nm
- **Yellow:** 570 - 585 nm
- **Orange:** 585 - 620 nm
- **Red:** 620 - 780 nm

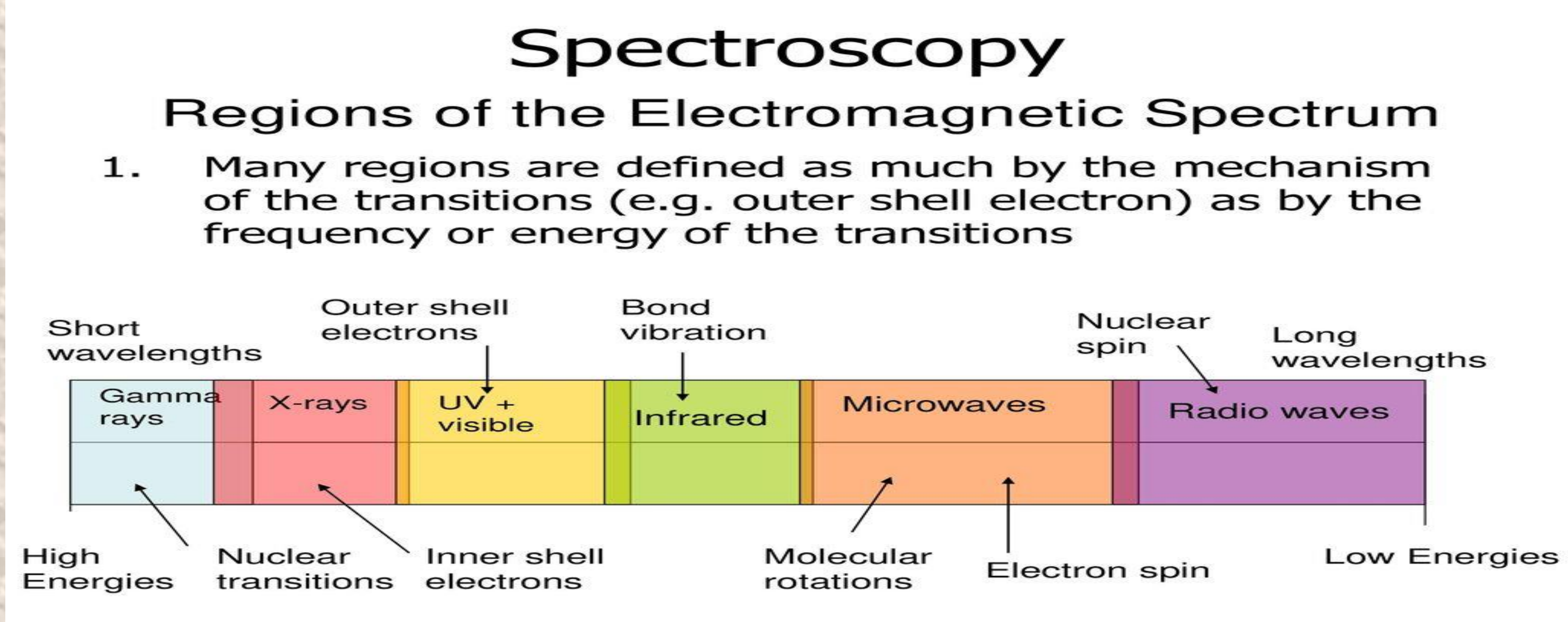

window shade
hole
white sunlight
glass prism
white card
spectrum
red
orange
yellow
green
blue
indigo
violet

Electromagnetic Radiation



Violet	400 - 420 nm	Yellow	570 - 585 nm
Indigo	420 - 440 nm	Orange	585 - 620 nm
Blue	440 - 490 nm	Red	620 - 780 nm
Green	490 - 570 nm		

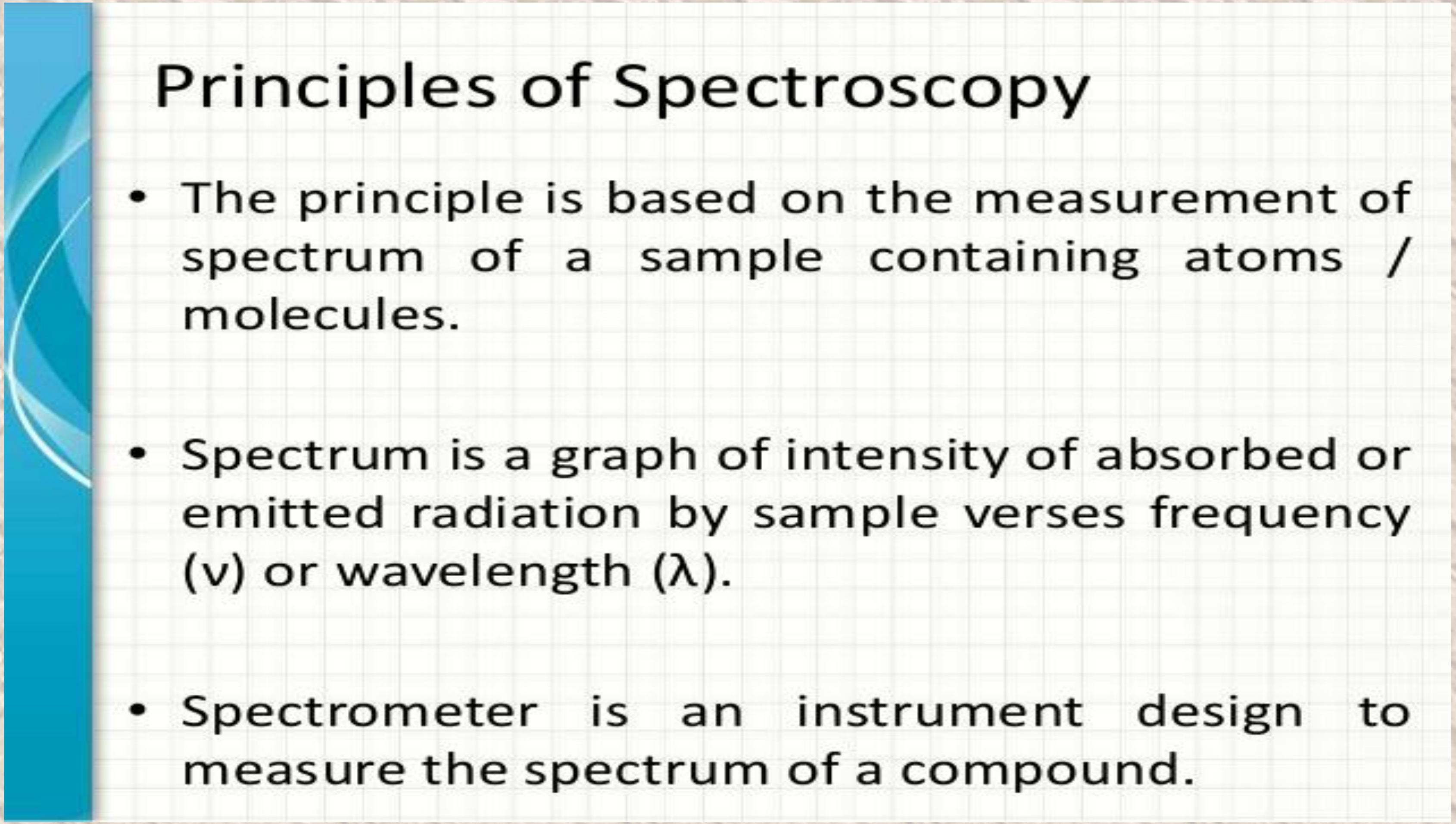




Spectroscopy

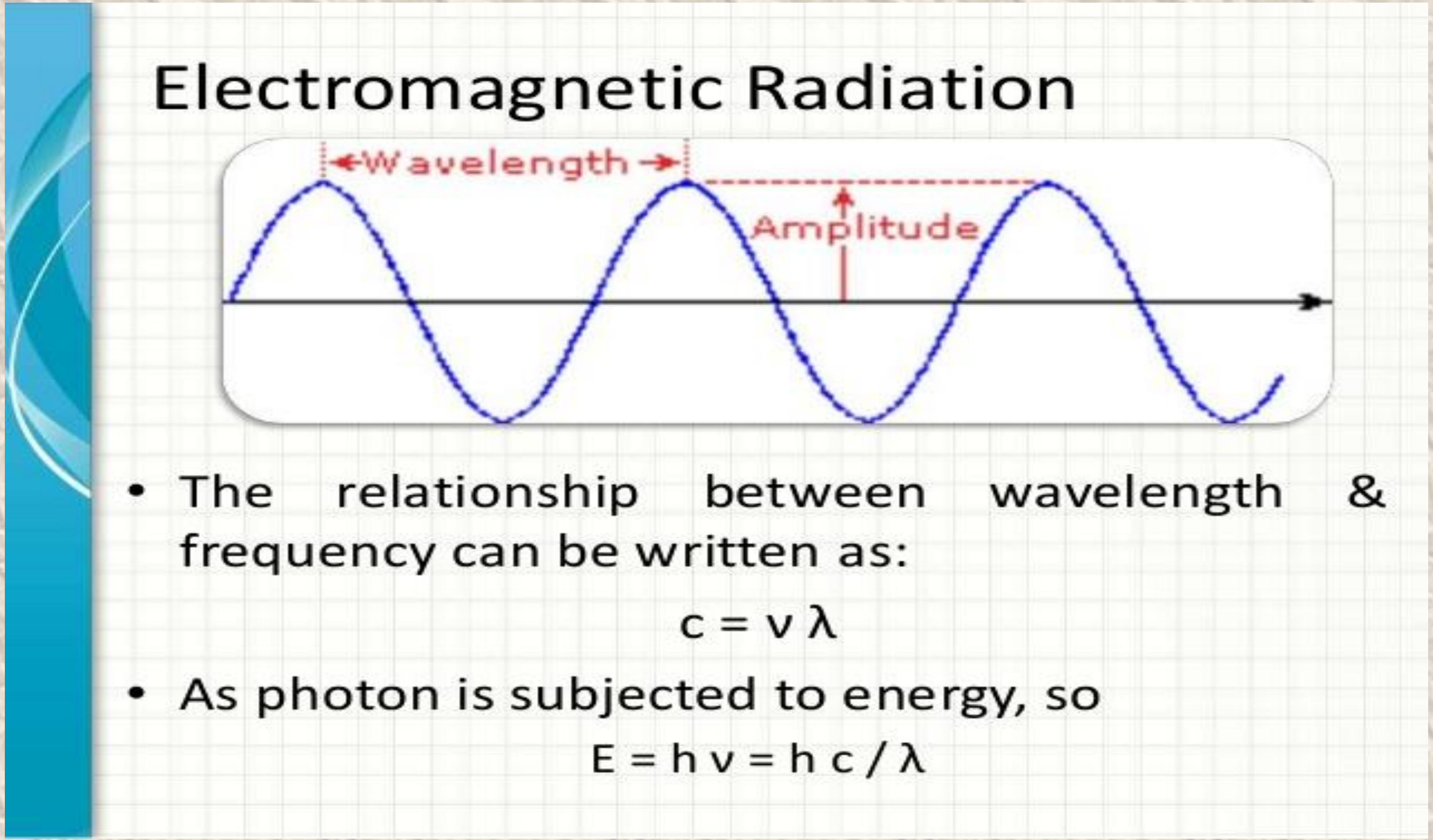
Regions of the Electromagnetic Spectrum

1. Many regions are defined as much by the mechanism of the transitions (e.g. outer shell electron) as by the frequency or energy of the transitions



Principles of Spectroscopy

- The principle is based on the measurement of spectrum of a sample containing atoms / molecules.
- Spectrum is a graph of intensity of absorbed or emitted radiation by sample verses frequency (ν) or wavelength (λ).
- Spectrometer is an instrument design to measure the spectrum of a compound.



Electromagnetic Radiation

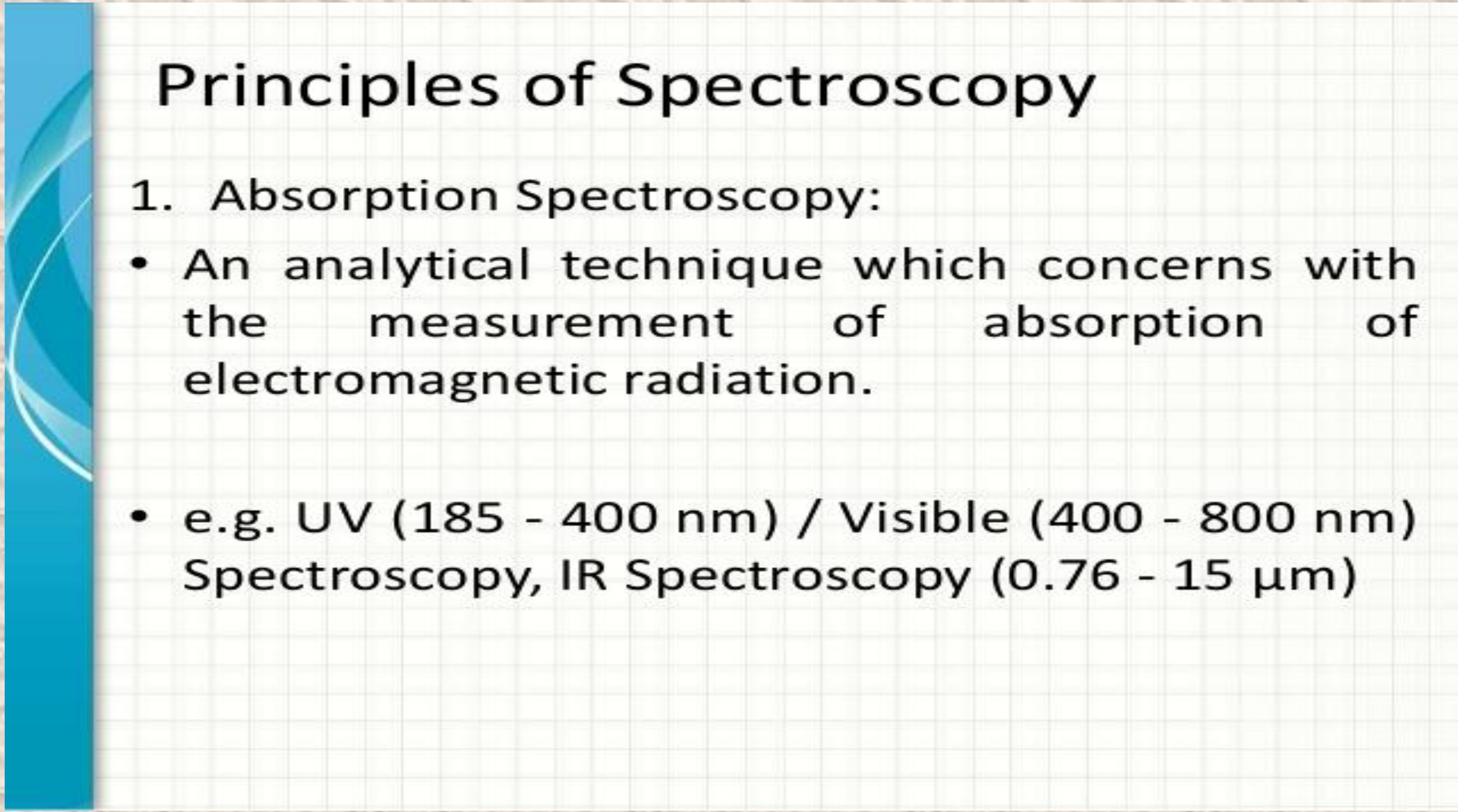
- The relationship between wavelength & frequency can be written as:

$$c = \nu \lambda$$

- As photon is subjected to energy, so

$$E = h \nu = h c / \lambda$$

$$E\ \alpha\ \lambda$$

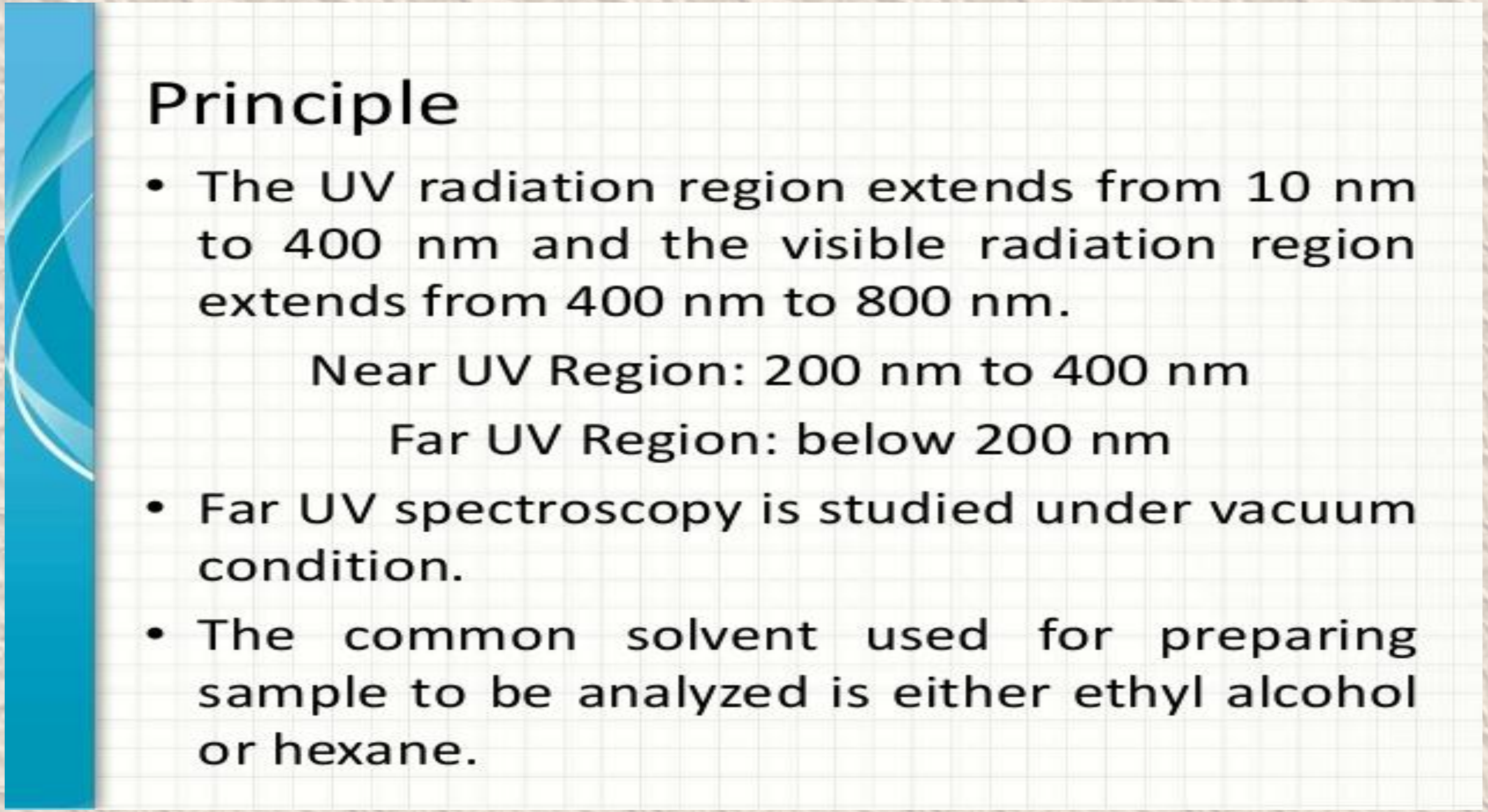


Principles of Spectroscopy

1. Absorption Spectroscopy:

- An analytical technique which concerns with the measurement of absorption of electromagnetic radiation.

- e.g. UV (185 - 400 nm) / Visible (400 - 800 nm) Spectroscopy, IR Spectroscopy (0.76 - 15 µm)



Principle

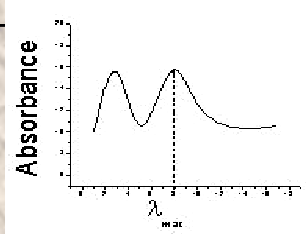
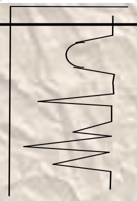
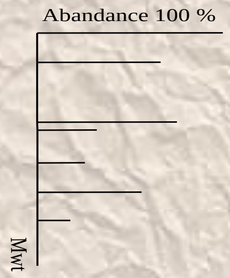
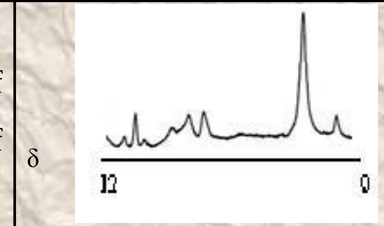
- The UV radiation region extends from 10 nm to 400 nm and the visible radiation region extends from 400 nm to 800 nm.

Near UV Region: 200 nm to 400 nm

Far UV Region: below 200 nm

- Far UV spectroscopy is studied under vacuum condition.
- The common solvent used for preparing sample to be analyzed is either ethyl alcohol or hexane.

Spectroscopic Techniques:

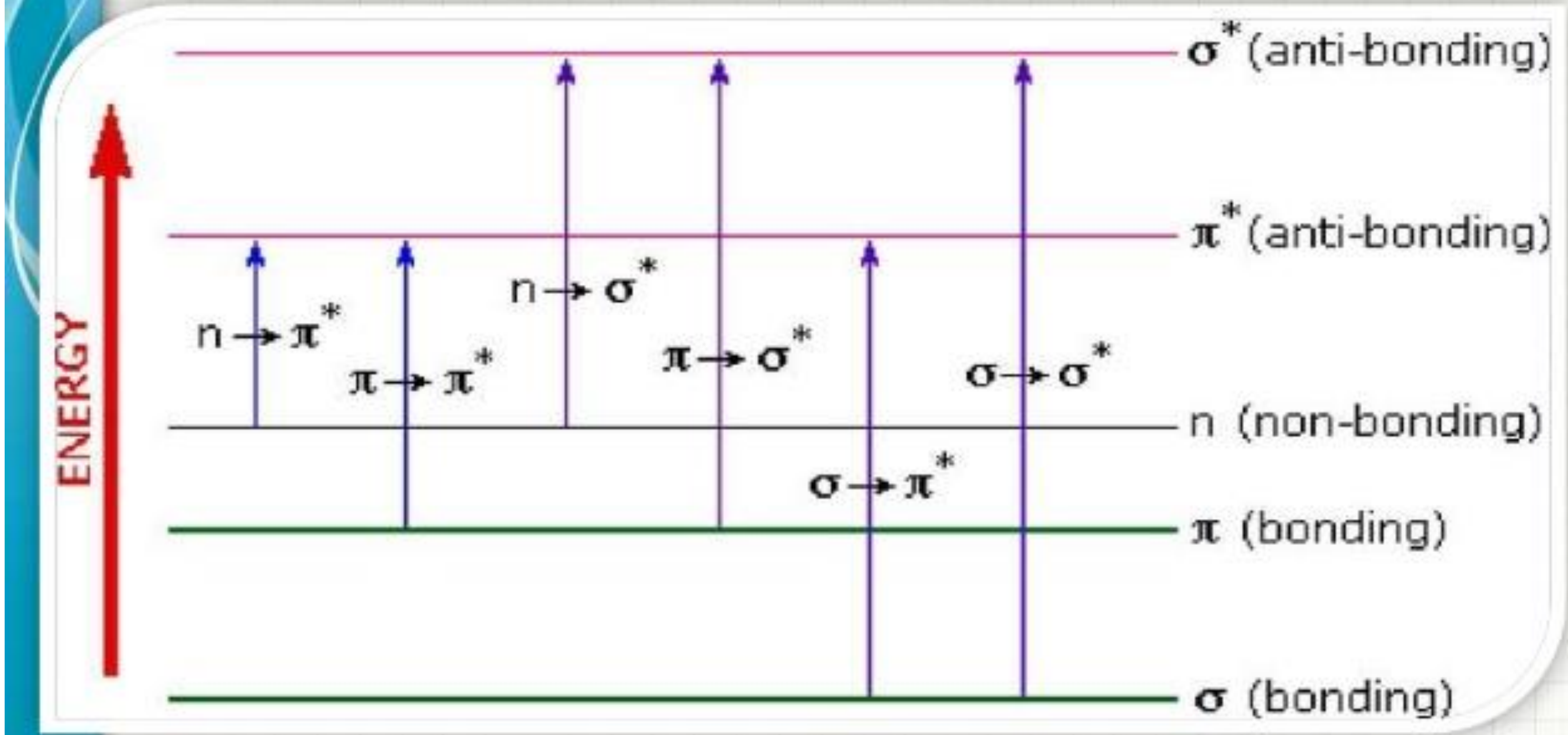
Type of technique	Effect of this "E" on the molecule	Shape of chart	Uses of this technique
U.V.	Cause changes in the electronic energy levels within a molecule Excitation of elec. from lower level her level		Identify for conjugation (= - =)
I.R	Vibration for bond between two atoms		Identify for the function J/gps in the molecule
M.S	Fragmentation of the molecule to small parts		Identify through wt. and M.wt. of some fragment to identify the structure
N.M.R	Microwave cause resonance of nucleus of atom under effect of strong magnet		Identification for the types of "H" in the compound and the structure

Chromophores is the atoms or groups responsible to absorption

N, S, Osuch as;

C=O, C=C, C-C, C=N, C=s

The possible electronic transitions can graphically shown as:



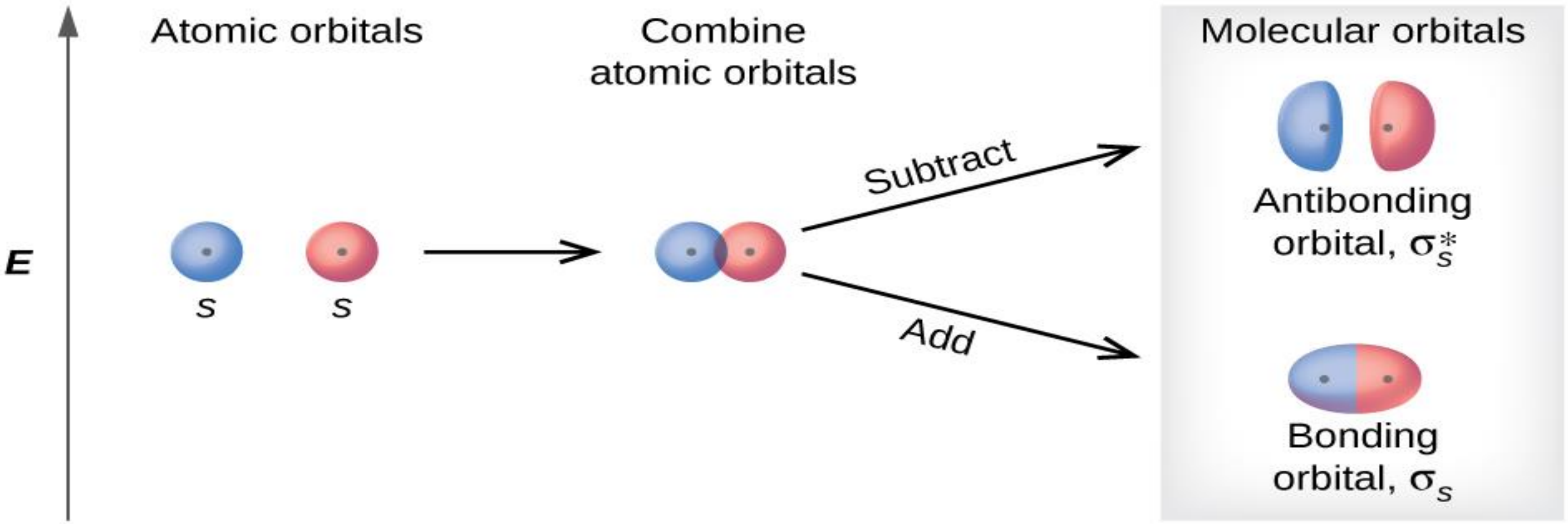
The possible electronic transitions are

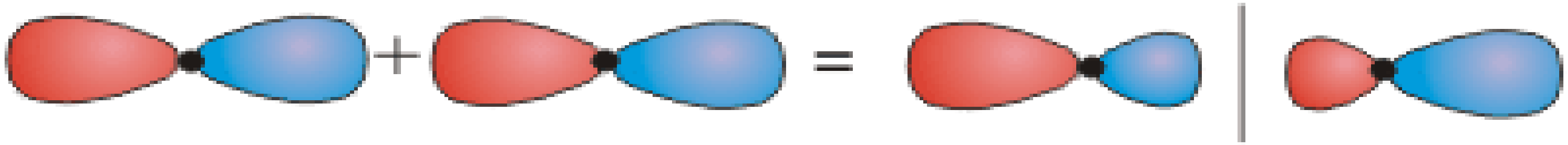
1. $\sigma \rightarrow \sigma^*$ transition
2. $\pi \rightarrow \pi^*$ transition
3. $n \rightarrow \sigma^*$ transition
4. $n \rightarrow \pi^*$ transition
5. $\sigma \rightarrow \pi^*$ transition
6. $\pi \rightarrow \sigma^*$ transition

1

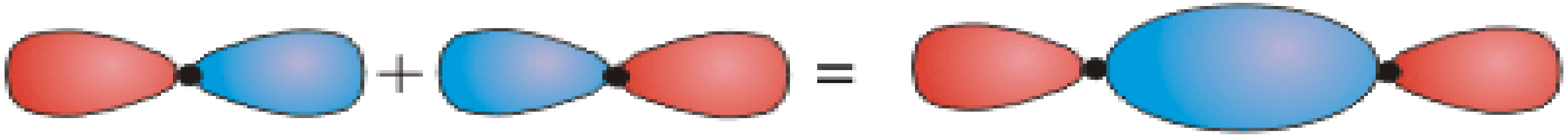
• σ → σ* transition

- σ electron from orbital is excited to corresponding anti-bonding orbital σ*.
- The energy required is large for this transition.
- e.g. Methane (CH_4) has C-H bond only and can undergo σ → σ* transition and shows absorbance maxima at 125 nm.

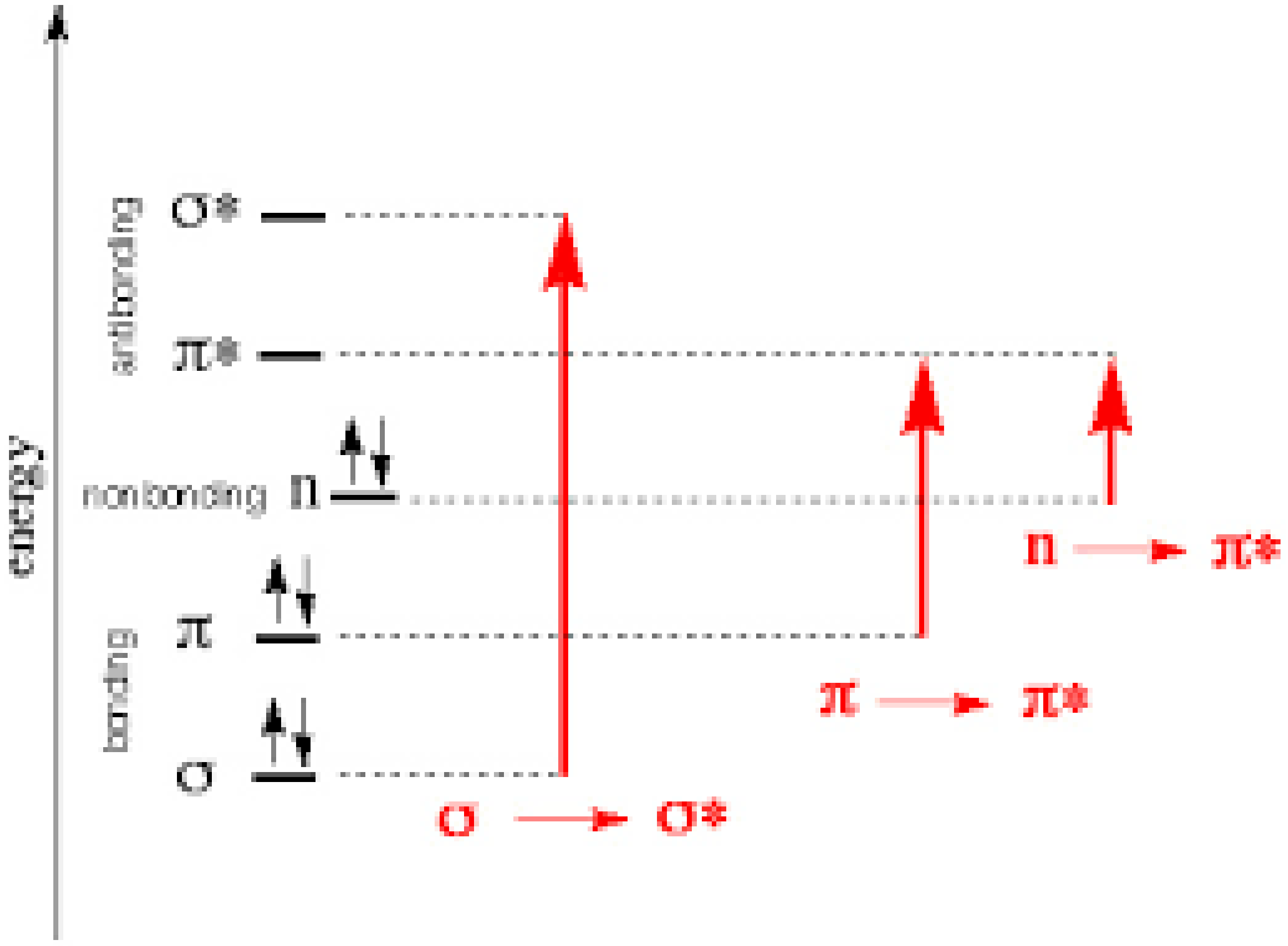




out of phase combination = $\sigma *$ MO

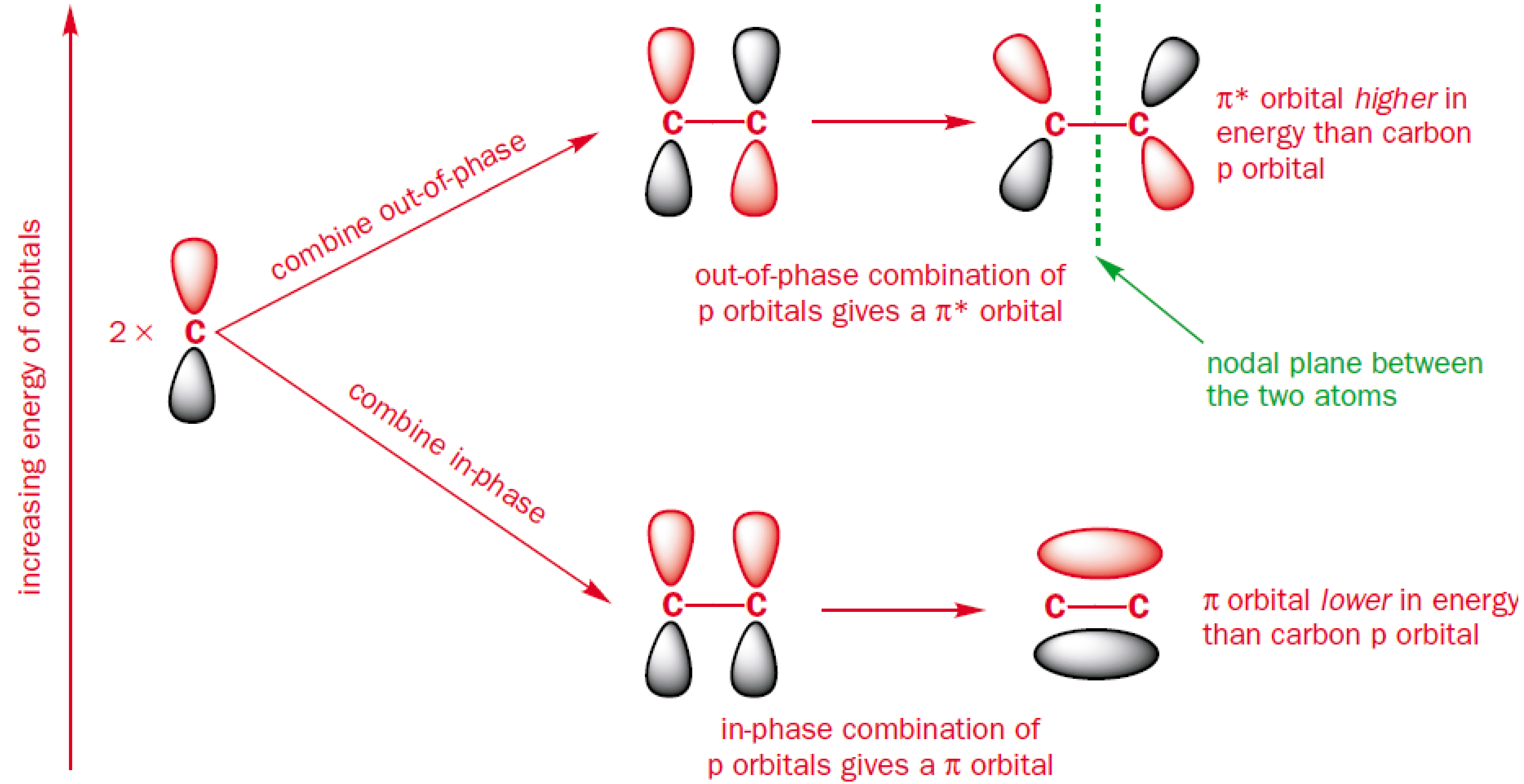


in-phase combination = σ MO


energy
antibonding
σ*
π*
nonbonding
n
bonding
π
σ
σ ⟶ σ*
π ⟶ π*
n ⟶ π*

2 • π → π* transition

- π electron in a bonding orbital is excited to corresponding anti-bonding orbital π*.
- Compounds containing multiple bonds like alkenes, alkynes, carbonyl, nitriles, aromatic compounds, etc undergo π → π* transitions.
- e.g. Alkenes generally absorb in the region 170 to 205 nm.


increasing energy of orbitals
2 × C
combine out-of-phase
combine in-phase
C–C
out-of-phase combination of p orbitals gives a π* orbital
π* orbital *higher* in energy than carbon p orbital
nodal plane between the two atoms
in-phase combination of p orbitals gives a π orbital
π orbital *lower* in energy than carbon p orbital

4

• $n \rightarrow \pi^*$ transition

- An electron from non-bonding orbital is promoted to anti-bonding π^* orbital.

- Compounds containing double bond involving hetero atoms (C=O, C≡N, N=O) undergo such transitions.

- $n \rightarrow \pi^*$ transitions require minimum energy and show absorption at longer wavelength around 300 nm.

Chromophore

The part of a molecule responsible for imparting color, are called as chromospheres.

OR

The functional groups containing multiple bonds capable of absorbing radiations above 200 nm due to n → π* & π → π* transitions.

e.g. NO_2, N=O, C=O, C=N, C≡N, C=C, C=S, etc

Chromophore

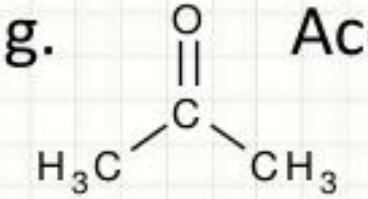
To interpretate UV – visible spectrum following points should be noted:

1. Non-conjugated alkenes show an intense absorption below 200 nm & are therefore inaccessible to UV spectrophotometer.

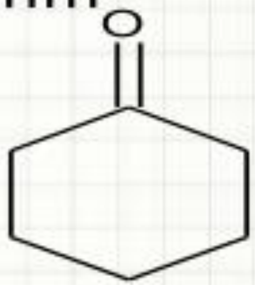
2. Non-conjugated carbonyl group compound give a weak absorption band in the 200 - 300 nm region.

Chromophore

e.g.



Acetone which has λ_{max} = 279 nm

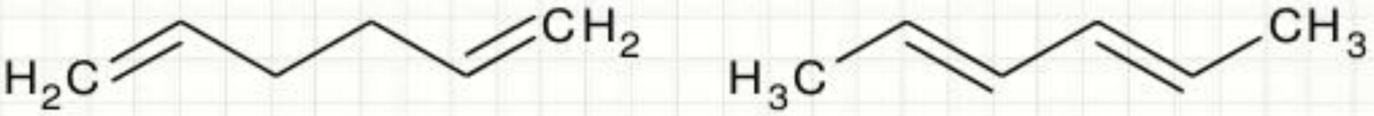


and that cyclohexane has λ_{max} = 291 nm.

When double bonds are conjugated in a compound λ_{max} is shifted to longer wavelength.

e.g. 1,5 - hexadiene has λ_{max} = 178 nm

2,4 - hexadiene has λ_{max} = 227 nm



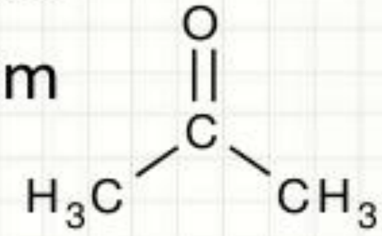
Chromophore

3. Conjugation of C=C and carbonyl group shifts the λ_{max} of both groups to longer wavelength.

e.g. Ethylene has λ_{max} = 171 nm

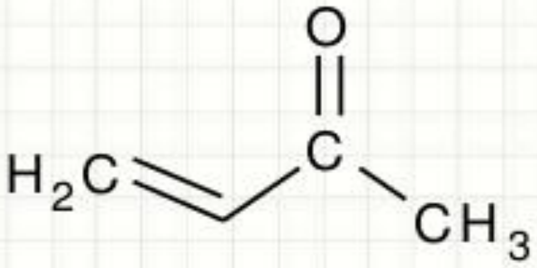
Acetone has λ_{max} = 279 nm

$H_2C{=}CH_2$



$H_3C{-}C({=}O){-}CH_3$

Crotonaldehyde has λ_{max} = 290 nm



Auxochrome

The functional groups attached to a chromophore which modifies the ability of the chromophore to absorb light , altering the wavelength or intensity of absorption.

OR

The functional group with non-bonding electrons that does not absorb radiation in near UV region but when attached to a chromophore alters the wavelength & intensity of absorption.

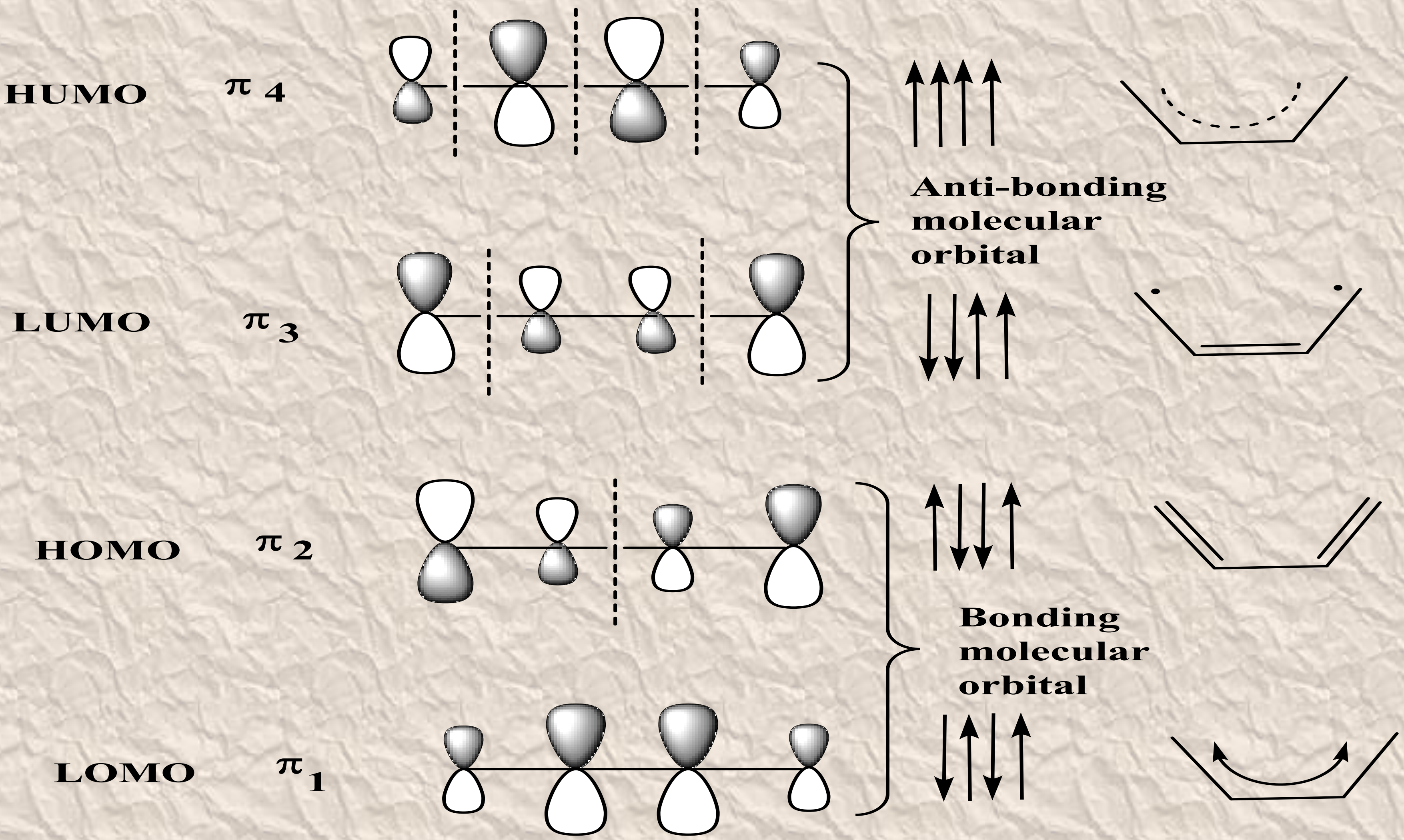
Auxochrome

e.g. Benzene λ_{max} = 255 nm

Phenol λ_{max} = 270 nm

Aniline λ_{max} = 280 nm

The π- π* transitions in π-molecular orbitals of 1,3-butadiene.



HUMO π_4

LUMO π_3

Anti-bonding
molecular
orbital

HOMO π_2

LOMO π_1

Bonding
molecular
orbital

π - Molecular orbitals of 1,3-butadiene

Chromophore

3. Conjugation of C=C and carbonyl group shifts the λ_{max} of both groups to longer wavelength.

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Acetone has λ_{max} = 279 nm

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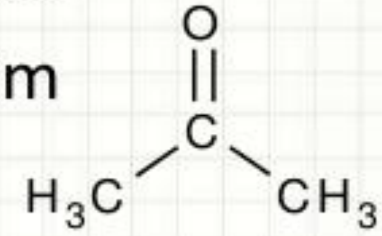
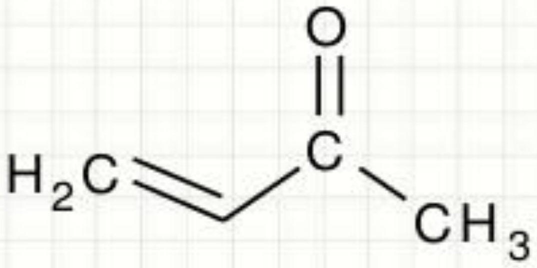
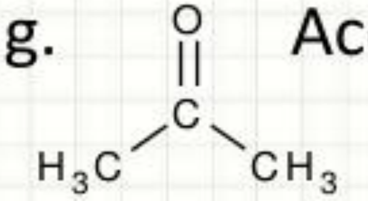
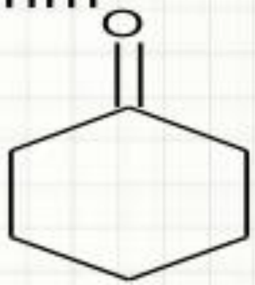


$H_3C-C(=O)-CH_3$

Crotonaldehyde has λ_{max} = 290 nm



Chromophore

e.g. Acetone which has λ_{max} = 279 nm

and that cyclohexane has λ_{max} = 291 nm.

When double bonds are conjugated in a compound λ_{max} is shifted to longer wavelength.

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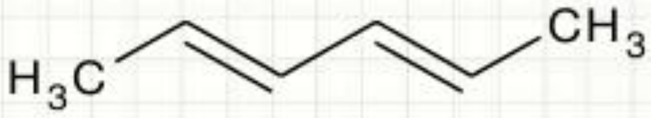
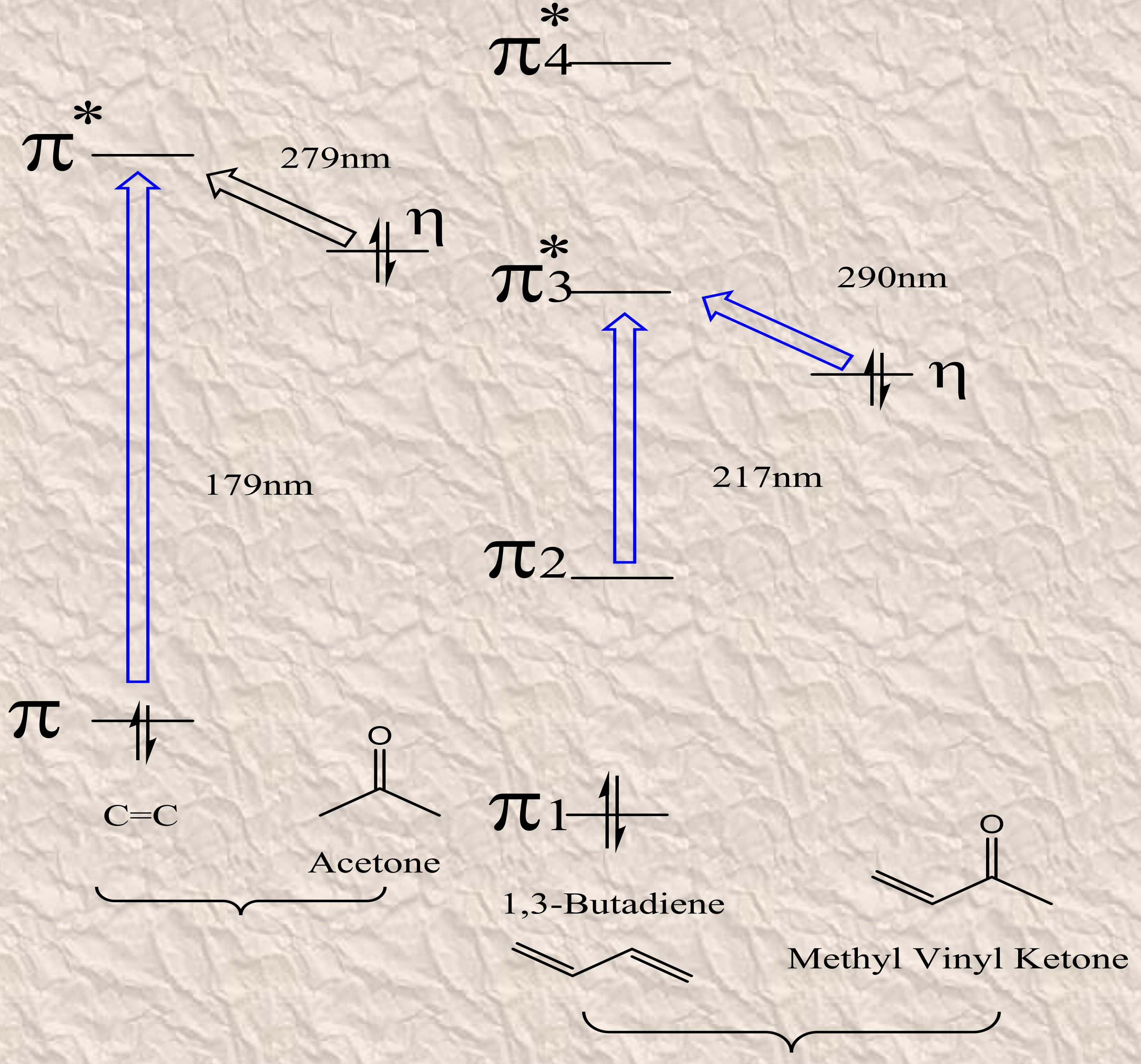




The Electronic Transitions of C=C, Acetone, 1,3-butadiene and Methyl vinyl ketone

Auxochrome

The functional groups attached to a chromophore which modifies the ability of the chromophore to absorb light , altering the wavelength or intensity of absorption.

OR

The functional group with non-bonding electrons that does not absorb radiation in near UV region but when attached to a chromophore alters the wavelength & intensity of absorption.

Auxochrome

e.g. Benzene λ_{max} = 255 nm

Phenol λ_{max} = 270 nm

Aniline λ_{max} = 280 nm

FOLLOW THE ULTRA-VIOLET SPECTROSCOPY

Woodward-Fieser rules

- In this lesson we discuss a few examples of how we can utilize the **Woodward-Fieser** rules to determine the wavelength of maximum absorption for some molecules. **You have to** read up the first two sections on the **Woodward rules to calculate the λmax for conjugated dienes** and **the Woodward rules to calculate the λmax for α,β-unsaturated carbonyl compounds**.

The Numerical values for Woodward-Fieser rules are in the following tables:

S	Conjugated polyenes	Base absorption (nm)
1	Homoannular diene	253
2	Heteroannular diene	214
	Function	
3	Alkyl	5
4	-OCOR	0
5	-OR	6
6	-SR	30
7	-Cl, -Br	5
8	-NR_2	60
9	Extended conjugation	30
10	**Exocyclic double bond**	5

It is recommended that you learn on how to apply these values on the structures and then you have to calculate the λmax value.

In these sample problems you will be shown the structure, then the structure is highlighted to show you key features which would affect the λmax of the molecule. Then the table will show you the solutions on how to solve to get the wavelength of maximum absorption, with a final calculated λmax using the Woodward-Fieser rules. In some cases if we have an observed λmax for comparison, it may be given as well.

Example 1

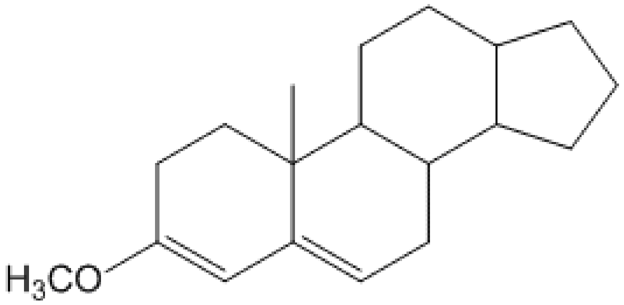
2,4-dimethylpenta-1,3-diene

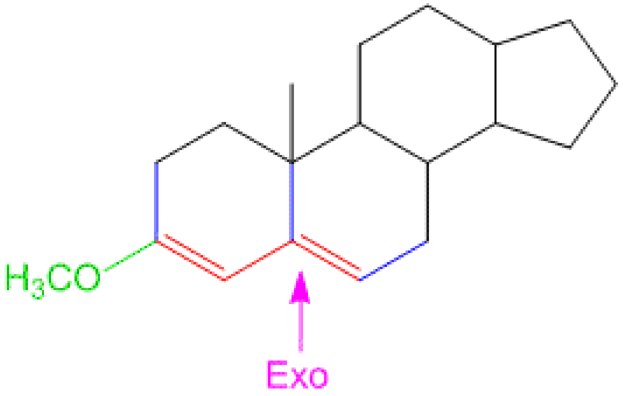
Woodward Component	Contribution
Parent base- Heteroannular Diene	+ 214 nm
Substituents- 3 alkyl groups	3 x 5 = 15 nm
Calculated λmax	**229 nm**

Example 2

Name of Compound	1-methylcyclohexa-1,3-diene
Woodward Component	**Contribution**
Parent base- Homoannular Diene	+ 253 nm
Substituents- 3 alkyl groups	3 x 5 = + 15 nm
Calculated λmax	**268 nm**

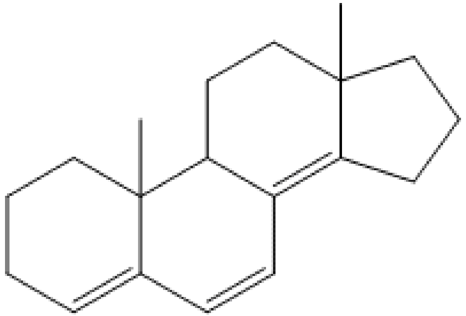
Example 3

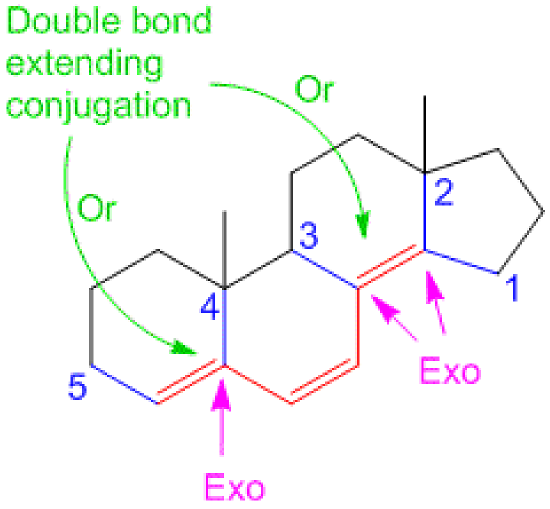




Name of Compound	3-methoxy-10-methyl-2,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene
Woodward Component	**Contribution**
Parent base- Heteroannular Diene	214 nm
Substituents- 3 alkyl groups	3 x 5 = 15 nm
1 alkoxy group	+ 6 nm
Exocyclic Double Bond	+ 5 nm
Calculated λmax	**240 nm**

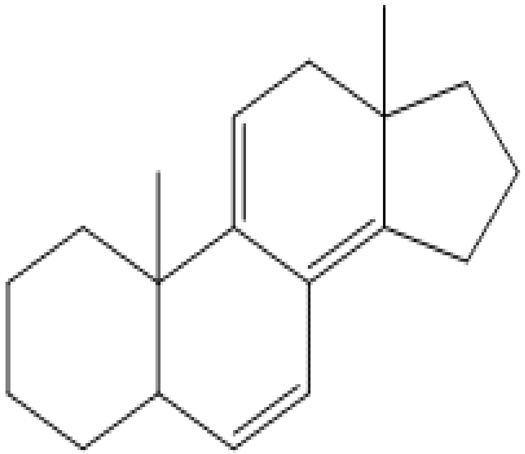
Example 4





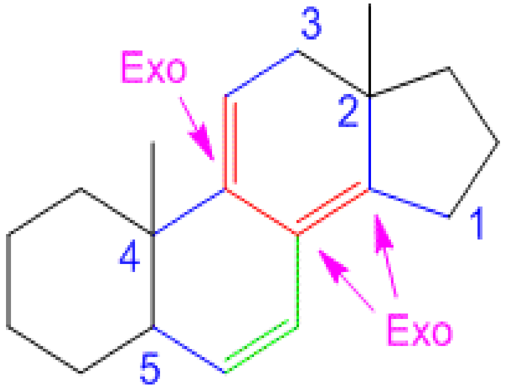
Name of Compound	10,13-dimethyl-2,3,9,10,11,12,13,15,16,17-decahydro-1H-cyclopenta[a]phenanthrene
Woodward Component	**Contribution**
Parent base- Heteroannular	+ 214 nm
Substituents- 5 alkyl groups 1 Double bond extending conjugation	5 x 5 = + 25 nm + 30 nm
3 Exocyclic Double Bond	+ 15 nm
Calculated λmax	**284 nm**

Example 5



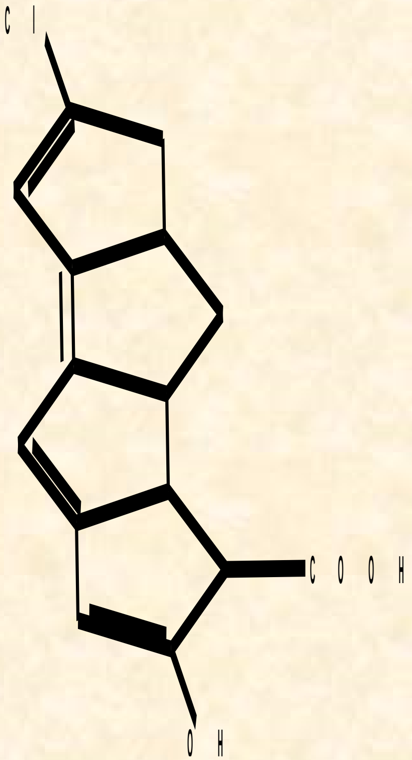
Note- In this example the molecule **contains both, a homoannular diene system and a heteroannular diene** system. In such a molecule the core chromophore is considered to be the homoannular system and accordingly the calculations are performed.

Homoannular system



Component	**Contribution**
Parent base- Homoannular	+ 253 nm
Substituents– 5 alkyl substituents	5 x 5 = + 25 nm
Double bond extending conjugation	+ 30 nm
3 Exocyclic double bonds	3 x 5 = + 15 nm
Calculated λ_{max}	**323 nm**

Parent base- α,β-unsaturated carbonyl compound cyclohexenone	+ 214 nm
Substituents: 5 alkyl group	+ 25 nm
Cl	5
OH	+ 6 nm
Other Effects: 2 Double bonds extending conjugation	+ 60 nm
3 Exocyclic double bond	+ 15 nm
Calculated λ_{max}	325 nm



Calculation of the λmax of α,β-unsaturated carbonyl compounds

In this lesson we discuss a few examples of how we can utilize the **Woodward-Fieser** rules to determine the wavelength of maximum absorption for some molecules. **The Woodward rules to calculate the λmax for α,β-unsaturated carbonyl compounds**.

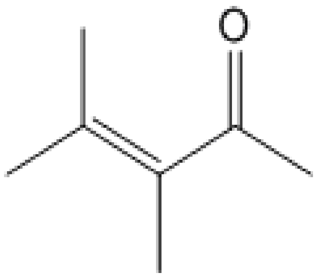
The Numerical values for Woodward-Fieser rules are in the following tables:

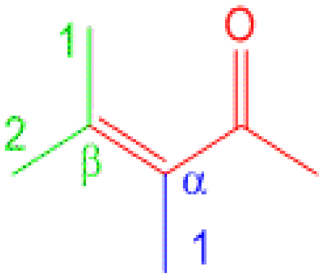
S	α , β- Unsaturated parent	Base absorption (nm)
1	Acyclic or six membered or higher ring ketones	215
2	Five-membered ring ketone	205
3	Aldehydes	210
4	Carboxylic acids and esters	195
5	Extended conjugation	30
6	Homodienic component	39
7	**Exocyclic double bond**	5

S	Substituent	α	β	γ or higher
1	Alkyl (R-)	10	12	18
2	Hydroxyl (-OH)	35	30	50
3	Alkoxyl (RO-)	35	30	17
4	Acetoxyl (CH_3COO-)	6	6	6
5	Dialkylamino (-NR_2	-	95	-
6	Chloro (Cl-)	15	12	-
7	Bromo (Br-)	25	30	-
8	**Alkylthio (RS-)**	-	85	-

It is recommended that you learn on how to apply these values on the structures and then you have to calculate the λmax value.

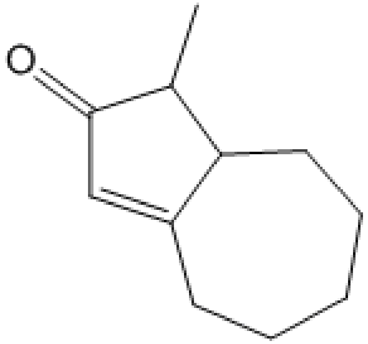
In these sample problems you will be shown the structure, then the structure is highlighted to show you key features which would affect the λmax of the molecule. Then the table will show you the solutions on how to solve to get the wavelength of maximum absorption of α,β-unsaturated carbonyl compounds, with a final calculated λmax using the Woodward-Fieser rules. In some cases if we have an observed λmax for comparison, it may be given as well.

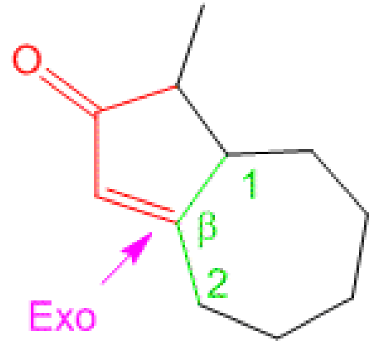




Name of Compound	3,4-dimethylpent-3-en-2-one
Component	**Contribution**
Parent base- α,β-unsaturated carbonyl compound	+ 215 nm
Substituents at α-position- 1 alkyl group	+ 10 nm
Substituents at β-position- 2 alkyl groups	2 x 12 = 24 nm
Calculated λ_{max}	**249 nm**

Example 1



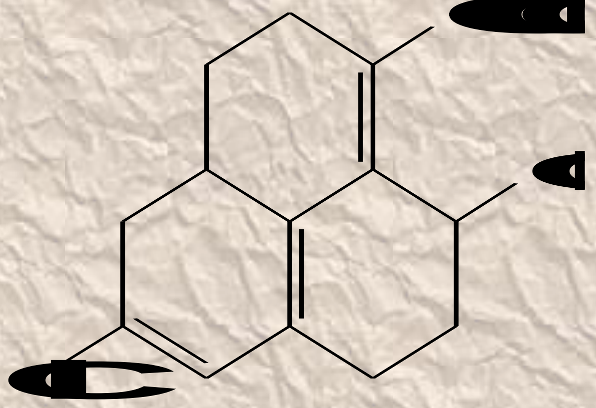


Name of Compound	1-methyl-4,5,6,7,8,8a-hexahydroazulen-2(1H)-one
Component	**Contribution**
Parent base- cyclopentenone	+ 205 nm
Substituents at α-position	0
Substituents at β-position- 2 alkyl groups	2 x 12= + 24 nm
1 Exocyclic Double Bond	+ 5 nm
Calculated λ_{max}	**234 nm**

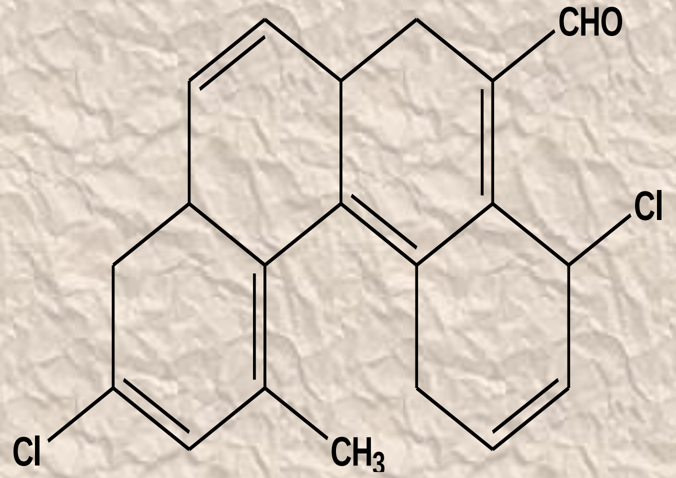
Example 2

Name of Compound	4,4a,5,6,7,8-hexahydrophenanthren-2(3H)-one
Component	**Contribution**
Parent base- α,β-unsaturated carbonyl compound cyclohexenone	+ 215 nm
Substituents at α-position:	0
Substituents at β-position: 1 alkyl group	+ 12 nm
Substituents at γ-position: 3 alkyl group	3 x 18 = + 54 nm
Other Effects: 2 Double bonds extending conjugation	2 x 30 = + 60 nm
Homoannular Diene system in ring B	+ 35 nm
1 Exocyclic double bond	+ 5 nm
Calculated λ_{max}	**381 nm**

Parent base- α,β-unsaturated carbonyl compound cyclohexenone	+ 195 nm
Substituents at α-position:	+ 10nm
Substituents at β-position: 1 alkyl group	+ 12 nm
Substituents at γ-position: 3 alkyl group	3 x 18 = + 54 nm
γ- Cl	0
Other Effects: 2 Double bonds extending conjugation	2 x 30 = + 60 nm
Homoannular Diene system in ring B	+ 35 nm
2 Exocyclic double bond	+ 10nm
Calculated λ_{max}	376 nm



Parent base- α,β-unsaturated carbonyl compound Aldehyde	**+ 210 nm**
Substituents at α-position:	+ 10nm
Substituents at β-position: 1 alkyl group	+ 12 nm
Substituents at γ-position: 4 alkyl group	4 x 18 = + 72 nm
γ- CH3	+18
γ- Cl	0
Other Effects: 2 Double bonds extending conjugation	3 x 30 = + 90 nm
Homoannular Diene system in ring B, D	2 x 39 nm
4 Exocyclic double bond	+ 20nm
Calculated λ_{max}	510 nm



IR

Infrared Spectroscopy

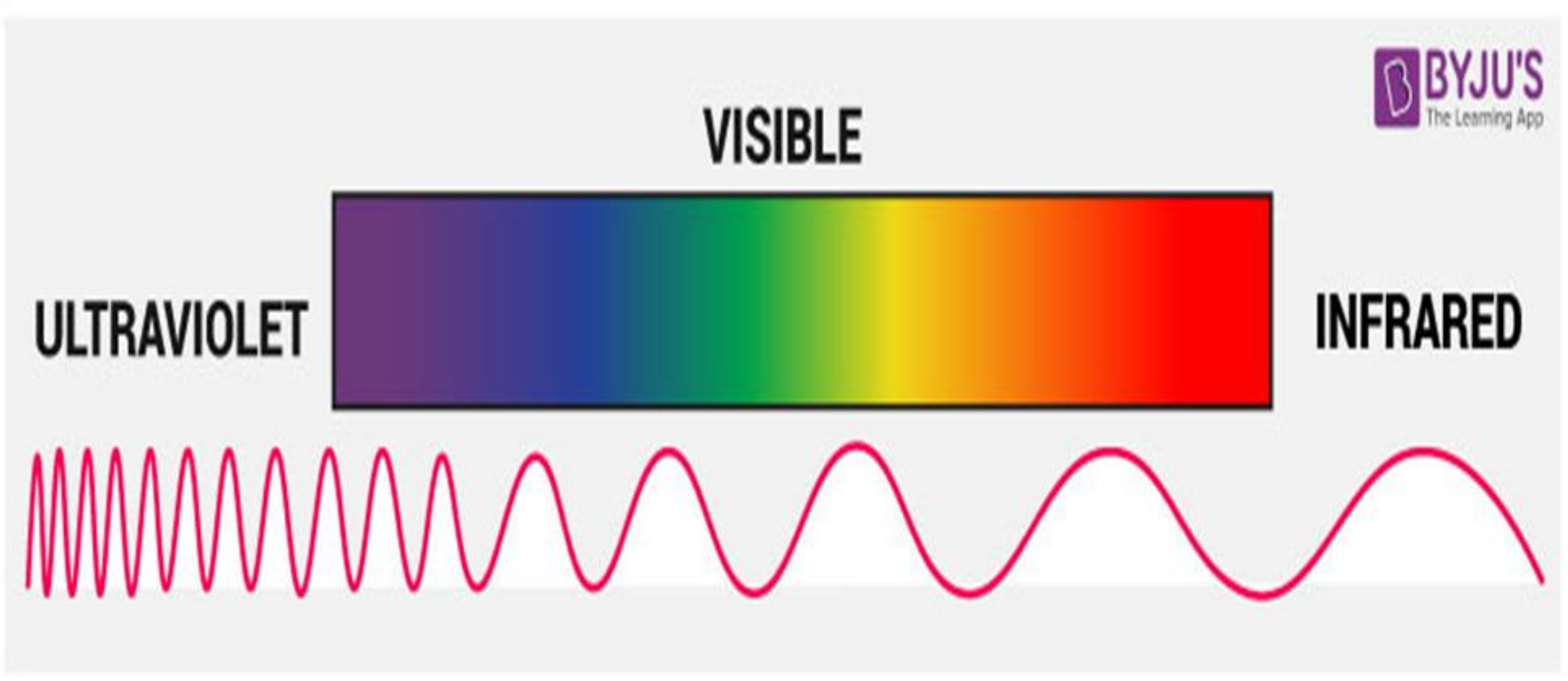
Infrared spectroscopy (IR spectroscopy) is the spectroscopy that deals with the infrared region of the electromagnetic spectrum, that is light with a longer wavelength and lower frequency than visible light. It covers a range of techniques, mostly based on absorption spectroscopy. As with all spectroscopic techniques, it can be used to identify and study chemicals. A common laboratory instrument that uses this technique is a Fourier transform infrared (FTIR) spectrometer. The IR spectroscopy theory utilizes the concept that molecules tend to absorb specific frequencies of light that are characteristic of the corresponding structure of the molecules.

Infrared spectroscopy (IR spectroscopy or vibrational spectroscopy) involves the interaction of infrared radiation with matter. It covers a range of techniques, mostly based on absorption spectroscopy. As with all spectroscopic techniques, it can be used to identify and study chemical substances. Samples may be solid, liquid, or gas. The method or technique of infrared spectroscopy is conducted with an instrument called an infrared spectrometer to produce an infrared spectrum.

Typical units of frequency used in IR spectra are wave numbers, with the symbol cm−1. Units of IR wavelength are commonly given in micrometers (formerly called "microns"), symbol µm, which are related to wave numbers in a reciprocal way. A common laboratory instrument that uses this technique is a Fourier transform infrared (FTIR) spectrometer. Two-dimensional IR is also possible.

The infrared portion of the electromagnetic spectrum is usually divided into three regions; the near- (0.75- 2.5 µm , mid- (2.5- 16 µm) and far- infrared (25- 1000 µm), named for their relation to the visible spectrum. The higher-energy near-IR, approximately 14000–4000 cm−1 (0.7–2.5 µm wavelength) can excite overtone or harmonic molecular vibrations. The mid-infrared, approximately 4000–400 cm−1 (2.5–25 µm) may be used to study the fundamental vibrations and associated rotational-vibrational structure. The far-infrared, approximately 400–10 cm−1 (25–1000 µm), lying adjacent to the microwave region, has low energy and may be used for rotational spectroscopy. The names and classifications of these subregions are conventions, and are only loosely based on the relative molecular or electromagnetic properties.

IR Spectroscopy detects frequencies of infrared light that are absorbed by a molecule. Molecules tend to absorb these specific frequencies of light since they correspond to the frequency of the vibration of bonds in the molecule.


BYJU'S
The Learning App
VISIBLE
ULTRAVIOLET
INFRARED

There are two types of vibrational motions:

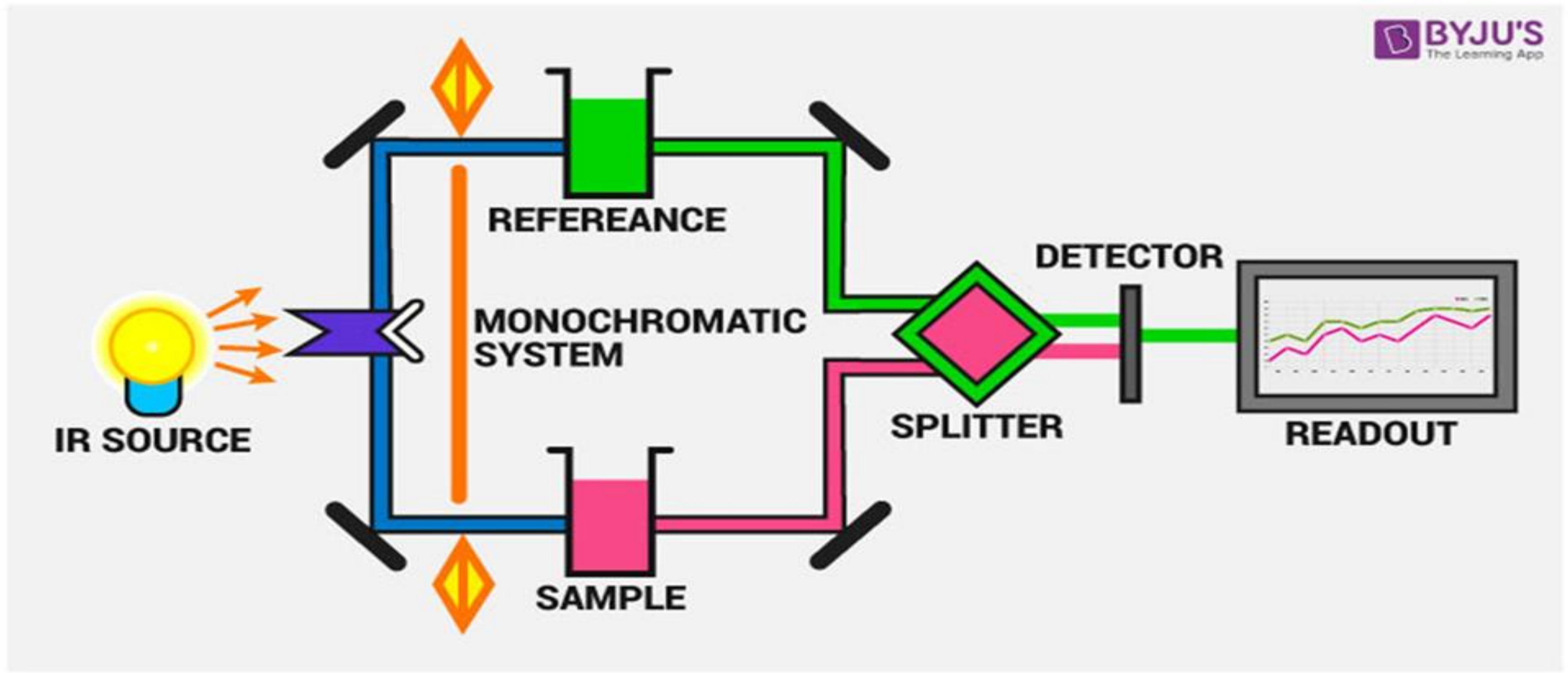
A) Stretching deformation: It is a vibrational motion of a bond along the bond axis within a molecule (Ʋ).

B) Bending deformation: It is a vibrational motion of a bond perpendicular to the bond axis within a molecule (δ).

Normal modes: A molecule can vibrate in many ways, and each way is called a vibrational mode. Linear molecules have 3N - 5 degrees of vibrational modes whereas nonlinear molecules have 3N - 6 degrees of vibrational modes (also called vibrational degrees of freedom). As an example H2O, a non-linear molecule, will have 3 × 3 - 6 = 3 degrees of vibrational freedom, or normal modes.

IR Spectroscopy Instrumentation

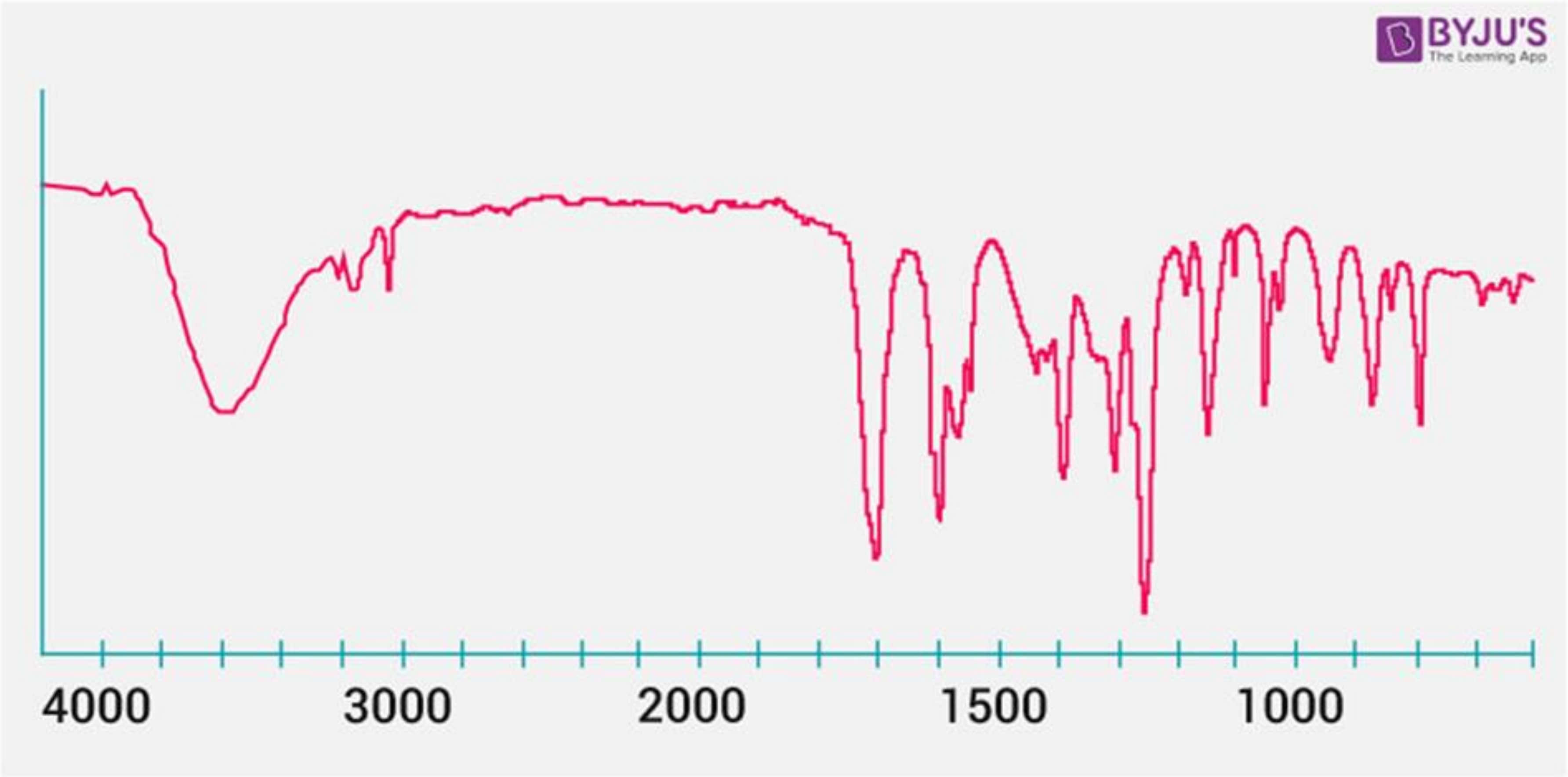
The instrumentation of infrared spectroscopy is illustrated below. First, a beam of IR light from the source is split into two and passed through the reference ant the sample respectively.



Now, both of these beams are reflected to pass through a splitter and then through a detector. Finally, the required reading is printed out after the processor deciphers the data passed through the detector.

Graph of the IR spectrum

Given below is a sample of typical Infrared Absorption Frequencies.

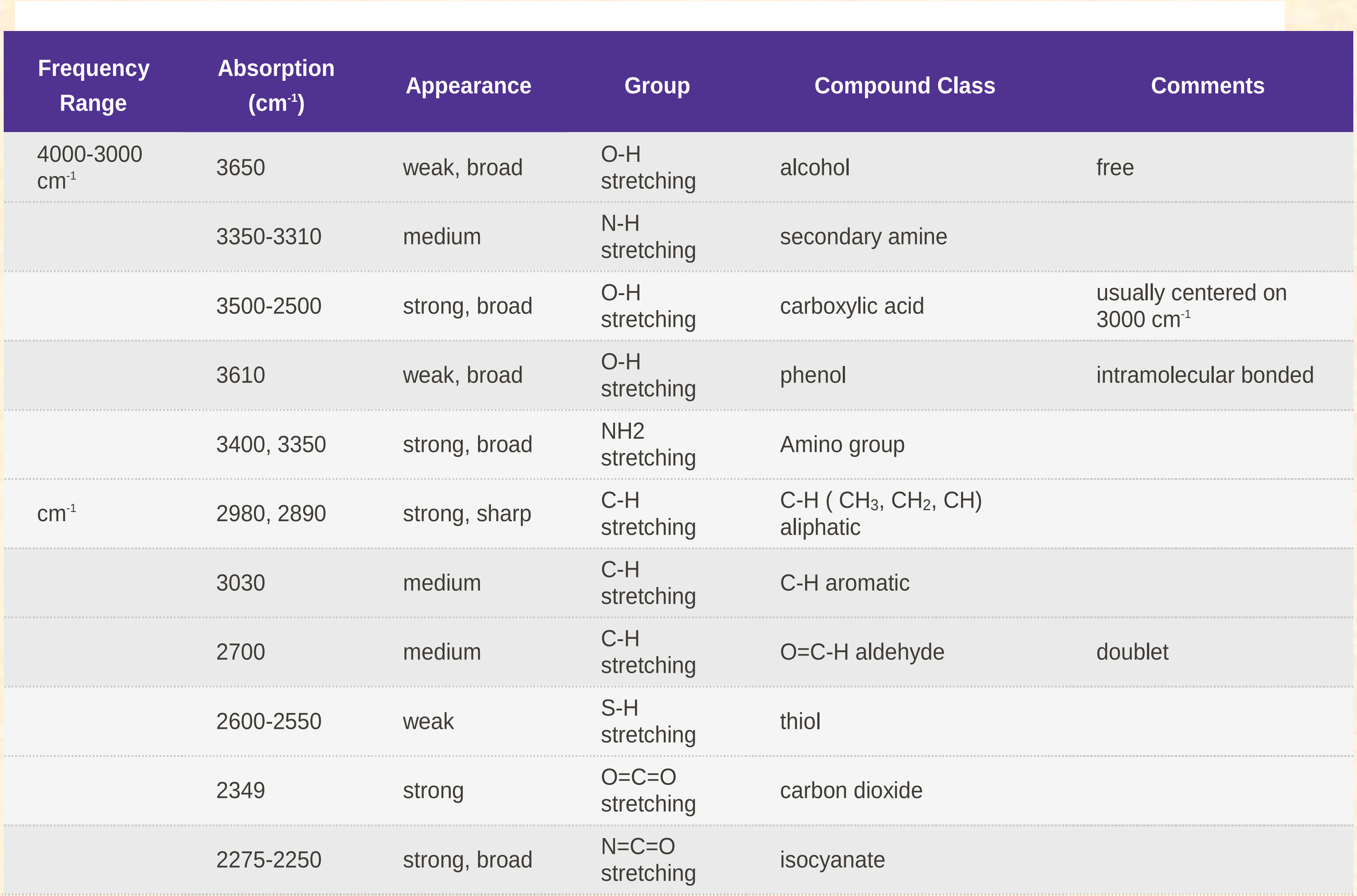


CHARACTERISTIC ABSORPTION BANDS

The IR Spectrum Table is a chart for use during infrared spectroscopy. The table lists IR spectroscopy frequency ranges, appearance of the vibration and absorptions for functional groups.

IR Spectrum Table by Frequency Range

Use the following table when you already know the frequency of your material. Find the frequency range in the first column on the left side of the chart and corresponding values in adjacent columns. (يحفظ الجدول كاملا)



Frequency Range	Absorption (cm^{-1})	Appearance	Group	Compound Class	Comments
4000-3000 cm^{-1}	3650	weak, broad	O-H stretching	alcohol	free
	3350-3310	medium	N-H stretching	secondary amine	
	3500-2500	strong, broad	O-H stretching	carboxylic acid	usually centered on 3000 cm^{-1}
	3610	weak, broad	O-H stretching	phenol	intramolecular bonded
	3400, 3350	strong, broad	NH2 stretching	Amino group	
cm^{-1}	2980, 2890	strong, sharp	C-H stretching	C-H (CH$_3$, CH$_2$, CH) aliphatic	
	3030	medium	C-H stretching	C-H aromatic	
	2700	medium	C-H stretching	O=C-H aldehyde	doublet
	2600-2550	weak	S-H stretching	thiol	
	2349	strong	O=C=O stretching	carbon dioxide	
	2275-2250	strong, broad	N=C=O stretching	isocyanate	

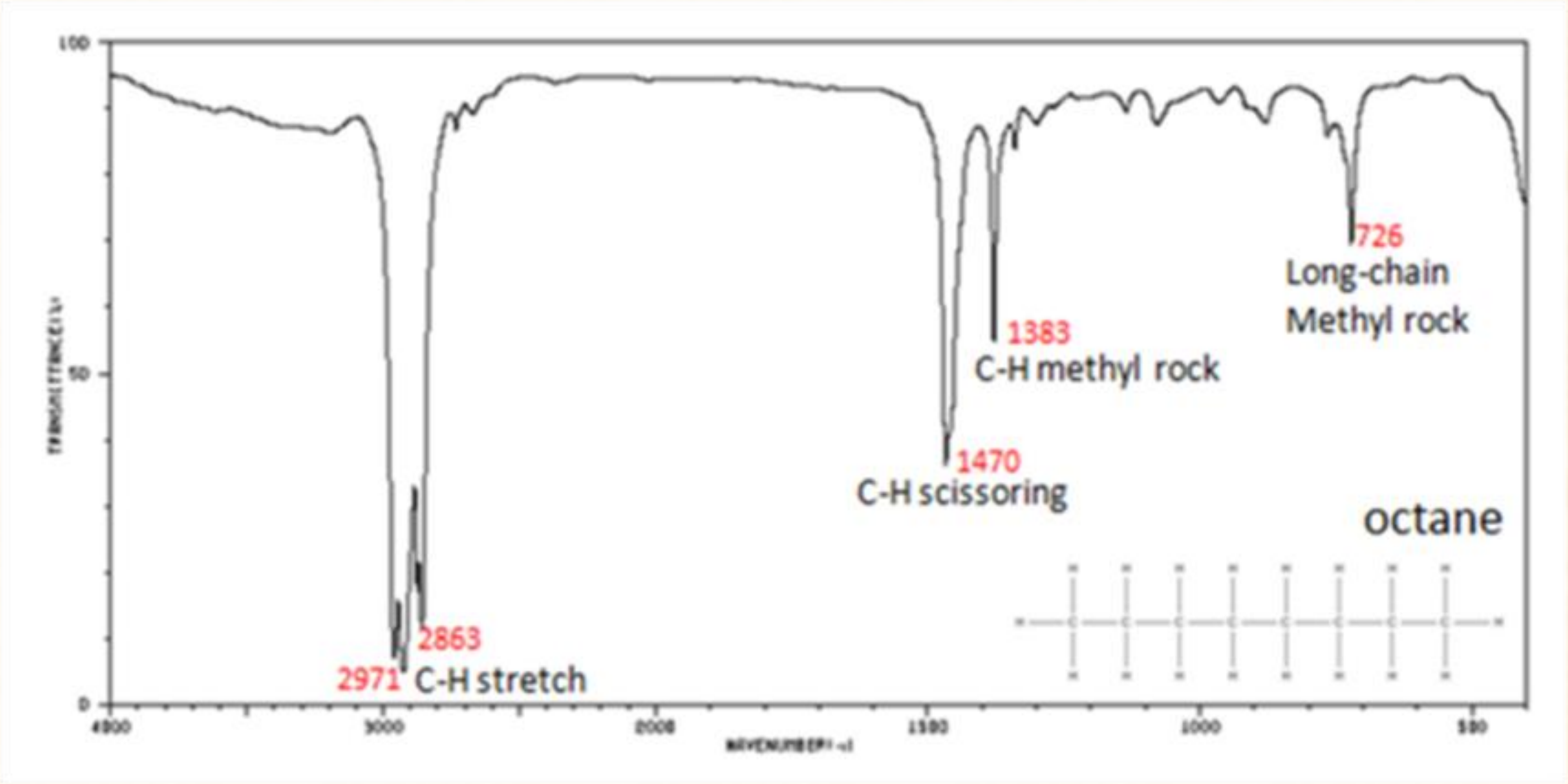
2220	weak	CΞN stretching	nitrile	
2260-2190	weak	CΞC stretching	alkyne	disubstituted
2175-2140	strong	S-CΞN stretching	thiocyanate	
2160-2120	strong	N=N=N stretching	N3 azide	
2150		C=C=O stretching	ketene	
2145-2120	strong	N=C=N stretching	carbodiimide	
2140-1990	strong	N=C=S stretching	isothiocyanate	
2000-1900	medium	C=C=C stretching	allene	
2000		C=C=N stretching	ketenimine	
2000-1650	weak	C-H bending	C-H aromatic compound	overtone

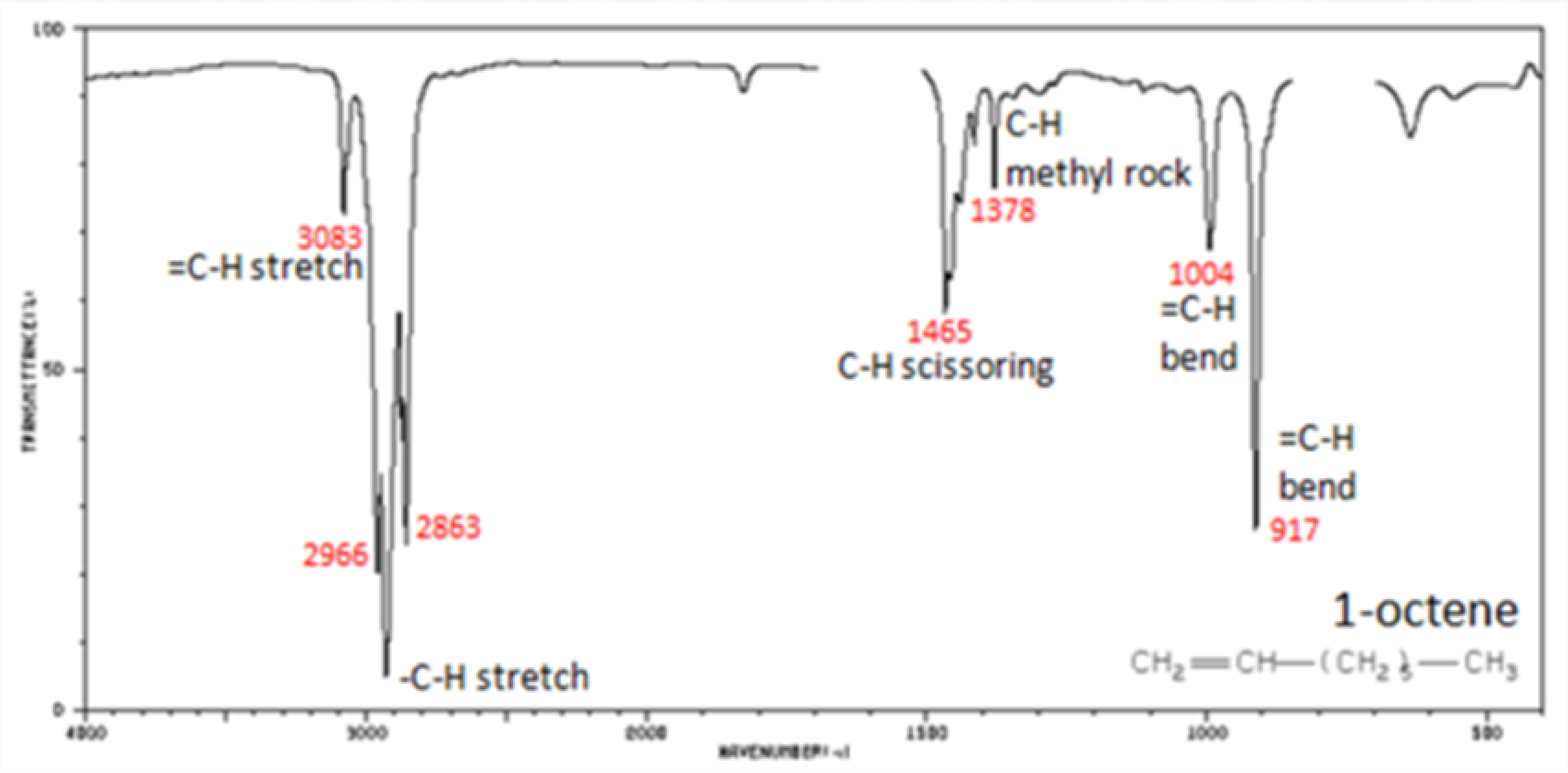
1820, 1760	strong	C=O stretching	anhydride	
1815-1785	strong	C=O stretching	O=C-X acid halide	
1760	strong	C=O stretching	carboxylic acid	monomer
1735	strong	C=O stretching	esters	6-membered lactone
1750	strong	C=O stretching	δ-lactone	γ: 1770
1745	strong	C=O stretching	cyclopentanone	
1720	strong	C=O stretching	aldehyde	
1725	strong	C=O stretching	aliphatic ketone	or cyclohexanone or cyclopentenone
1690	strong	C=O stretching	$CONH_2$ primary amide	
1620	medium	C=N stretching	imine / oxime	
1640	strong	C=O stretching	secondary amide	

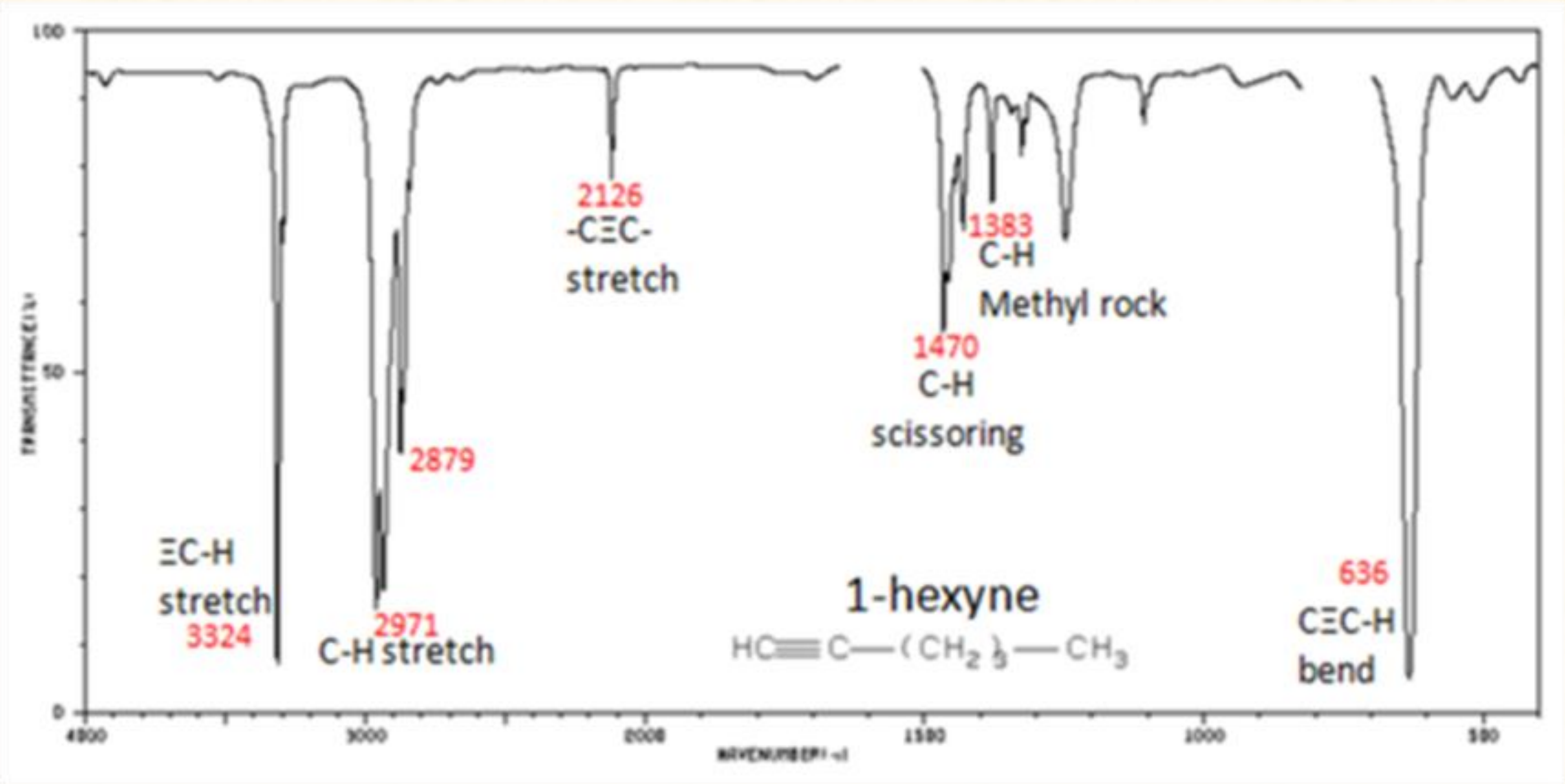
1630	strong	C=O stretching	tertiary amide	
1650	strong	C=O stretching	δ-lactam	
1678-1668	weak	C=C stretching	alkene	disubstituted (trans)
1662-1626	medium	C=C stretching	alkene	disubstituted (cis)
1650-1600	medium	C=C stretching	C=C-C=C conjugated alkene	
1620-1610	strong	C=C stretching	C=C-C=O α,β-unsaturated ketone	
1550-1500	strong	N-O stretching	NO_2 nitro group	
1415-1380	strong	S=O stretching	SO_4 sulfate	
1200-1185				

1410-1380	strong	S=O stretching	SO_2Cl sulfonyl chloride	
1204-1177				
1400-1000	strong	C-F stretching	fluoro compound	
1372-1335	strong	S=O stretching	sulfonate	
1370-1335	strong	S=O stretching	SO_2NH_2 sulfonamide	
1170-1155				
1350-1342	strong	S=O stretching	SO_3H sulfonic acid	anhydrous
1070-1030	strong	S=O stretching	sulfoxide	
690-515	strong	C-Br stretching	halo compound	
600-500	strong	C-I stretching	halo compound	
880	strong	C-H bending	1,2,4-trisubstituted benzene	
860	strong	C-H bending	1,3-disubstituted benzene	
780	strong	C-H bending	1,4-disubstituted or	
780	strong	C-H bending	1,2,3-trisubstituted benzene	
755	strong	C-H bending	1,2-disubstituted benzene	
700	strong	C-H bending	monosubstituted	
			benzene derivative	

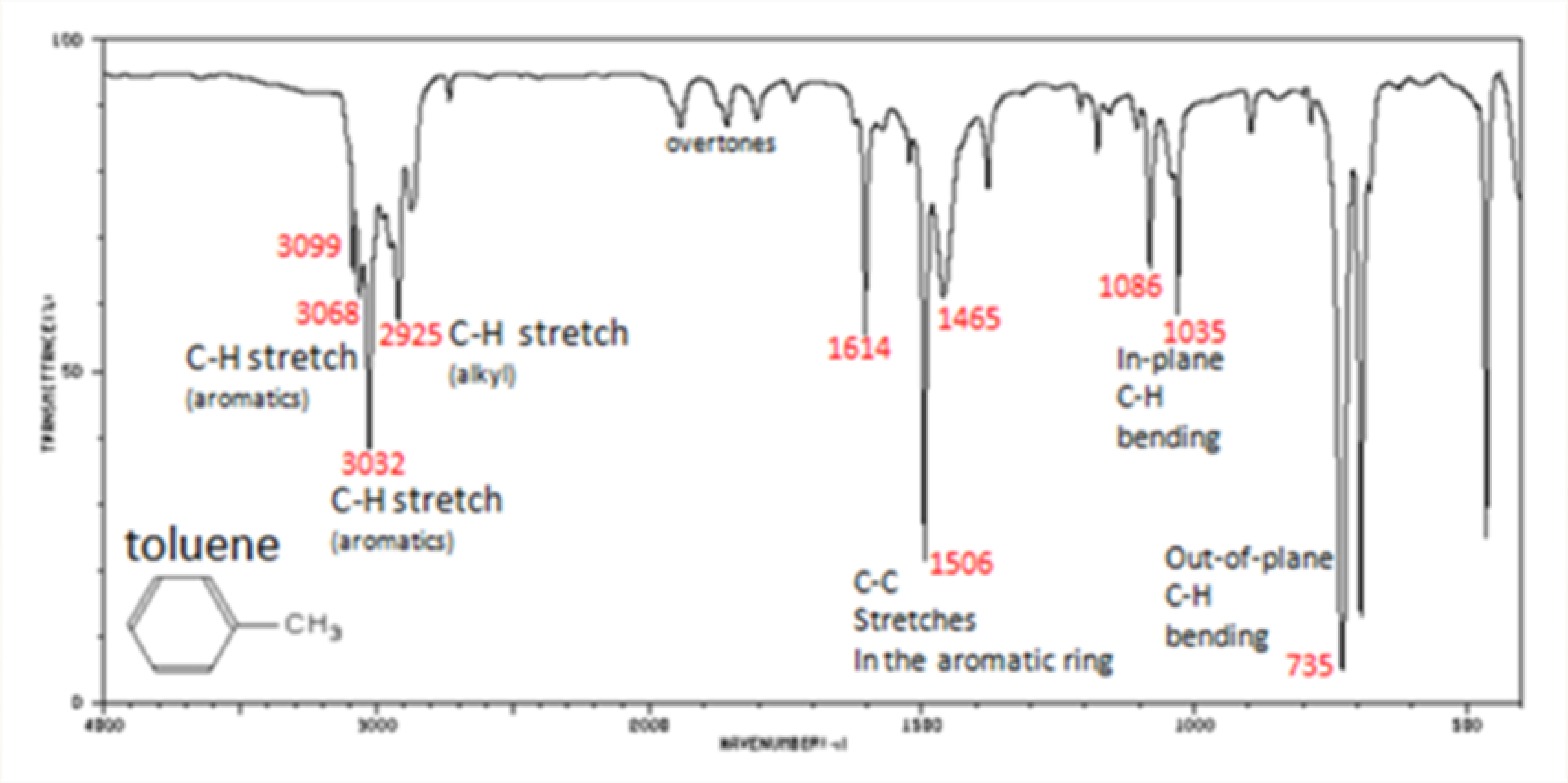
Examples

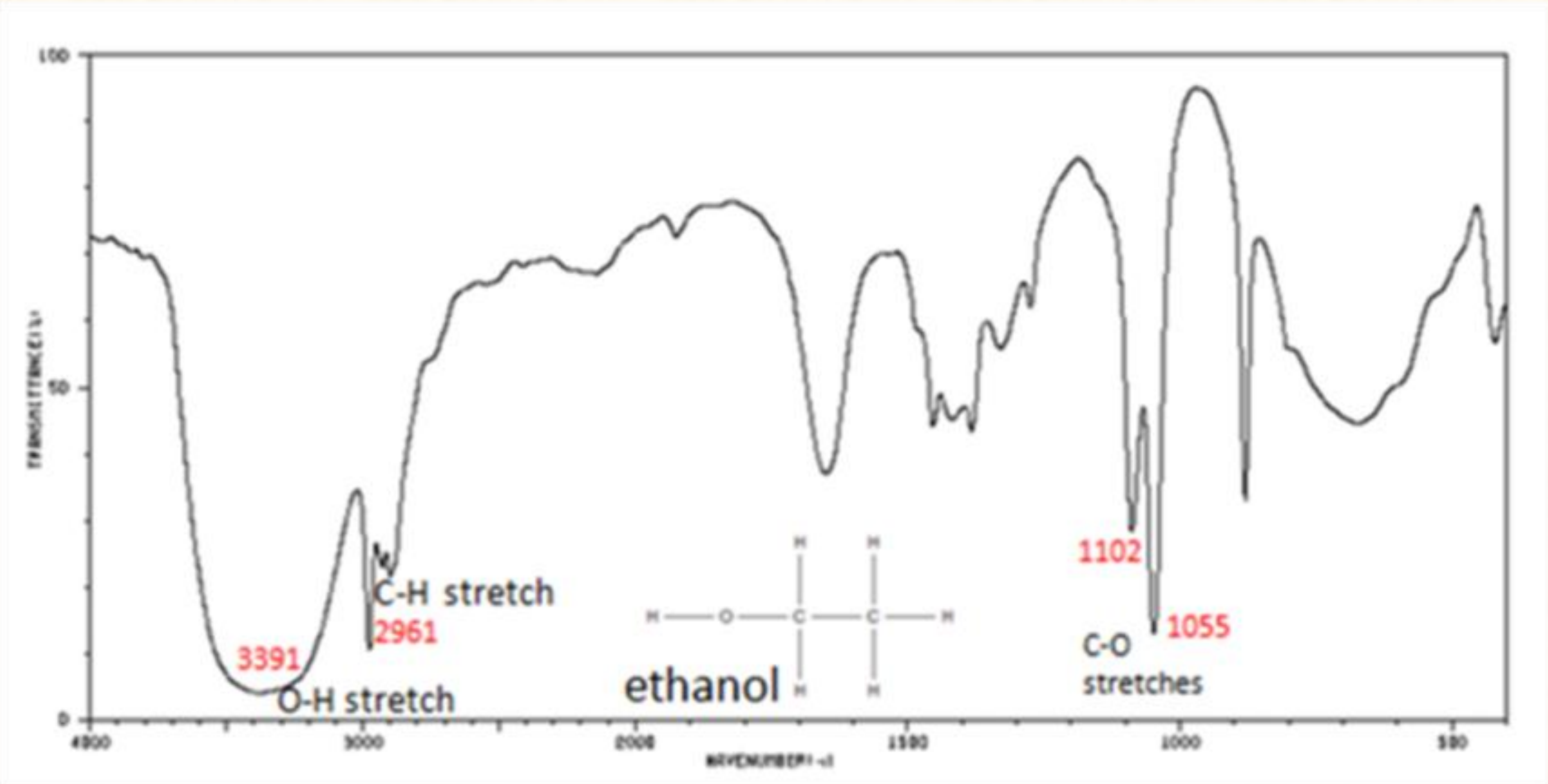

100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(cm-1)
2971
2863
C-H stretch
1470
C-H scissoring
1383
C-H methyl rock
726
Long-chain
Methyl rock
octane

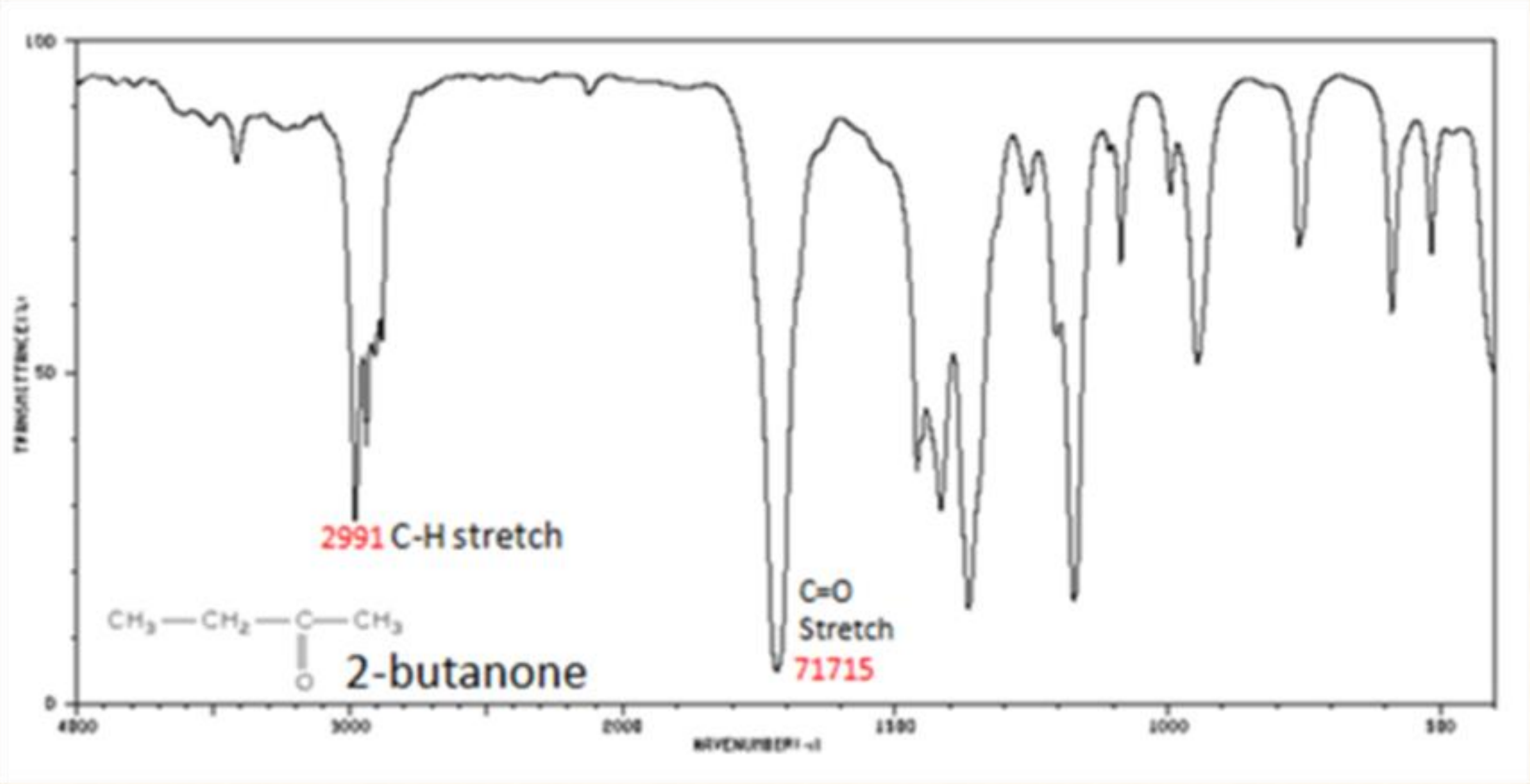

100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(-1)
3083
=C-H stretch
2966
2863
-C-H stretch
1465
C-H scissoring
1378
C-H
methyl rock
1004
=C-H
bend
917
=C-H
bend
1-octene
CH2=CH—(CH2)5—CH3



100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(-1)
2126
-C≡C-
stretch
1383
C-H
Methyl rock
1470
C-H
scissoring
2879
≡C-H
stretch
3324
2971
C-H stretch
1-hexyne
HC≡C—(CH$_2$)$_3$—CH$_3$
636
C≡C-H
bend


100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(cm-1)
overtones
3099
3068
C-H stretch
(aromatics)
2925
C-H stretch
(alkyl)
3032
C-H stretch
(aromatics)
toluene
CH3
1614
1465
1506
C-C
Stretches
In the aromatic ring
1086
1035
In-plane
C-H
bending
Out-of-plane
C-H
bending
735


100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(-1)
3391
O-H stretch
C-H stretch
2961
ethanol
H
O
C
1102
1055
C-O
stretches

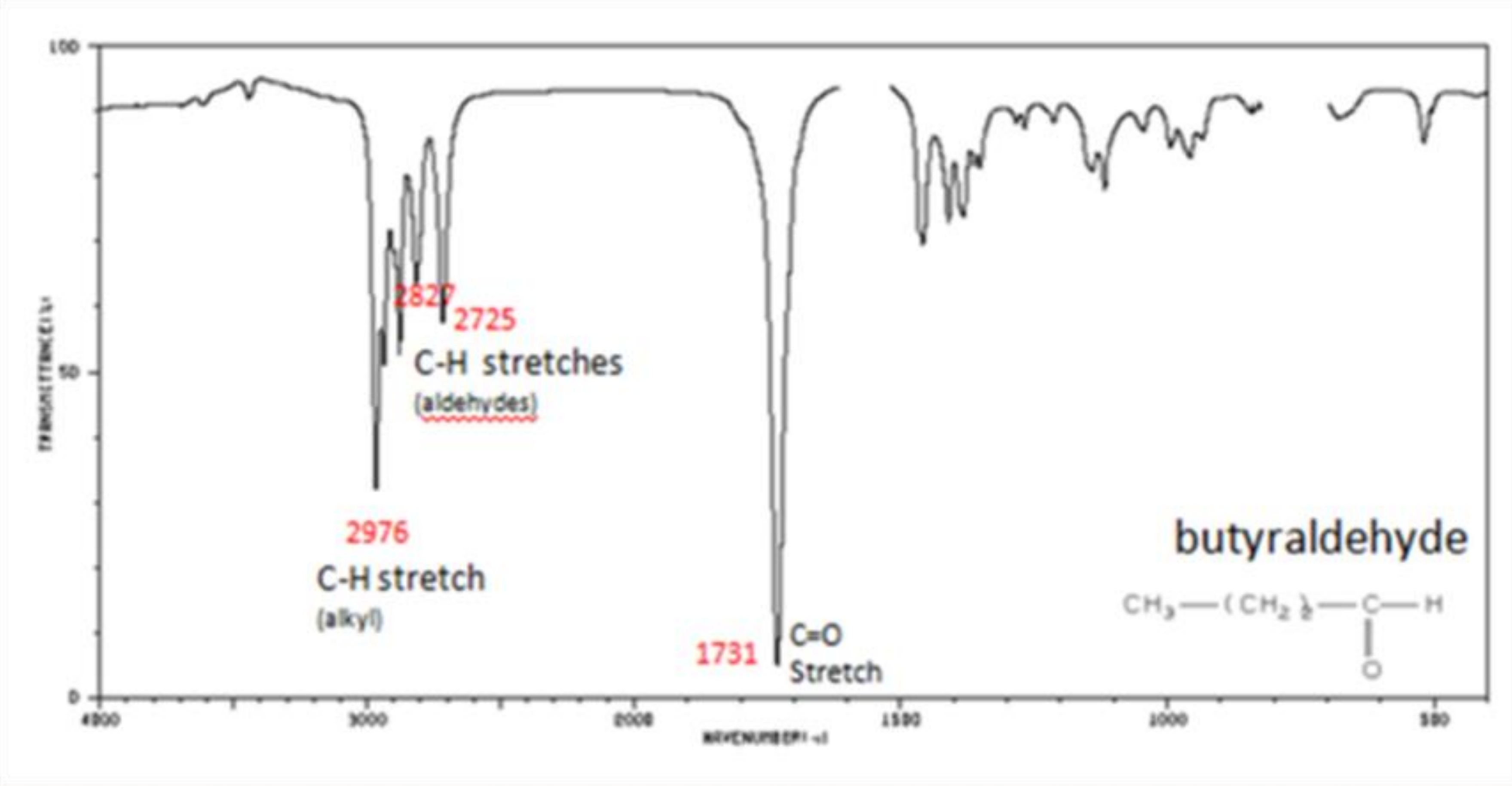


2991 C-H stretch

C=O
Stretch
71715

2-butanone

$CH_3-CH_2-C(=O)-CH_3$



2827 2725

C-H stretches

(aldehydes)

2976

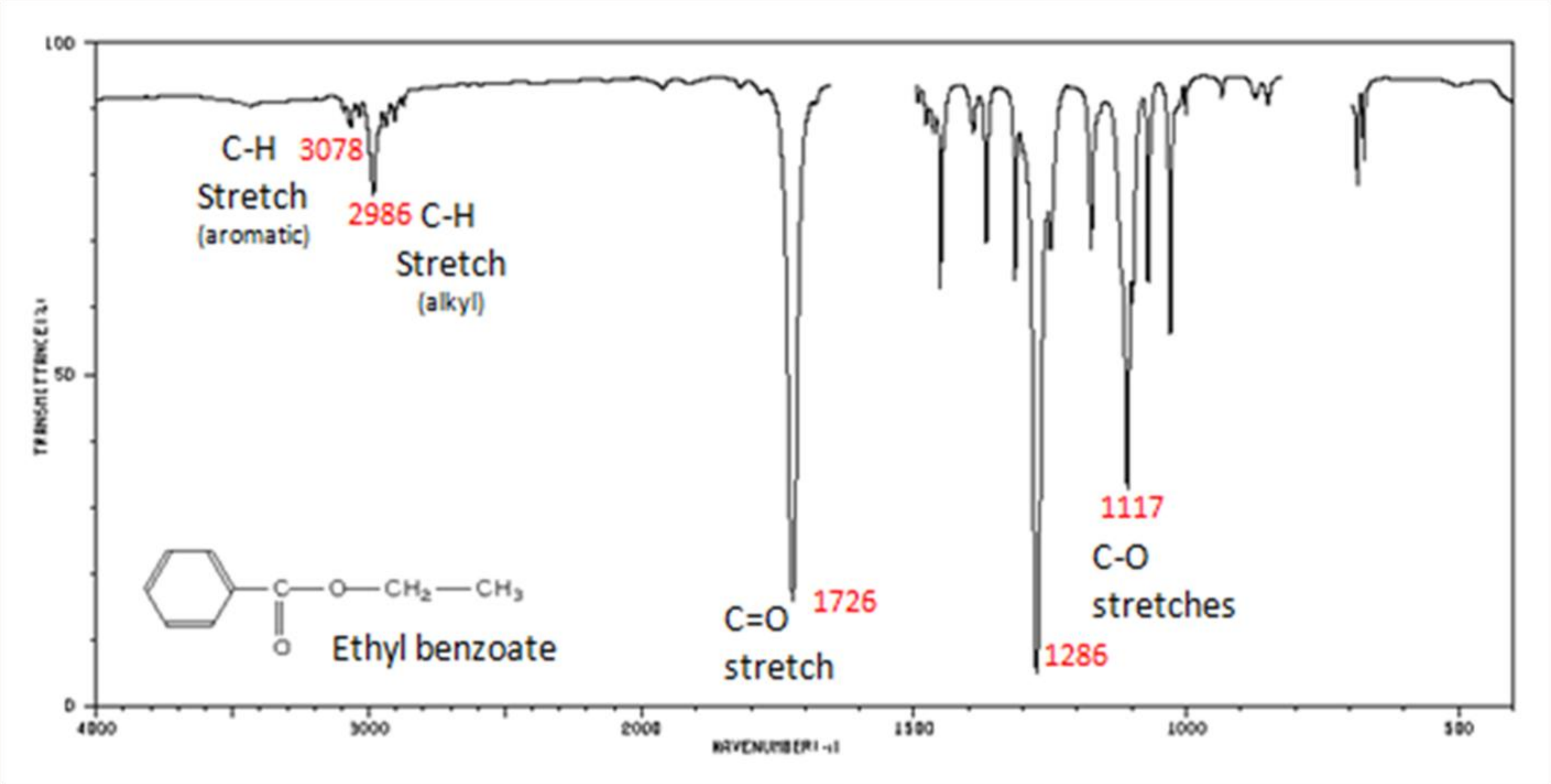
C-H stretch

(alkyl)

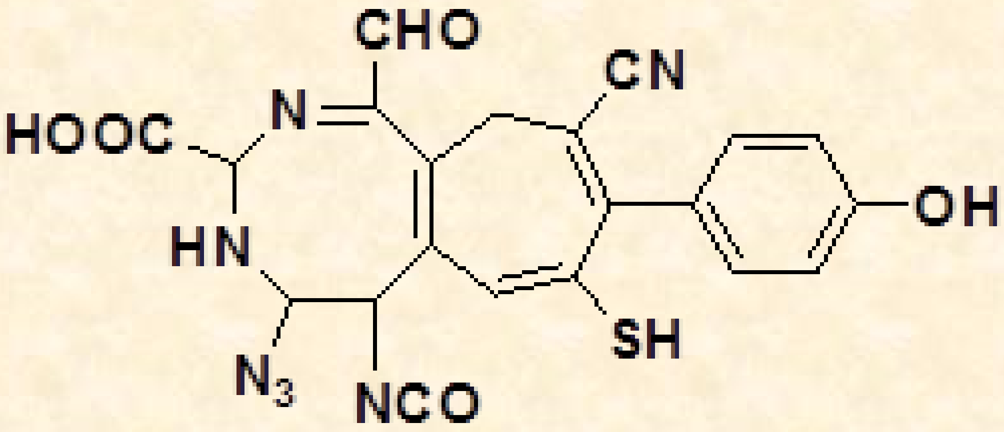
1731 C=O Stretch

butyraldehyde

$$CH_3-(CH_2)_2-\underset{\underset{O}{\|}}{C}-H$$


100
50
0
TRANSMITTANCE(%)
4000
3000
2000
1500
1000
500
WAVENUMBER(-1)
C-H Stretch (aromatic)
3078
2986
C-H Stretch (alkyl)
1726
C=O stretch
1286
1117
C-O stretches
Ethyl benzoate
C
O
CH2
CH3

Indicate the expected IR bands for the following compound:



The Answer:

-CN 2220 cm-1, NH 3350-3310 cm-1, C=O (COOH) 1760 cm-1, carboxylic -OH 2500-3500 cm-1, -SH 2600-2550 cm-1, -CHO 2700 cm-1, 1720 cm-1, CH 2980, 2890 cm-1, N3 2160-2120 cm-1, NCO 2275-2250 cm-1 , C=N 1620 cm-1, OH 3610 cm-1, CH aromatic 3030 cm-1.