استخدام ضوء لتحليل المادة كـ كمية ونوعية

qualtitive or quantitive

Spectroscopy is any procedure that uses the interaction of **Electromagnetic Radiation (EMR)** with matter to *identify* and/or to *estimate* an analyte.

Quantitative Analysis

molecules	solid
ions	liquid
atoms	gas
Mixtures	solutions

Qualitative Analysis

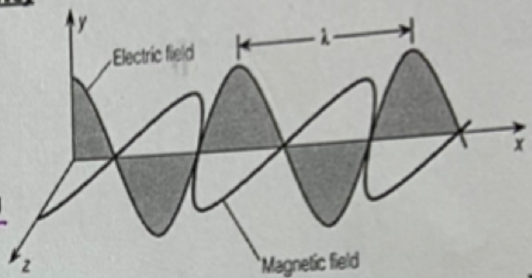
Electromagnetic radiation (light)

trans the Light for the space ?

1- particles (photons)

2- waves

- EMR can be described in terms of both particles and waves (Dual nature of light)
- Light waves consist of perpendicular and oscillating electric and magnetic fields ?



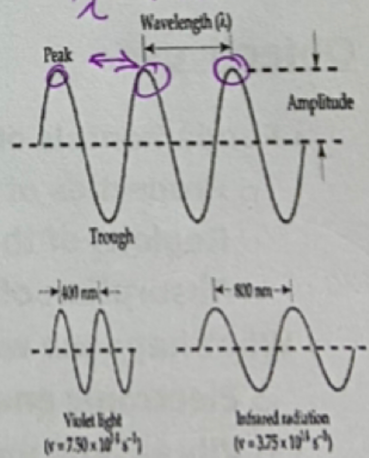
مسافة بين قمتين :

the distance between two peaks

Light waves can be characterized By:

λ = fixed

Wavelength (λ, *Greek lambda*):
Distance from one wave peak to the next.
Units: m, cm, <u>µm</u>, <u>nm</u> or Å



هون عندك نقطة ادي دائرة

Frequency (υ, *Greek nu*):
Number of peaks that pass a given point per second.
Units: Cycles/second or s^{-1} or Hertz (Hz)

ضوء

ضوء كم مرة لف دائرة خلال وحدة زمن

frequency

Wavenumber
Number of waves per cm.

$$\bar{\upsilon} = \frac{1}{\lambda} \quad cm^{-1}$$

→ (wave Length) λ مكانها

Wave nature of light can explain phenomena such as reflection, refraction and diffraction.

① Frequency (ν) = $\dfrac{\text{velocity of light (c) fixed}}{\text{wave length } (\lambda)}$.

② wavenumber = $\dfrac{1}{\lambda}$
$\bar{\nu}$

Ex: calculate the wavelength of Light in nm of Light with a frequency of $3.52 * 10^{14}$?

$\Rightarrow f = \dfrac{c}{\lambda} \longrightarrow \lambda = \dfrac{c}{\nu} = \dfrac{3 * 10^{8}}{3.52 * 10^{14}} = 8.52 * 10^{-7}$

هان تحويل بس

$w.L = \dfrac{1}{\lambda} \Rightarrow \lambda = 8.52 * 10^{-7} \cancel{m} * \dfrac{10^{9}\ nm}{\cancel{m}}$

$= 852\,nm$

* energy (E) $= h * \nu = h * \frac{c}{\lambda}$

$\rightarrow \boxed{h \times c \times \bar{\nu}}$

planks constant

6.6×10^{-27} 6.6×10^{-34} joule.sec

cm^2

(حسب ما يبغى السؤال)

Calculate the energy (in joules) of a photon with a wavelength of 700.0 nm

$\lambda = 700.0nm$

$\boxed{E = h \times \upsilon}$

$\upsilon = \frac{c}{\lambda} = \frac{3 \times 10^{8} m/s}{7 \times 10^{-7}}$

$$\lambda = 700.0\ \text{nm} \times \frac{10^{-9}\ \text{m}}{\text{nm}} = 7.00 \times 10^{-7}\ \text{m}$$

هاد تحويل وحدة بس

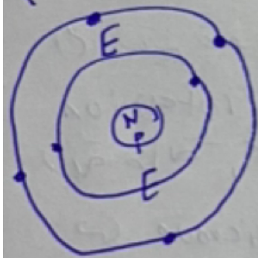
$$\upsilon = \frac{3.00 \times 10^{8}\ \text{m/s}}{7.00 \times 10^{-7}\ \text{m}} = 4.29 \times 10^{14}\ \text{s}^{-1}$$

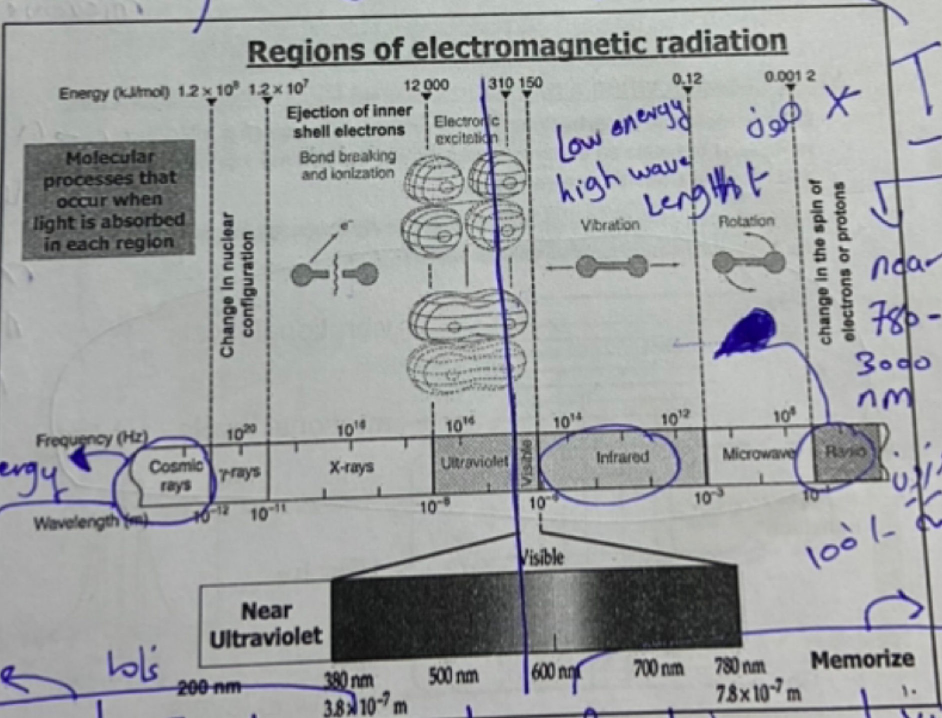
$$E = (6.63 \times 10^{-34}\ \text{J} \cdot \text{s})(4.29 \times 10^{14}\ \text{s}^{-1})$$

$$E = 2.84 \times 10^{-19}\ \text{J}$$

* هون كنا حين تنتقل على الأرض بتطلع أطوال موجية وأشعاعات مختلفة على حسب الأطوال

(near > mid > far) energy من حيث





Low energy high wave Length

* هون IR(infrared)

near	Middle	far
780 - 3000 nm	3000 - 30000	30000 - 3000
	زيادة (c)	

تنفذ من الأوزون نحن بس نسبة 100%

high energy Low wave Length

لا تنفذ من الأوزون

خطر

cosmic rays	γ	X-rays	UV-far	UV near	visible	micro wave
$< 10^{-4}$	$10^{-4} - 10^{-3}$	$10^{-3} - 10^{-10}$	10-200	200-380	380-780 can you see	3000,000 - 10^{-9}
بفتت	بفتت E ذاتية ونارية قفة	خطر من الالياف ضوئية في العظام وسنتر حاد ضوء في العظام	تعرف الأشعة التي كمشعة limital volume			

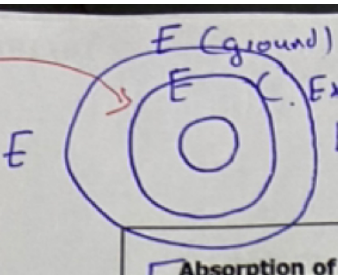
F, N, P بفتت

ضوء في العظام → العظام density بسبب

ثانية للنظام فقط

5

Light



E (Excited)

UV (visible)

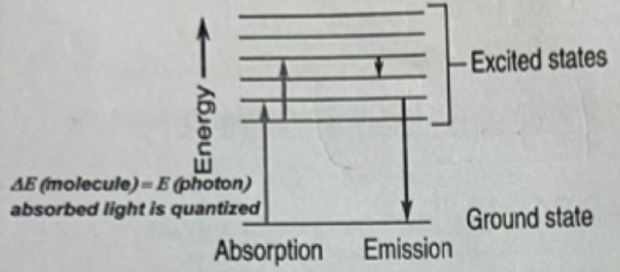
E (ground)

زيادة في الطاقة الحركية للالكترونات ← 2,

تنتقل الالكترونات من ground لـ Excited

Absorption of light

A **molecule** that absorbs light photons will end up with increased energy. The molecule will be promoted to an **excited** state. Microwave energy will cause rotation of compounds. IR energy is high enough to promote bond stretching. UV/Vis energy promotes electrons into higher orbitals. Short-λ UV and X-rays can ionize molecules or even break bonds.



Most excited molecules relax again to the ground state emitting the excess energy in the form of heat.

E electronic >> E vibrations >> E rotations

energy (E) مهم ★

microve

① اذا سقط microve

ح تتغير فقط rotation (r₀ → r₁)

لانه طاقة قليلة

microve ←

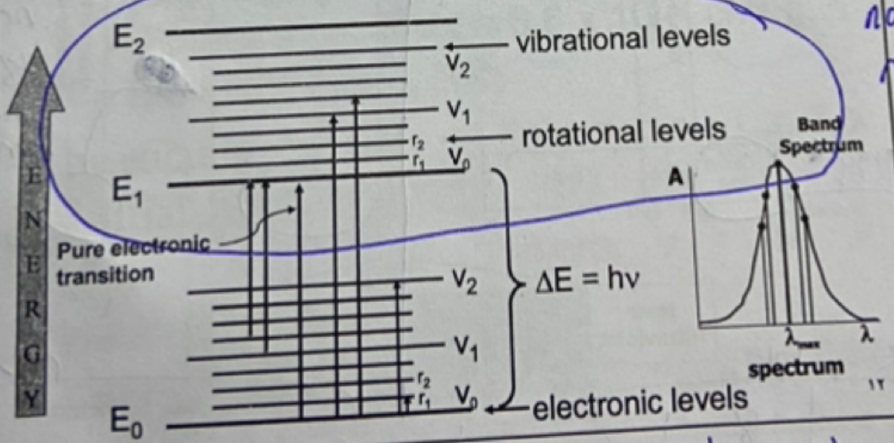
no vibration

no Electronic

Ultraviolet-Visible Spectrophotometry

What happens when a molecule absorbs UV-Visible radiations?

- **When a molecule absorbs light having sufficient energy (e.g. UV-Vis radiation) to cause an electronic transitions, (additional vibration and rotation transitions also occur)**
- **Molecule can absorb one photon of just the right energy to cause the following simultaneous changes:**



② اذا سقط IR ,2 تتغير vibration

rotational و

③ اذا سقط UV-visible ، الثلاثة ح يتغيروا مع بعض

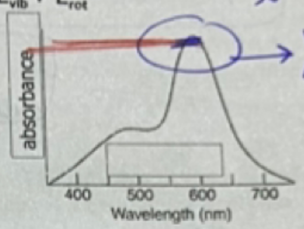
هون عشان لنميزهن اذا ما بعرف بالالوان:
electronic → blues colors
vibrations → colors in red
rotations → blue
مهمة.

1. A transition from the ground electronic state E_0 to the E_1 excited electronic state
2. A change in the vibrational energy from the ground vibrational state of E_0 to an excited vibrational state of E_1
3. A transition from one rotational state of E_0 to a different rotational state of E_1
4. All the above transitions are quantized which means that they required certain exact amount of energy
5. Thus, total energy absorbed = $E_{elec} + E_{vib} + E_{rot}$

$$\Delta E_{elec} >> \Delta E_{vib} >> \Delta E_{rot}$$

تعريف λmax

As a result, a large numbers of photons of certain wavelengths are absorbed by a molecule. These individual wavelengths are too numerous and too close to each other and a spectrum of broad bands of absorbed wavelengths are obtained



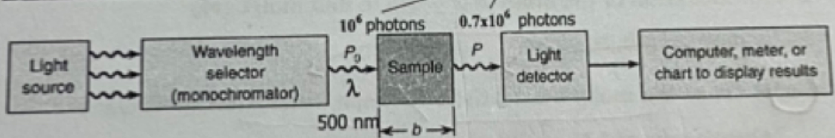
Spectrum (a graph that shows how absorbance varies with wavelength)

λ max اعلى قمة
λ max
الكثر صوبة امتصها بـ next step
اذا كانو متشابهين بالامتصاص بنعتمد على density

solution → solvent, solute (solid) (مادة بلا يديها اعرفها)
ذوبتها وحولتها لـ solution

Transmittance and Absorbance

T = 0.7, %T = 70%, A = 0.155



There are two quantities that relate the change in the intensity or radiant power of EMR before, P_0, and after, P, interaction with matter.

1. Transmittance, T, is simply defined as "the fraction of light that reaches a detector after passing through a sample"

ع الكوبات بلي استقرت للعينة

$$T = \frac{P}{P_0}$$

الخارج
الساقط

$0 \leq T \leq 1$

انه انا عندي مادة سقطت عليها ضوء فاي الكادة اح تمتص اطوال موجية مختلفة فونا انا باخذ quantity & quality

The percent transmittance, %T, is simply 100 T

$$\%T = \frac{P}{P_0} \times 100$$

$0 < \%T < 100$

unitless

اذا كان الضوء الساقط نفسه 100% transmittance
الخارج ← الساقط

2. Absorbance, defined as:

$$A = -\log T \Longrightarrow A = -\log\frac{P}{P_0} \Longrightarrow A = \log\left(\frac{P_0}{P}\right)$$

quality
quality ماي الاطوال الموجية بيرجع على pharmacopie ويعرف quality بعد التجربة مرة ثانية اذا بدي احسب quantity بعينها الطول الموجي الي امتصه فا بتمثيلي الكمية.

absronce → unit- less سأتشر وحدة

For purpose of chemical analysis

Absorbance is directly proportional to:

1. concentration, c, of absorbing species in the sample ($A \propto c$)
2. path length of light, b, through the sample ($A \propto b$)

A = absorbce → A=1

Beer's law $\boxed{A = \varepsilon bc}$

(absronce)

The previous equation is the heart of spectrophotometry as applied to analytical chemistry, it is called Beer-Lambert law or simply Beer's law

ε → molar absorptivity
c → concentration
b → thickness, Length Light
وحدة الطول

1- Concentration of the analyte is given in unit mol/L (M)

2-The path length, b, in cm

3-ε, is called the molar absorptivity or molar absorption coefficient

"Absorbance of 1 M solution measured in a cell of 1 cm path length"

مهم →
$$\varepsilon = \frac{A}{bc} = \frac{1}{\frac{mol}{L}\,cm} = L\,mol^{-1}cm^{-1} = M^{-1}cm^{-1}$$

ε, is characteristic for each substance at a particular wavelength, λ.