SPEKTROSKOPI

Fundamental of Spectroscopy
Emission Spectrometry
Atomic Absorption Spectrometry
UV – Vis Spectrometry
Infra Red Spectrometry
Mass Spectrometry

Oleh : Umar Hafidz A.H., M.Sc.

What is:

- Spectroscopy ?
- Spectrometry ?
- Spectrometer ?
- Spectrophotometry ?
- Spectrophotometer ?

- ❑ What for are they ?
- ❑ How to use it ?
- ❑ How it is work ?

Spectroscopy is
The study of interaction of electromagnetic radiation with matter

Spectrometry is
Analysis method of the measurement and interpretation of electromagnetic radiation absorbed, or emitted by atoms, molecules, or other chemical species

Spectrometer is
The instrumen that use spectrometry method

Spectrophotometry is
Analog with spectrometry, but specially for photon measurement

Bohr Atomic Theory

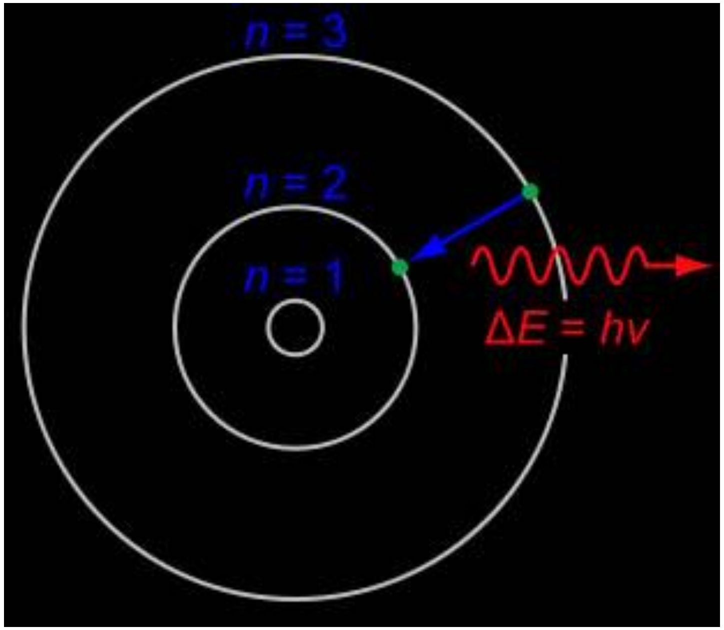
In this model electrons have only certain energies allowed corresponding to particular distances from nucleus.

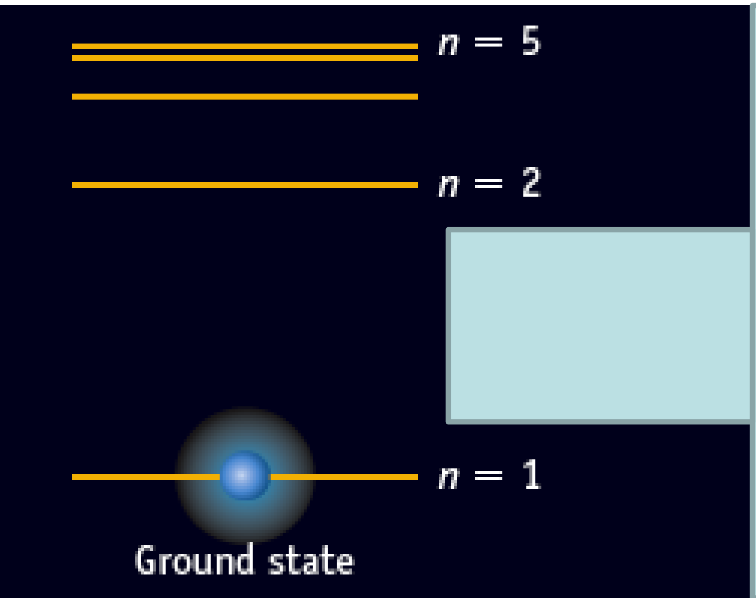
As long as the electron is in one of those energy orbits, it will not lose or absorb any energy.

The orbits closer to the nucleus have lower energy.

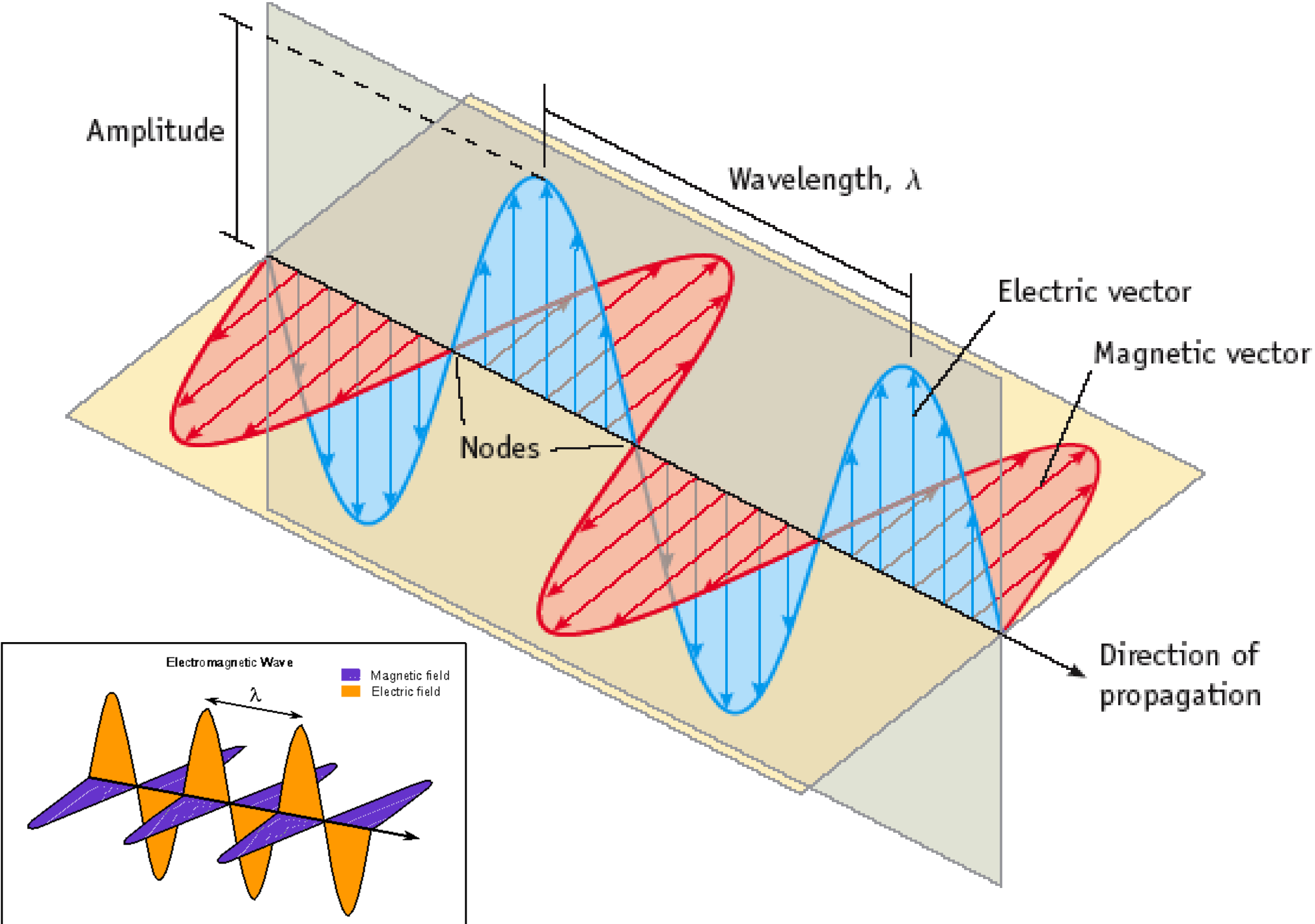
Electrons want to be in the lowest possible energy state called **the ground state.**

However, the electron can go to a higher orbit after absorbing energy, or the electron can go to a lower orbit after emitting energy.
When you heat the atoms, electrons go to higher orbits.
When they cool off, they give the energy back by **radiating electromagnetic waves.**

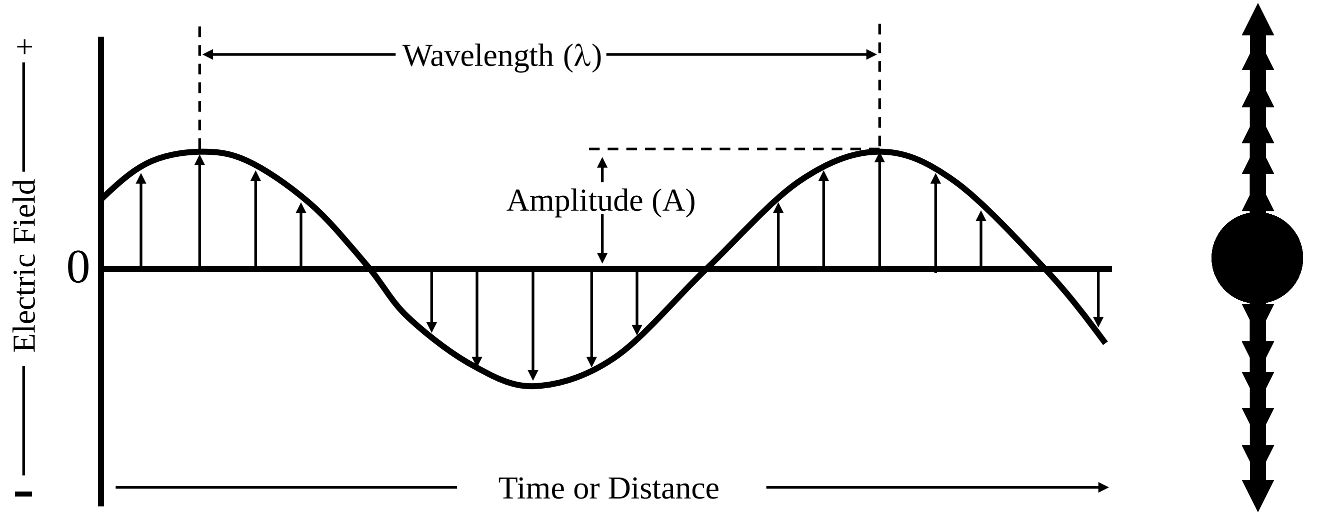




What is Electromagnetic (EM) Radiation ?



Wave Parameters



Period **(p)** – the time required for one cycle to pass a fixed point in space.

Frequency **(ν)** – the number of cycles which pass a fixed point in space per second.

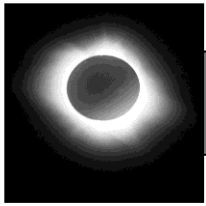
$$\nu = 1/p \; (s^{-1} = Hz)$$

- ν depends on the source, but is independent of the propagating (transmitting) material.

Amplitude **(A)** – The maximum length of the electric vector in the wave (Maximum height of a wave).

Wavelength **(λ)** – The distance between two identical adjacent points in a wave (usually maxima or minima).

- Frequency: the number of wavelengths that pass a point per unit time
- Wavelength: the mean distance between maximums (or minimums)
- Common units: micrometers (μm) or nanometers (nm)
- One cycle per second is termed one hertz (1 Hz)



Wave Model of Electromagnetic Energy

The relationship between the wavelength (λ) and frequency (ν) of electromagnetic radiation is based on the following formula, where *c* is the speed of light:

$$c = \lambda \cdot \nu \qquad \nu = \frac{c}{\lambda} \qquad \lambda = \frac{\nu}{c}$$

Note that frequency (ν) is inversely proportional to wavelength (λ) The longer the wavelength, the lower the frequency, and vice-versa

- Einstein had proposed a relationship between energy and frequency of light in 1905:

$$E = h\nu$$

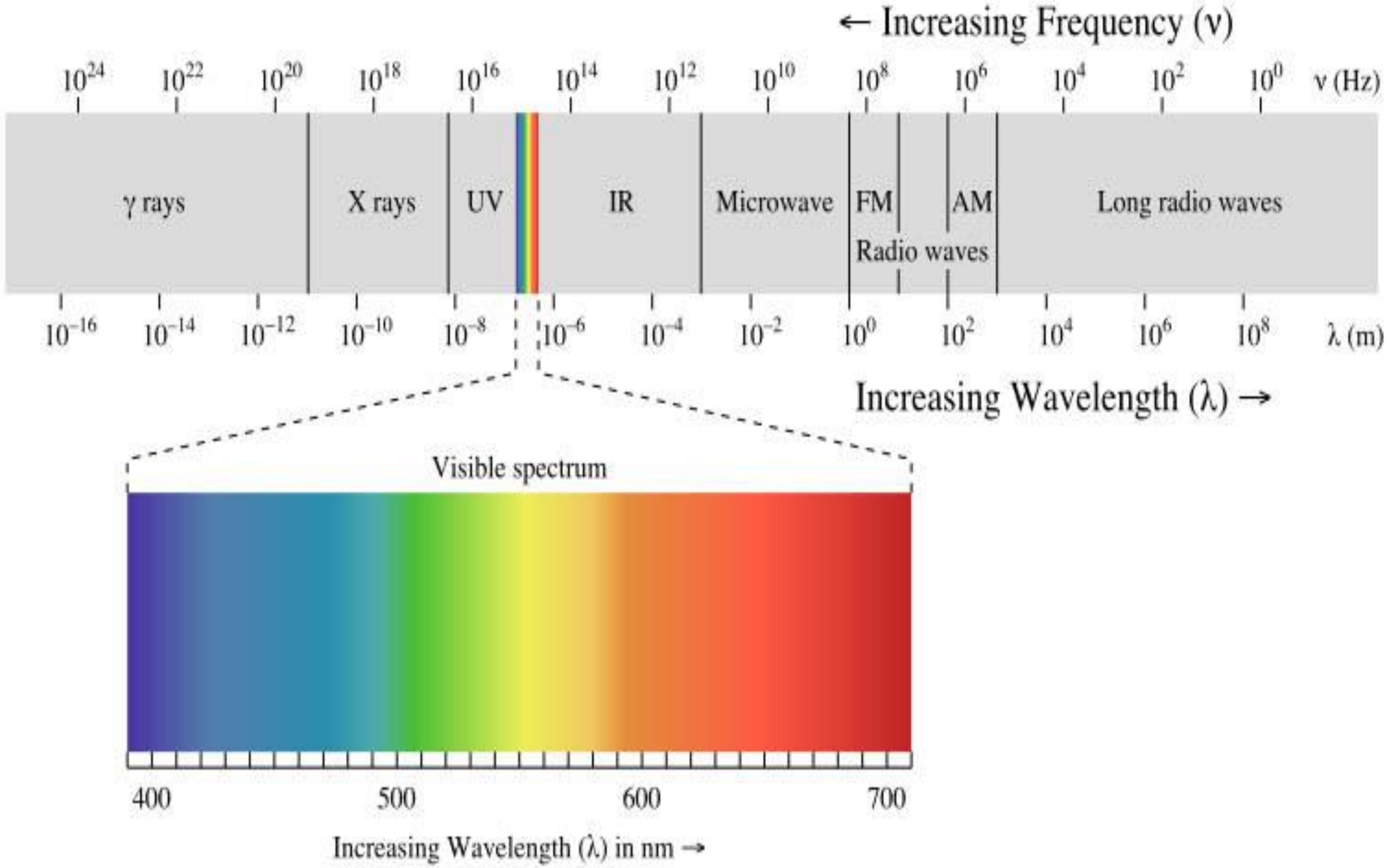
where h is Planck's constant (6.62618×10^{-34} J·s)

- Recasting Einstein's equation in terms of wavelength of radiation.

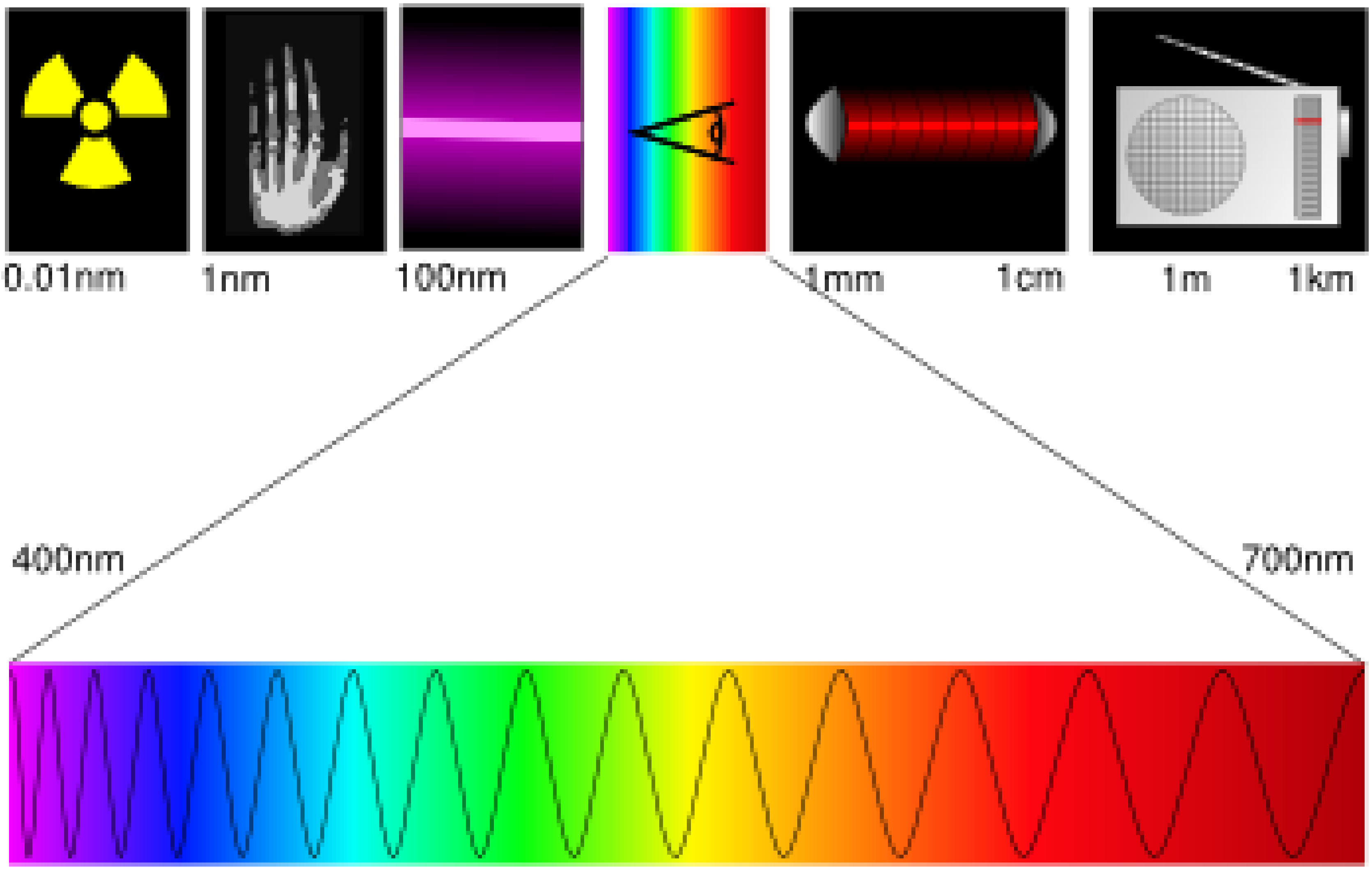
$c = \nu\lambda$ **or** $\nu = c/\lambda$

$$E = h\frac{c}{\lambda}$$

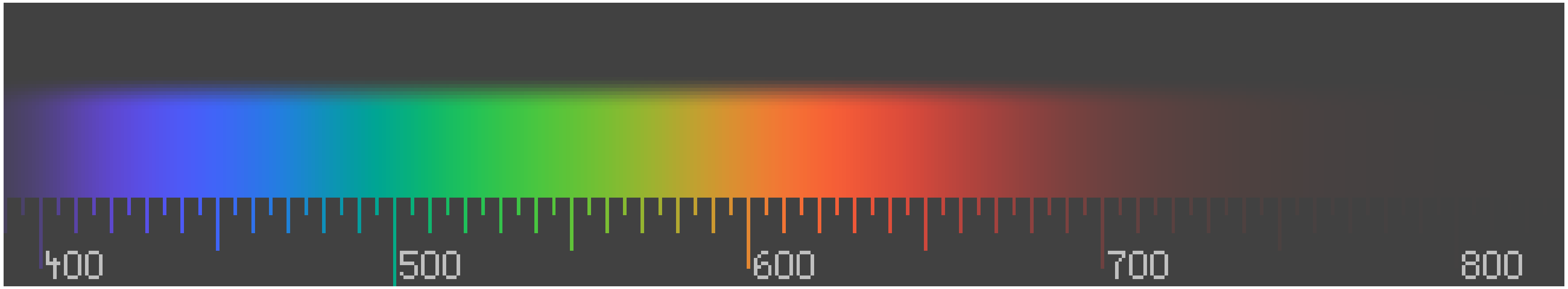
Electromagnetic waves travel through a vacuum at a constant velocity of 2.99792×10^{8} m/s, which is known as the speed of light(C)


← Increasing Frequency (ν)
10^{24} 10^{22} 10^{20} 10^{18} 10^{16} 10^{14} 10^{12} 10^{10} 10^{8} 10^{6} 10^{4} 10^{2} 10^{0} ν (Hz)
γ rays
X rays
UV
IR
Microwave
FM
AM
Radio waves
Long radio waves
10^{-16} 10^{-14} 10^{-12} 10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} 10^{2} 10^{4} 10^{6} 10^{8} λ (m)
Increasing Wavelength (λ) →
Visible spectrum
400 500 600 700
Increasing Wavelength (λ) in nm →

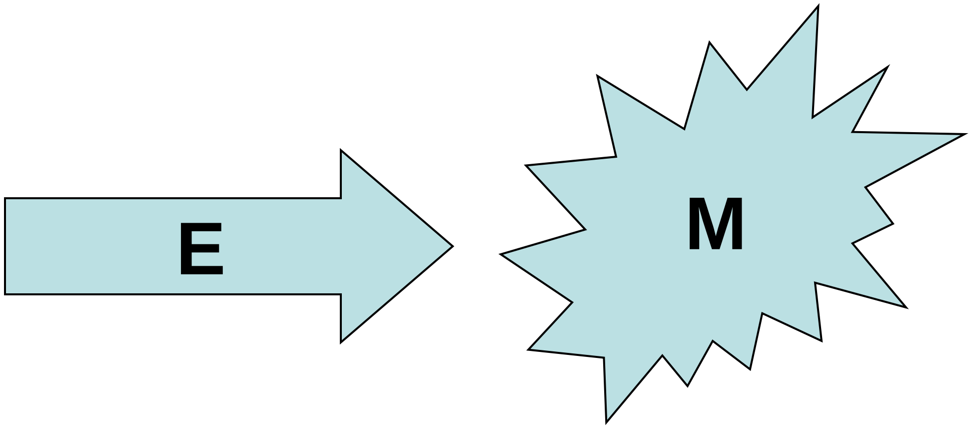
Type of Radiation	Frequency Range (Hz)	Wavelength Range	Type of Transition
gamma-rays	10^{20}-10^{24}	<1 pm	nuclear
X-rays	10^{17}-10^{20}	1 nm-1 pm	inner electron
ultraviolet	10^{15}-10^{17}	400 nm-1 nm	outer electron
visible	4-7.5x10^{14}	750 nm-400 nm	outer electron
near-infrared	1x10^{14}-4x10^{14}	2.5 µm-750 nm	outer electron molecular vibrations
infrared	10^{13}-10^{14}	25 µm-2.5 µm	molecular vibrations
microwaves	3x10^{11}-10^{13}	1 mm-25 µm	molecular rotations, electron spin flips*
radio waves	<3x10^{11}	>1 mm	nuclear spin flips*


0.01nm
1nm
100nm
1mm
1cm
1m
1km
400nm
700nm

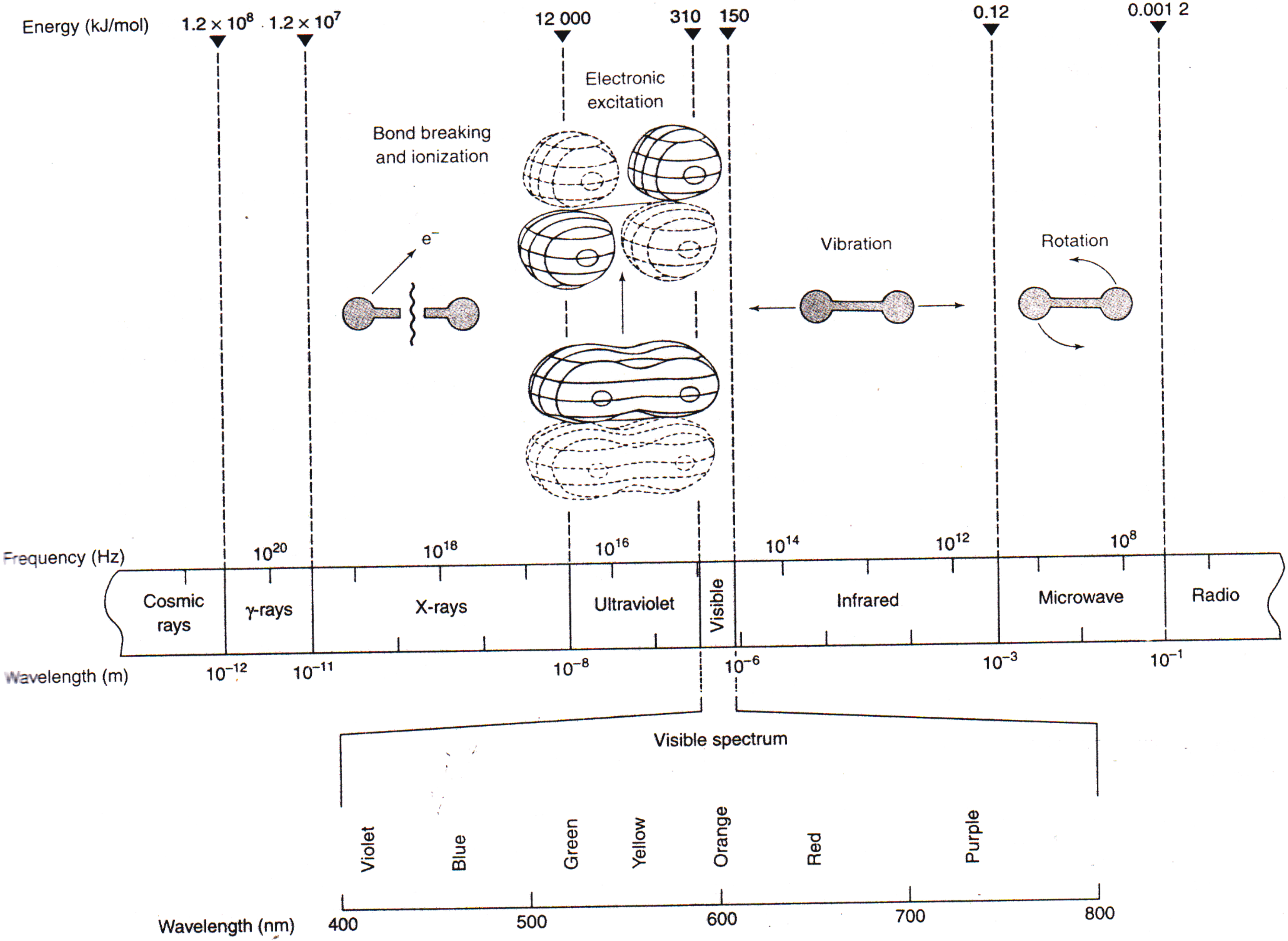
Color	Wavelength interval	Frequency interval
violet	~ 380 to 430 nm	~ 790 to 700 THz
blue	~ 430 to 500 nm	~ 700 to 600 THz
cyan	~ 500 to 520 nm	~ 600 to 580 THz
green	~ 520 to 565 nm	~ 580 to 530 THz
yellow	~ 565 to 590 nm	~ 530 to 510 THz
orange	~ 590 to 625 nm	~ 510 to 480 THz
red	~ 625 to 740 nm	~ 480 to 405 THz



The chemical and physical effects of interaction



- Gamma rays can cause changes in the nucleus
- X rays cause the ejection of inner electrons from matter
- Ultraviolet dan Visible rays causes change in the energy of the valence electron
- Infra red rays causes in rotational and vibration energy state of molecul
- Microwave region, causes change in electron spin states for substances with unpaired electrons when in a magnetic field
- Radio wave range, energy transitions are concerned with reorientation of nuclear spin states of substances



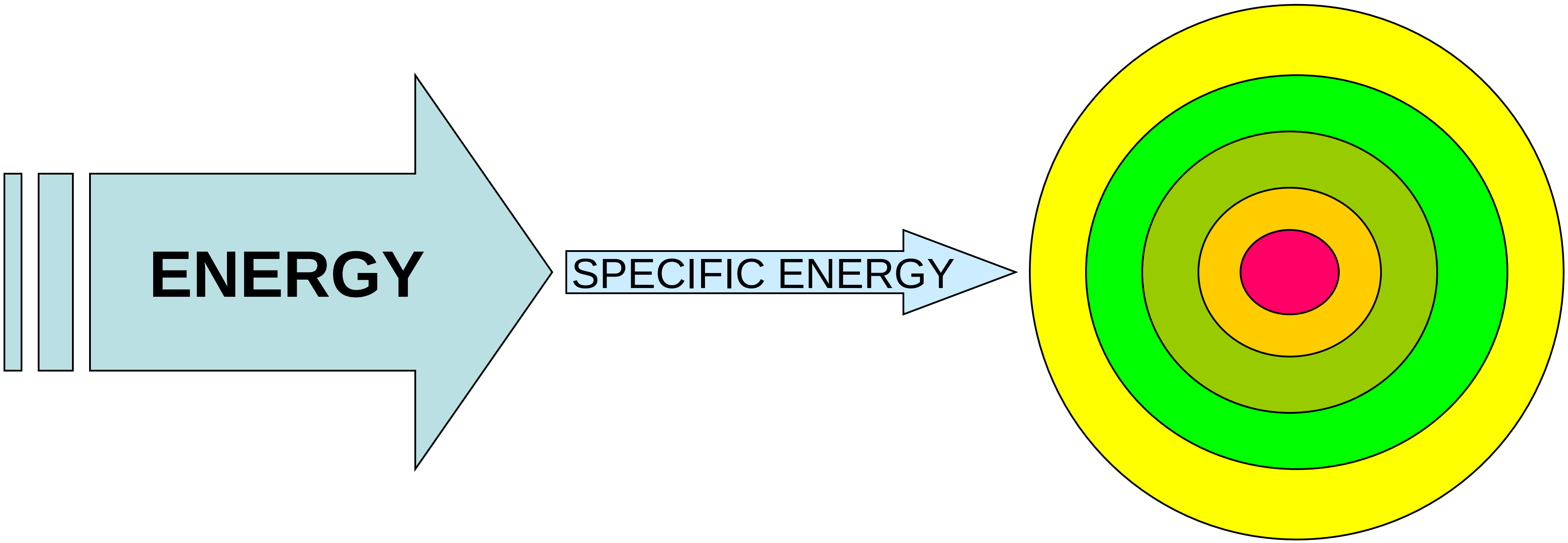
Energy (kJ/mol)
1.2 × 10^8
1.2 × 10^7
12 000
310
150
0.12
0.001 2
Electronic excitation
Bond breaking and ionization
e⁻
Vibration
Rotation
Frequency (Hz)
10^20
10^18
10^16
10^14
10^12
10^8
Cosmic rays
γ-rays
X-rays
Ultraviolet
Visible
Infrared
Microwave
Radio
Wavelength (m)
10^-12
10^-11
10^-8
10^-6
10^-3
10^-1
Visible spectrum
Violet
Blue
Green
Yellow
Orange
Red
Purple
Wavelength (nm)
400
500
600
700
800

Spectrometry Classification

Energy	Matter	Interaction effect	Name of Technique	Application
Gamma Ray	Atom Substances	nuclear transition	Gamma Spect	Qualitative & quantitative
X - Ray	Atom Substances	Transition of Inner shell elect	XRF	Qualitative & quantitative
			XRD	
UV – Visble Ray	Atom	Transition of Valence elect	A.A.S	Quantitative
			Spectrofluorometry	Quantitative
	Mol. / Subst.	Transition of Valence elect	UV-Vis Spectr.	Quantitative
			Spectrofluorometry	Quantitative
I.R. Ray	Mol. / Subst	Vibration rotation	IR Spectr.	Identification of functional
			FT IR Spect	
MW - Radio	Mol. / Subst	Elctron spin transition	NMR Spect	Identification and structure analysis
Electron	Mol. / Subst	fragmentation	MS Spect	Identification and structure analysis

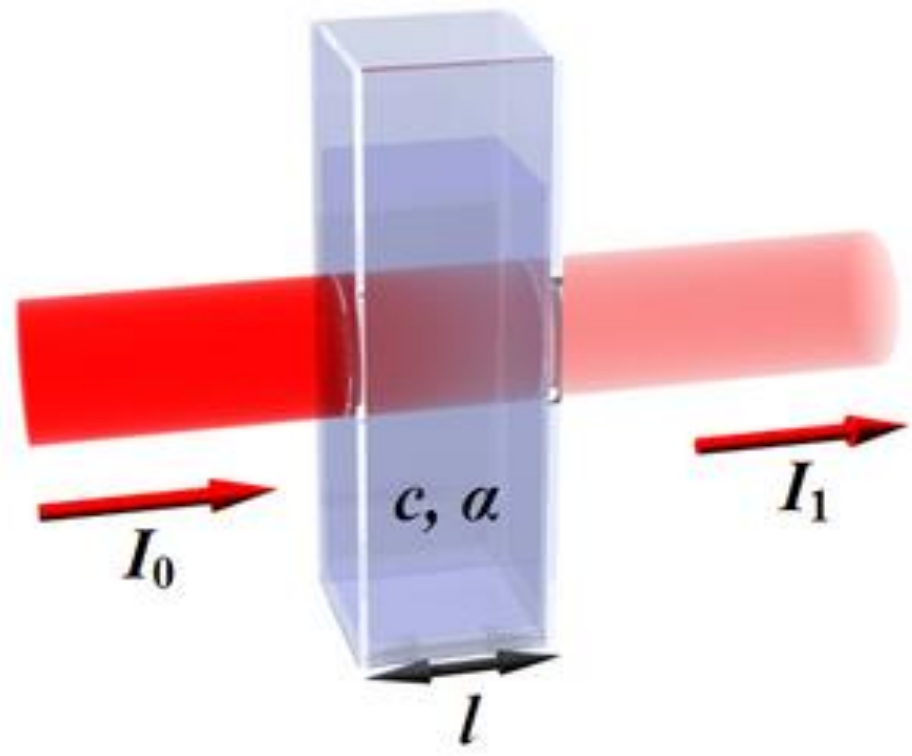
HOW THIS METHOD CAN USE FOR QUALITATIVE & QUANTITATIVE ANALYSIS ?

Qualitative



ONLY SPECIFIC ENERGY
WILL BE INTERACTION

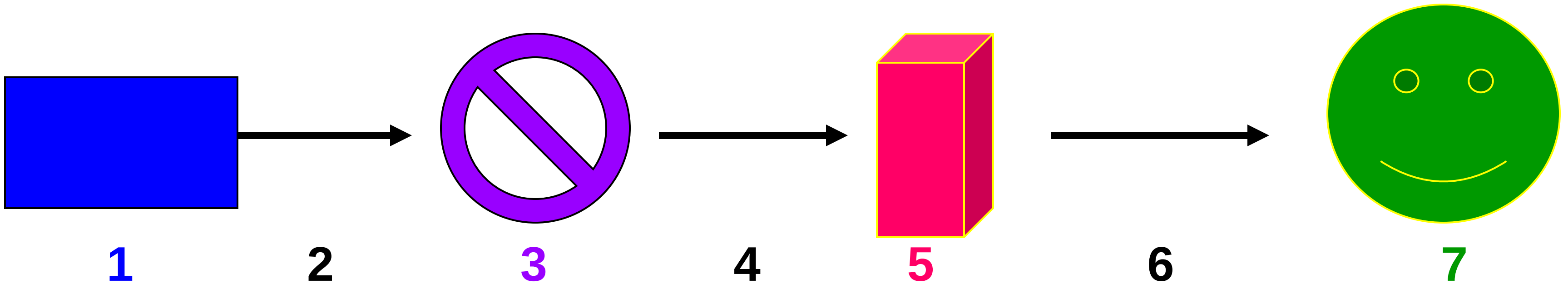
Quantitative



Pierre Bouguer (1729), Johann Heinrich Lambert (1760) and August Beer (1852) :

$$A = a.b.c$$

Schematic of basic diagram of Spectrophotometer



1 Source of electromagnetic radiation

2 Polychromatic rays

3 Wavelength selector

4 Monochromatic rays with Io

5 Matter (atom or molecules or substances)

6 Monochromatic ray with I_1 (transmitancy)

7 Electromagnetic radiation detector