Spectroscopic Methods in Organic Chemistry

CHEM-664/476, Organic Chemistry (Minor)

Online Lectures (Introduction)

Dr Abdul Rauf Raza

(*Associate Professor*)

Institute of Chemistry

University of Sargodha, Sargodha

Spectroscopy

Spectroscopy

to visualize an image

Latin language

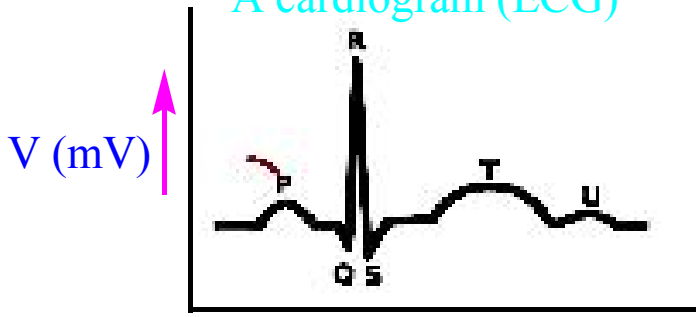
Spectrum

Image

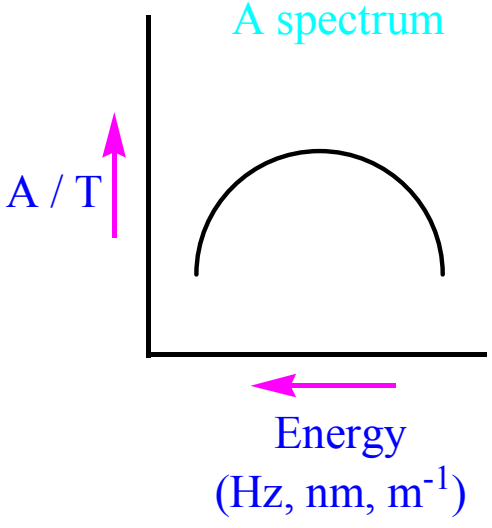
Scopian

to view

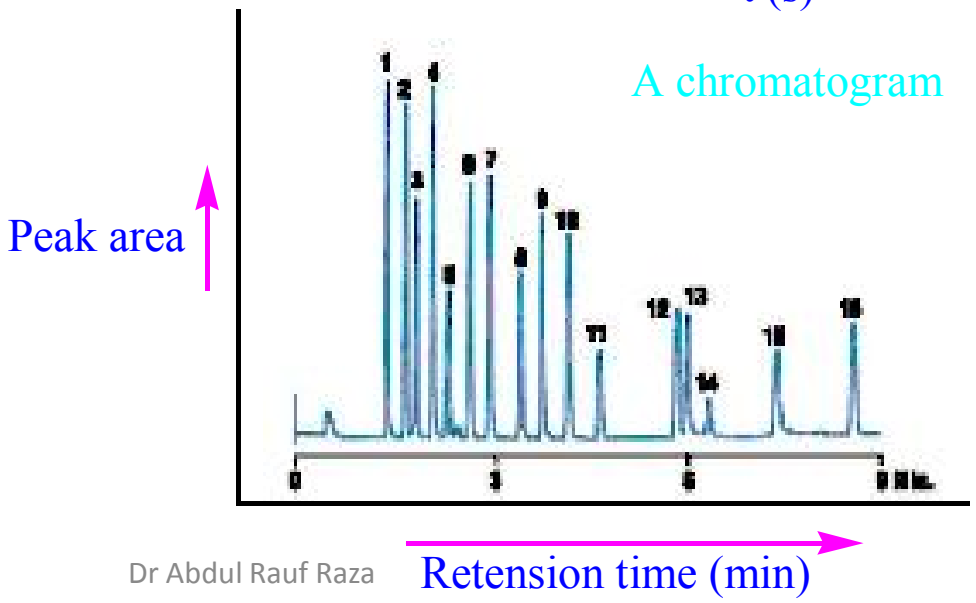
A cardiogram (ECG)



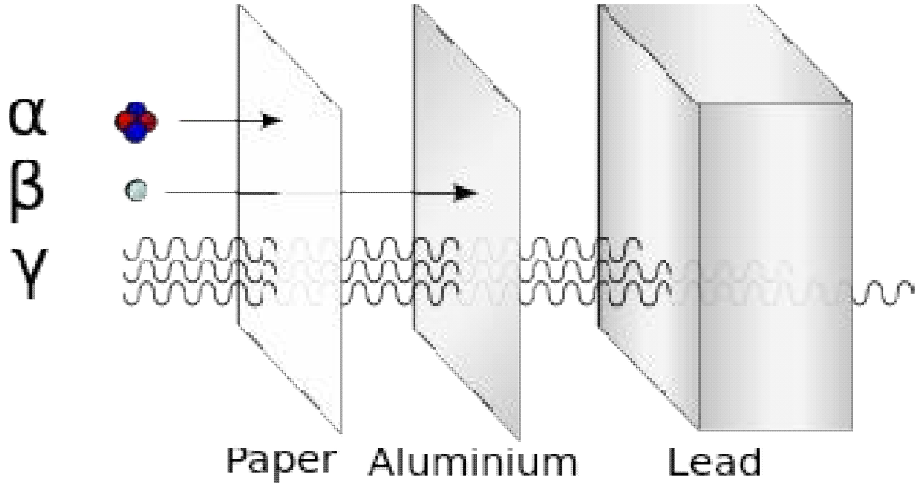
A spectrum



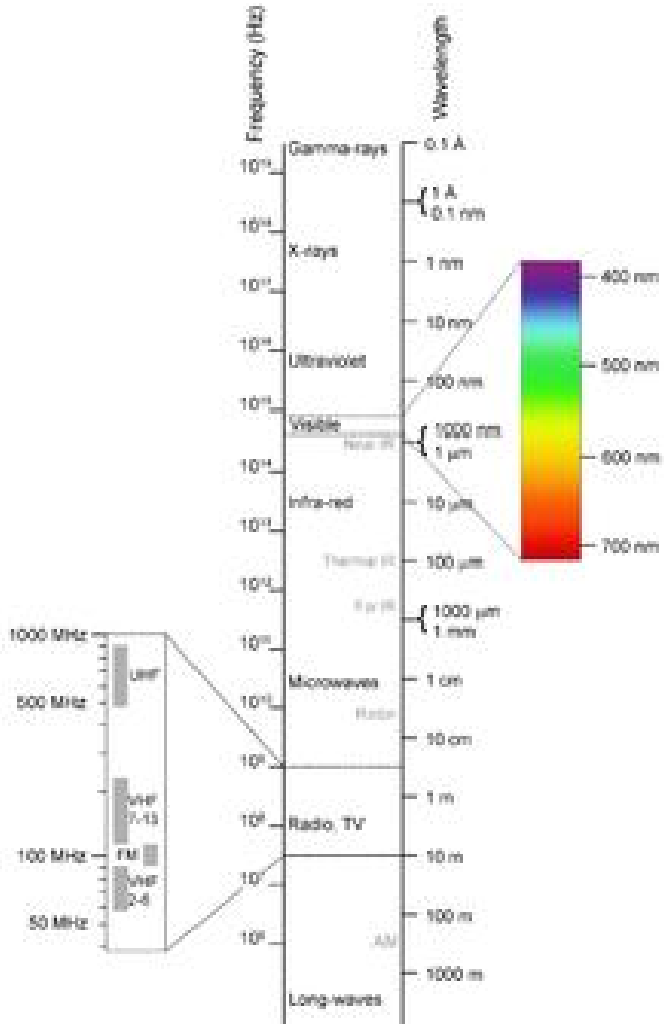
A chromatogram



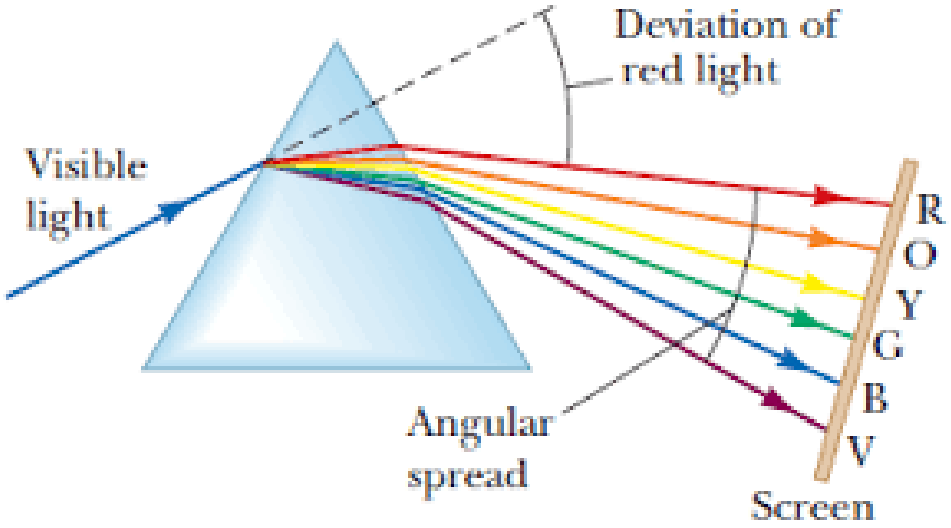
Spectroscopy



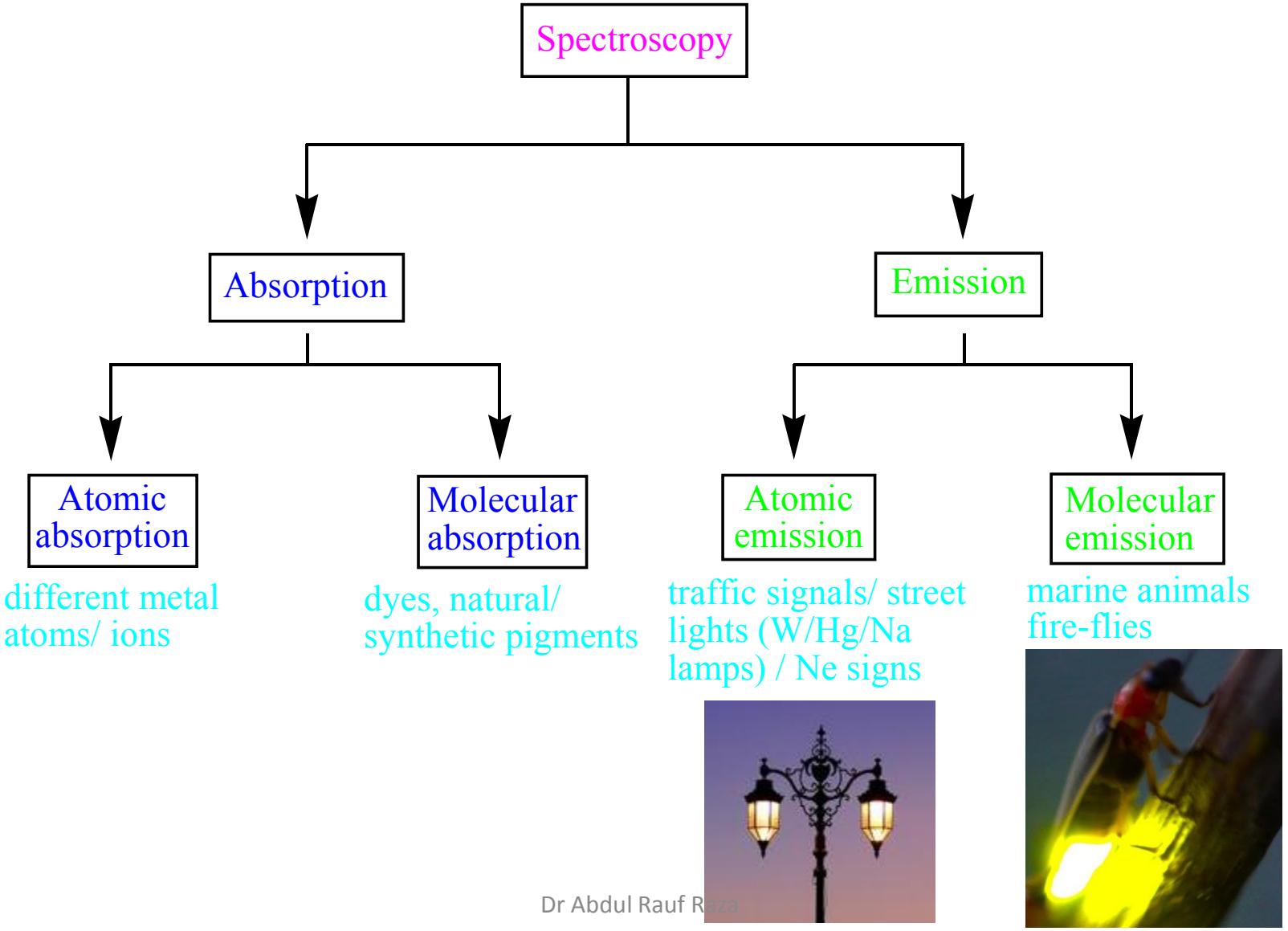
The international symbol for types and levels of radiation that are unsafe for unshielded humans. Radiation, in general, exists throughout nature, such as in light and sound.



Spectroscopy

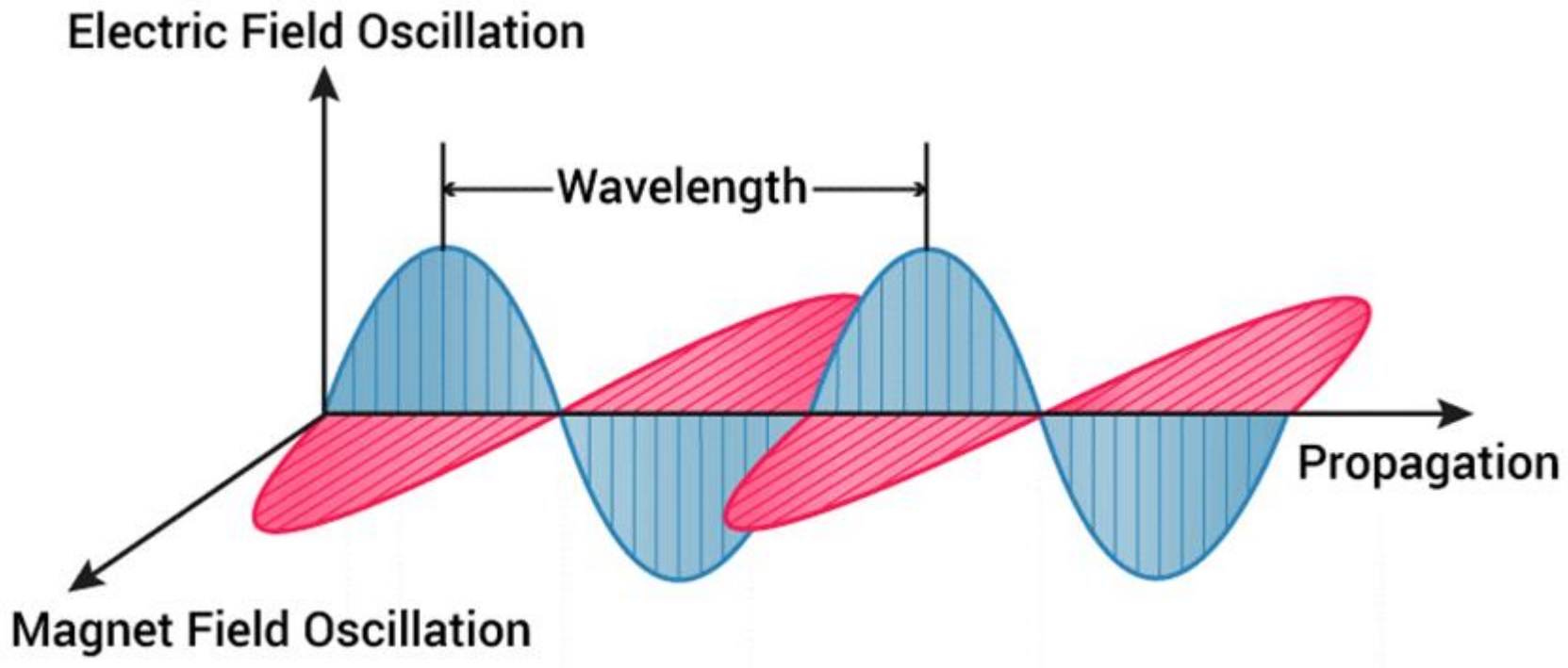


Classification of Spectroscopy

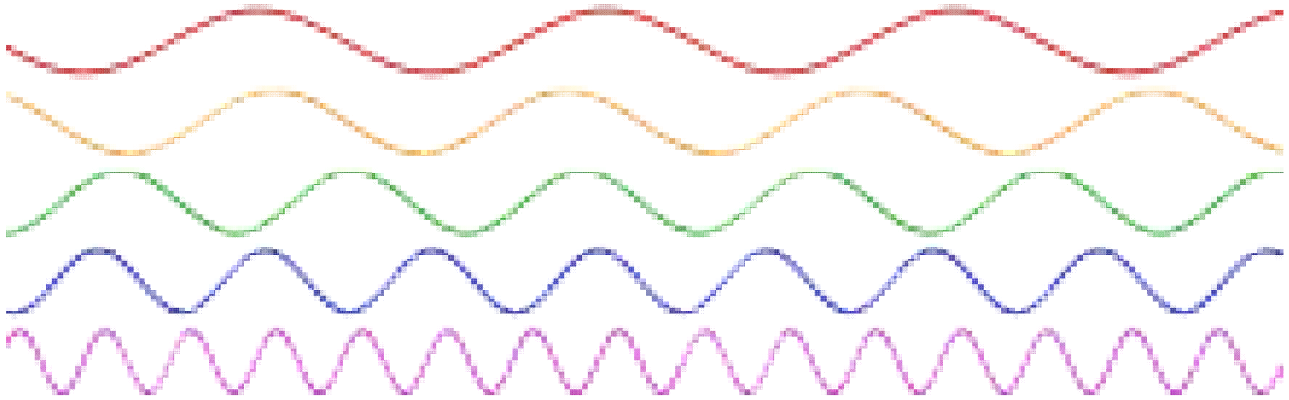


Electromagnetic Radiations (EMR)

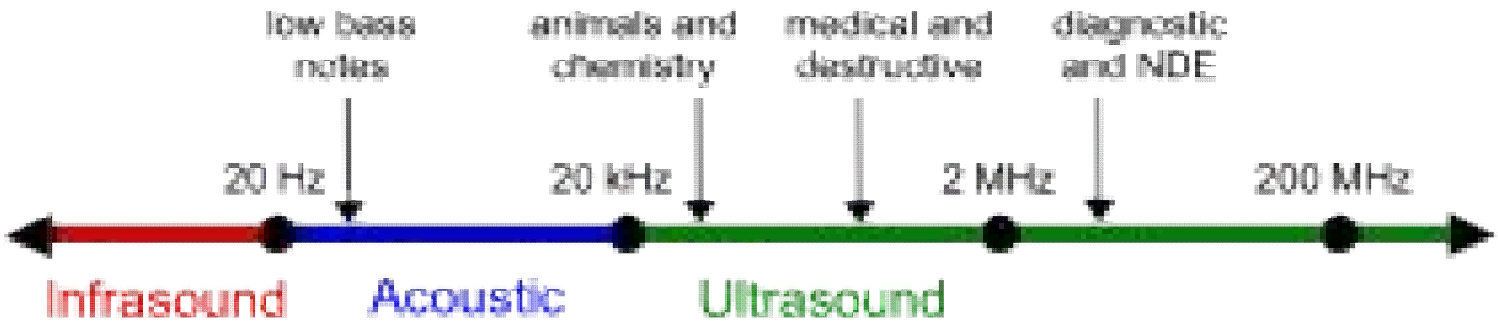
Waves: (sound, ocean etc.) propagates with frequency less than 100 Hz and needs a medium
Rays: (sun) propagates with frequency higher than 100 Hz and needs not a medium
EMR: composed of electrical and magnetic components (perpendicular to each other), propagates with velocity of light (3.0×10^8 m/s) in space and frequency in MHz or higher.



Sound waves



The direction of propagation is same to oscillation (non-polarized).
What is ν, λ and ύ?



ν, λ and ύ

The direction of propagation of EMR is perpendicular to oscillation (polarization) and moves with c. James Clerk Maxwell postulated it and Heinrich Hertz confirmed it. No effect on speed of EMR is observed in vacuum but is affected in crystals (Faraday effect) or solids (Kerr effect).

$E\ (EMR) = h\nu$ ⟶ eq. 1

$h = 6.6 \times 10^{-34}$ J.s

$E = mc^2$ (Einstein's theory) ⟶ eq. 2

$c = 3.0 \times 10^8$ m.s^{-1}

$h\nu = mc^2$ (since LHS of eq 1 & 2 are equal)

if $c > v$; $h\nu = mv^2$ ⟶ $\nu = mv^2/h$

because $\nu = c/\lambda$, therefore $1/\lambda = mv^2/ch$

$\lambda = h / mv$ ⟶ $\lambda \alpha (1/v)$

UNITS: $\nu = s^{-1}$, Hz, cycles/s, revolutions/s

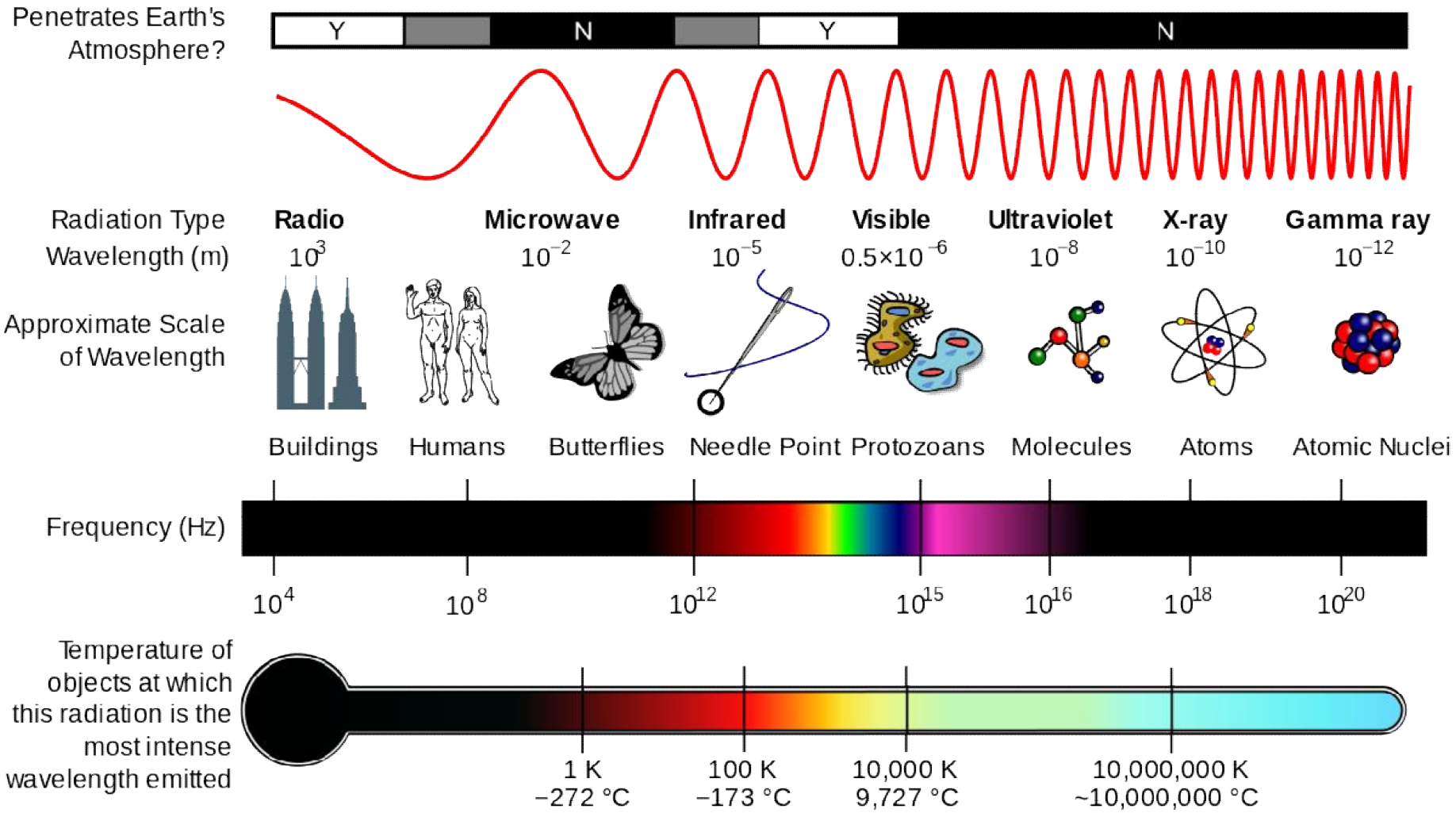
λ = m, μm, nm, pm

wave number = m^{-1}, cm^{-1}

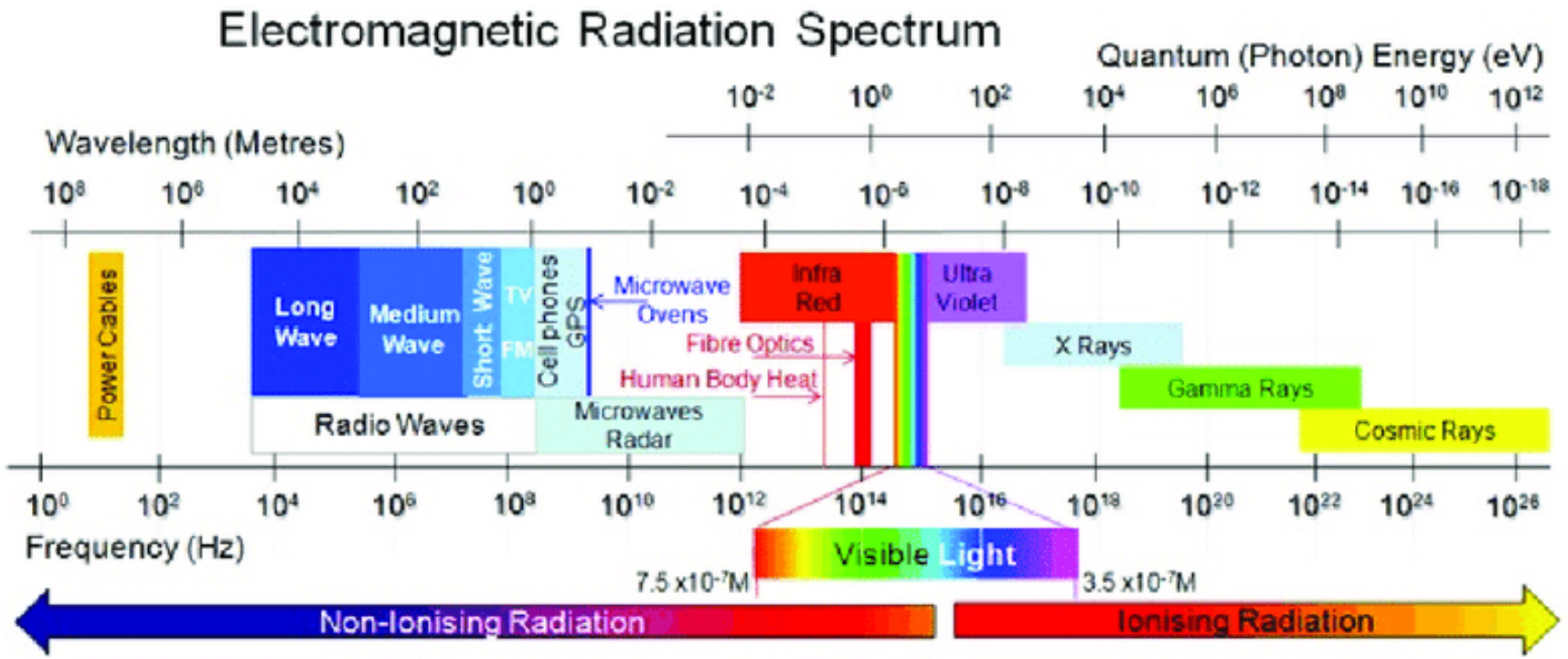
$E = h\nu$ (per photon)
$E = h\nu/\lambda$
$E = hc\bar{\nu}$

$E = N_A h\nu$
(per mole of photon)
$E = N_A h\nu/\lambda$
$E = N_A hc\bar{\nu}$
$N_A = 6.02 \times 10^{23}$
(Avogadro's number)

EMR Spectrum



EMR Spectrum

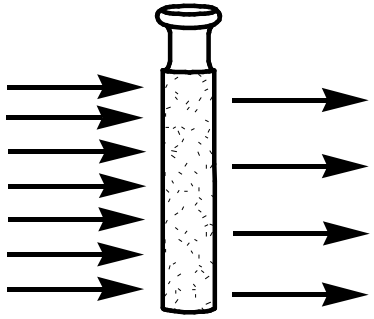


Merits of Spectroscopy

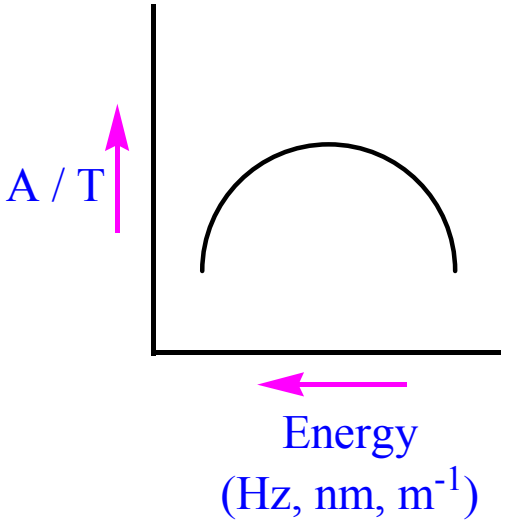
Bond lengths between bonds	Microwave (MW), XRD spectroscopy
Force constants between two atoms	Infrared (IR) spectroscopy
Bond energies of different bonds/ Energy levels	UV/Visible (UV/Vis) spectroscopy
Nature of atomic states	Electron spin resonance (ESR) spectroscopy
Configuration of an asymmetric centre/ Conformational analysis	Optical rotary dispersion (ORD) Circulatory dichroism (CD) spectroscopy
Molecular mass of a molecule/ Exact molecular formula of a molecule	Mass spectrometry
Total structure of a molecule	IR, UV/Vis, NMR, MS

Spectroscopy *vs* Spectrometry

1) Involves a physical change

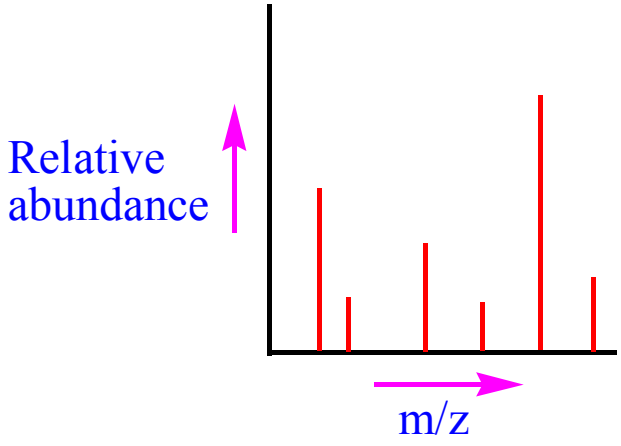


2) a spectrum



1) Involves a chemical change

2) a spectrum



Transition

Quick change of state (lower energy level to higher or vice versa) is called transition.
Transition from lower energy level to higher is called absorption.
Transition from higher energy level to lower is called emission.

i) Rotational transition (J)
ii) Vibrational transition (V)
i) Translational transition (T)
i) Electronic transition (E)