TRINITY COLLEGE FOR WOMEN
NAMAKKAL
Department of Chemistry

QUANTUM CHEMISTRY

BY

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HOD (PG)

QUANTUM THEORY

- Quantum chemistry is also called **MOLECULAR QUANTUM MECHANICS**, is a branch of chemistry focused on the applied of quantum mechanics
- It studies with the ground state of individual atoms and molecules, and the excited statesand transition states.
- Quantum theory is based on experimental observations of light and particles.

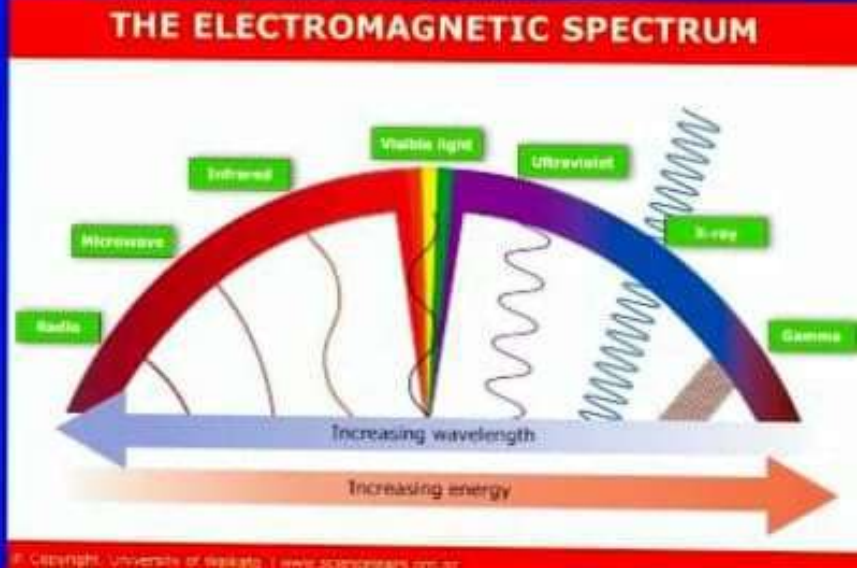
ELECTROMAGNETIC RADIATION

- Energy that exhibits **wave** like behaviour
- In a vacuum, Electromagnetic energy travels through space at the speed of the lights
- It is described by the Electromagnetic spectrum

Ultraviolet = 100nm - 400nm

Visible = 400nm- 700nm
Light

Infrared = 780nm- 1mm



WAVES

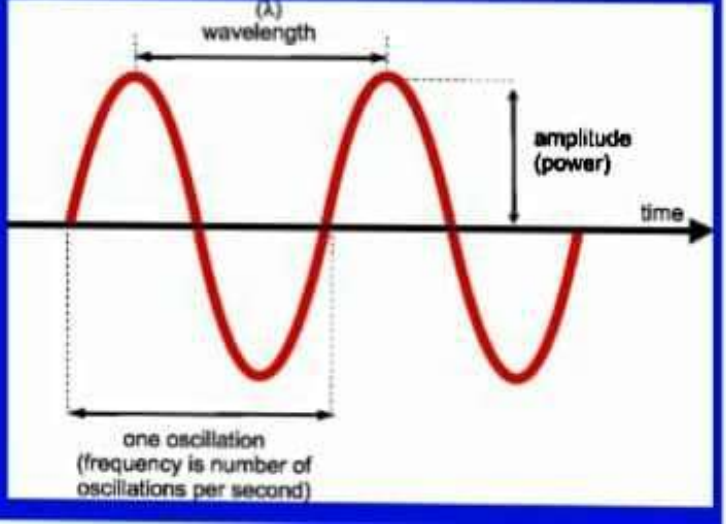
Waves have 4 primary characteristics;

1) Wavelength : distance between two peaks in a wave

2) Frequency : number of waves per second that pass a given Point in space

3) Amplitude : the height of the wave

4) speed : speed of light is 2.9979×10^{8} m/s.



PLANCK'S CONSTANT

Transfer of energy is quantised, and can only in discrete Units, called QUANTA

$$\Delta E = h\nu = \frac{hc}{\lambda}$$

(h= Planck 's constant)

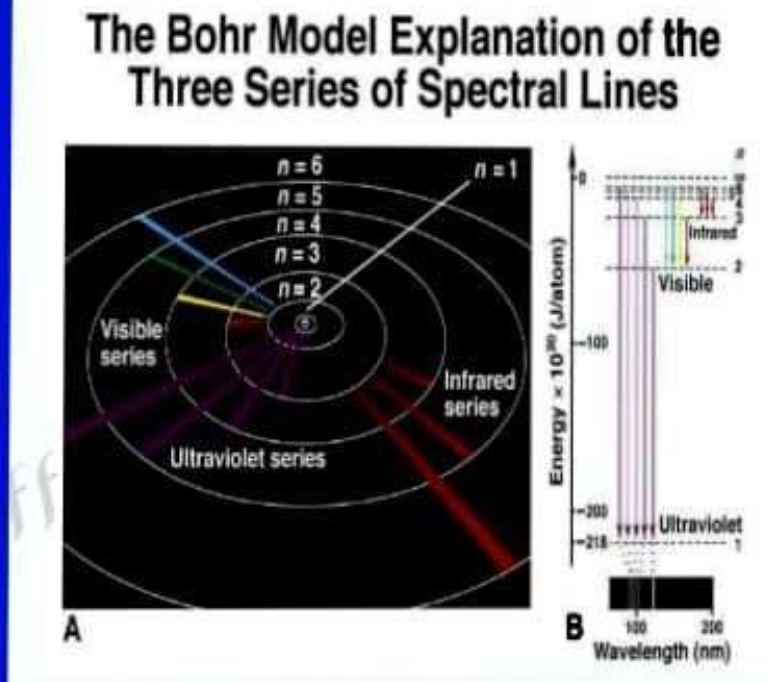
DE BROGLIE 'S EQUATION

$$\lambda = \frac{h}{mv}$$

BOHR MODEL

" The electron in a hydrogen atom moves around the nucleus only in certain allowed circuit orbits "

$$E = -2.178 \times 10^{-18} \text{J} \, (z^2 / n^2)$$



Where,

E = energy of the levels in hydrogen atom

Z = nuclear charge

n = nuclear charge

HEISENBERG'S UNCERTAINTY PRINCIPLE

"It states that it is impossible to determine the position and velocity of the particle cannot be accurately measured at the same time".

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

(OR)

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

Δx = uncertainty in position

Δp = uncertainty in Momentum

h = Planck's constant

QUANTUM NUMBERS

★ **PRINCIPAL QUANTUM NUMBER** (integer n= 1, 2, 3. . .) :
Relates to Size and Energy of the orbitals.

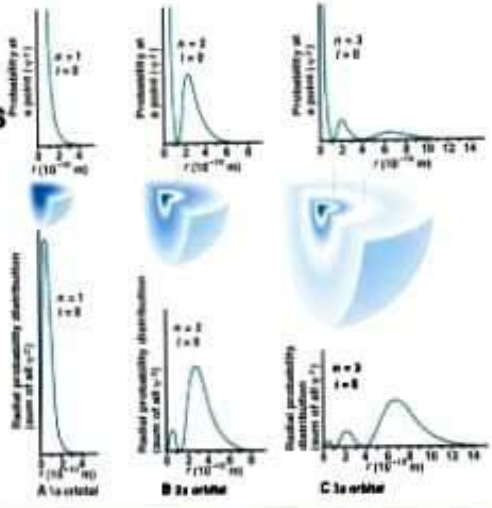
★ **ANGULAR MOMENTUM QUANTUM NUMBER** :
(integer 1)= 0 to n-1 . Relates to shape of the orbital

★ **MAGNETIC QUANTUM NUMBER**:
(Integer m = +1 to -1) Relates to orientation of the orbital in space relative to other orbitals.

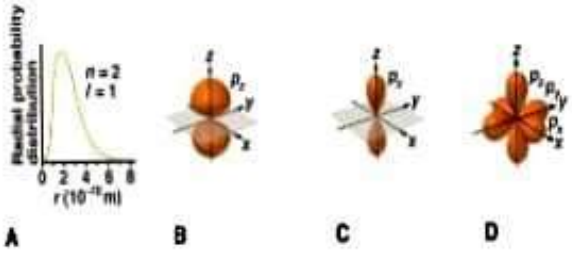
★ **SPIN QUANTUM NUMBER** :
(+1/2 and -1/2) relates to the spin state of the electrom

ORBITALS

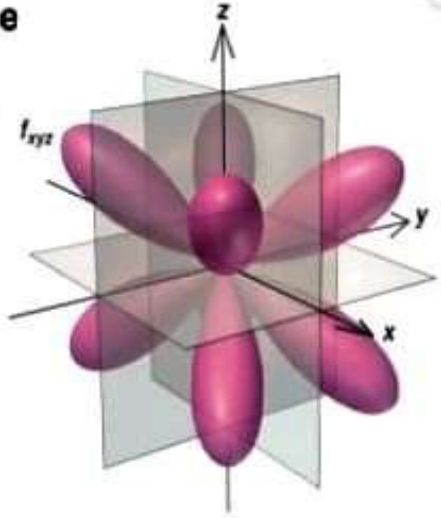
The 1*s*, 2*s*, 3*s* Orbitals



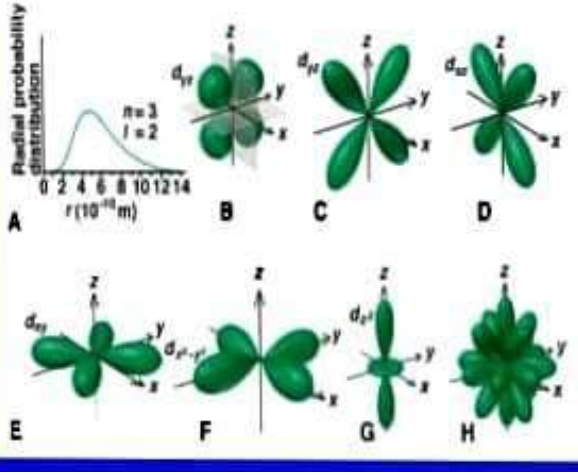
The 2*p* Orbitals



One of the Seven Possible 4*f* Orbitals



The 3*d* Orbitals



Application of quantum chemistry

Important applications of quantum theory include quantum chemistry, quantum optics, quantum computing, superconducting magnets, light-emitting diodes, the optical amplifier and the laser, the transistor and semiconductors such as the microprocessor, medical and research imaging such as magnetic resonance imaging and electron microscopy. .