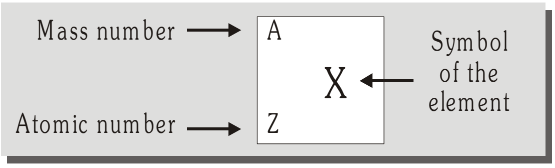
ATOMIC STRUCTURE

IMPORTANT DEFINITIONS

Proton (m_p) /anode rays	**Neutron (m_n)**	**Electron(m_e) / cathode rays**
mass $=1.67 \times 10^{-27}$ kg	mass $= 1.67 \times 10^{-27}$ kg	mass $= 9.1 \times 10^{-31}$ kg
mass $= 1.67 \times 10^{-24}$ g	mass $= 1.67 \times 10^{-24}$ g	mass $= 9.1 \times 10^{-28}$ g
mass = 1.00750 amu	mass = 1.00850 amu	mass = 0.000549 amu
e/m value is dependent on the nature of gas taken in discharge tube.		e/m of electron is found to be independent of nature of gas & electrode used.

REPRESENTATION OF AN ELEMENT



Terms associated with elements :

- Atomic Number (Z) : = No. of protons

  Electron = Z – C (charge on atom)

- Mass number (A) =Total number of neutron and proton present

  A = Number of proton + Number of Neutrons

- **Isotopes :** Same atomic number but different mass number

  Ex. : ${}_6C^{12}$, ${}_6C^{13}$, ${}_6C^{14}$

- **Isobars :** Same mass number but different atomic number

  Ex. ${}_1H^3$, ${}_2He^3$

- **Isodiaphers :** Same difference of number of Neutrons & protons

  Ex. ${}_5B^{11}$, ${}_6C^{13}$

- **Isotones** : Having same number of neutron

  Ex. ${}_1H^3$, ${}_2He^4$

- **Isosters**: They are the molecules which have the same number of atoms & electrons

  Ex. CO_2, N_2O

- **Isoelectronic**:Species having same no. of electrons

  Ex. Cl^-, Ar

ATOMIC MODELS

- **Thomson** : An atom considered to be positively charged sphere where e^- is embedded inside it.
- **Drawback** : Cannot explain stability of an atom.
- **Rutherford Model of an atoms :**

  Electron is revolving around the nucleus in circular path.

  $R_N = R_0(A)^{1/3}$, $R_0 = 1.33 \times 10^{-13}$ cm

  [A = mass number, R_N = Radius of nucleus]

SIZE OF NUCLEUS

- The volume of the nucleus is very small and is only a minute fraction of the total volume of the atom. Nucleus has a diameter of the order of 10^{-12} to 10^{-13} cm and the atom has a diameter of the order of 10^{-8} cm.
- Thus, diameter (size) of the atom is 1,00,000 times the diameter of the nucleus.

ELECTROMAGNETIC SPECTRUM

- RW →MW →IR →Visible →UV →X-rays →CR (Radiowaves →Microwaves →Infrared rays →Visible rays →Ultraviolet rays →X-rays →Cosmic rays)
- Wavelength decreases ⟶
- Frequency increases ⟶
- • $c = \nu\lambda$ • $\lambda = \dfrac{c}{\nu}$ • $\bar{\nu} = \dfrac{1}{\lambda} = \dfrac{\nu}{c}$

  • $T = \dfrac{1}{\nu}$ • $E = \dfrac{hc}{\lambda} = h\nu$, $h = 6.626 \times 10^{-34}$ Js

  • $E(ev) = \dfrac{12400}{\lambda(\text{Å})}$

  •Total amount of energy transmitted

  $E = nh\nu = \dfrac{nhc}{\lambda}$

BOHR'S ATOMIC MODEL

Theory based on quantum theory of radiation and the classical laws of physics

- $\frac{K(Ze)(e)}{r^2} = \frac{mv^2}{r}$
- $mvr = \frac{nh}{2\pi}$ or $mvr = n\hbar$
- Electron remains in stationary orbit where it does not radiate its energy.
- **Radius :** $r = 0.529 \times \frac{n^2}{Z} \text{Å}$
- **Velocity :** $v = 2.188 \times 10^6 \frac{Z}{n} ms^{-1}$
- Energy(KE + PE)

  =Total energy $= -13.6 \times \frac{Z^2}{n^2}$ eV/atom
- $TE = -\frac{KZe^2}{2r}$, $PE = \frac{-KZe^2}{r}$, $KE = \frac{KZe^2}{2r}$

  PE = –2KE, KE = –TE, PE = 2TE
- Revolutions per sec $= \frac{v}{2\pi r}$
- Time for one revolution $= \frac{2\pi r}{v}$
- Energy difference between n_1 and n_2 energy level

$$\Delta E = E_{n_2} - E_{n_1} = 13.6Z^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)\frac{eV}{atom} = IE \times \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

where IE = ionization energy of single electron species.

- **Ionization energy** $= E_\infty - E_{G.S.} = 0 - E_{G.S.}$

  $E_{G.S.}$ = Energy of electron in ground state

HYDROGEN SPECTRUM

- **Rydberg's Equation** :

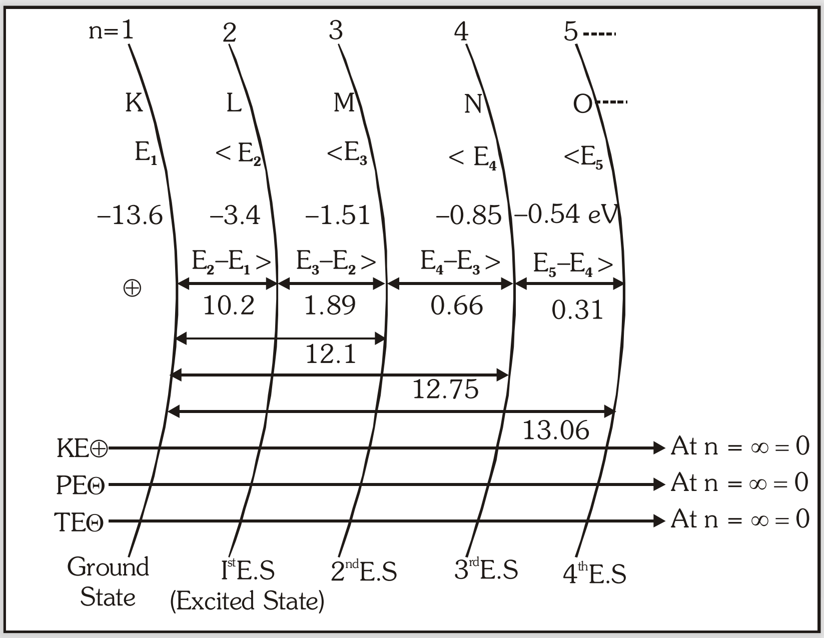
$$\frac{1}{\lambda} = \bar{v} = R_H\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] \times Z^2$$

$R_H \cong 109700\ cm^{-1}$ = Rydberg constant

- For first line of a series $n_2 = n_1 + 1$
- Limiting spectral line (series limit) means $n_2 = \infty$
- H_α line means n_2=n+1; also known as line of longest λ, shortest ν, least E
- Similarly H_β line means $n_2 = n_1 + 2$
- When electrons de-excite from higher energy level (n) to ground state in atomic sample, then number of spectral lines observed in the spectrum $= \frac{n(n-1)}{2}$
- When electrons de-excite from higher energy level (n_2) to lower energy level (n_1) in atomic sample, then number of spectral line observed in the spectrum

$$= \frac{(n_2 - n_1)(n_2 - n_1 + 1)}{2}$$

- No. of spectral lines in a particular series $= n_2 - n_1$



DE-BROGLIE HYPOTHESIS

- All material particles posses wave character as well as particle character.
- $\lambda = \dfrac{h}{mv} = \dfrac{h}{p}$
- The circumference of the n^{th} orbit is equal to n times of wavelength of electron i.e., $2\pi r_n = n\lambda$
  Number of waves = n = principal quantum number
- Wavelength of electron $(\lambda) \cong \sqrt{\dfrac{150}{V(\text{volts})}}$ Å
- $\lambda = \dfrac{h}{\sqrt{2mKE}}$

HEISENBERG UNCERTAINTY

- According to this principle, " it is impossible to measure simultaneously the position and momentum of a microscopic particle with absolute accuracy"
  If one of them is measured with greater accuracy, the other becomes less accurate.
- $\Delta x.\Delta p \geq \dfrac{h}{4\pi}$ or $(\Delta x)(\Delta v) \geq \dfrac{h}{4\pi m}$
  where Δx = Uncertainty in position
  Δp = Uncertainty in momentum
  Δv = Uncertainty in velocity
  m = mass of microscopic particle
- Heisenberg replaced the concept of orbit by that of orbital.

QUANTUM NUMBER

- **Principal Quantum number (By Bohr)**
  ⇒ Indicates = Size and energy of the orbit, distance of e^- from nucleus
  ⇒ Values n = 1, 2, 3, 4, 5....................
  ⇒ Angular momentum = $n \times \dfrac{h}{2\pi}$
  ⇒ Total number of e^-s in an orbit = $2n^2$
  ⇒ Total number of orbitals in an orbit = n^2
  ⇒ Total number of subshell in an orbit = n
- **Azimuthal/Secondary/Subsidiary/Angular momentum quantum number (ℓ)**
  ⇒ Given by = Sommerfeld
  ⇒ Indicates = Sub shells/sub orbit/sub level
  ⇒ Values ⇒ 0, 1..............(n–1)
  ⇒ Indicates shape of orbital/Sub shell

Value of n	Values of ℓ [Shape]	Initial from word
eg. If n = 4	ℓ = 0 (s) [Spherical]	Sharp
	ℓ=1 [p] [Dumb bell]	Principal
	ℓ=2 [d] [Double dumb bell]	Diffused
	ℓ=3 [f] [Complex]	Fundamental

  ⇒ Total no. of e^-s in a suborbit = 2(2l + 1)
  ⇒ Total no. of orbitals in a suborbit = (2l + 1)
  ⇒ Orbital angular momentum
  $= \sqrt{\ell(\ell+1)}\dfrac{h}{2\pi} = \sqrt{\ell(\ell+1)}\hbar$
  h = Planck's constant
  ⇒ For H & H like species all the subshells of a shell have same energy.
  i.e. 2s = 2p 3s = 3p = 3d
- **Magnetic Quantum number (m)**
  ⇒ Given by Linde
  ⇒ Indicates orientation of orbitals i.e. direction of electron density.
  ⇒ Value of m = $-\ell$ ....0.........$+\ell$
  ⇒ Maximum no of e's in an orbital = 2 (with opposite spin)
  m for p sub shell = p_x p_y p_z
  -1 $+1$ 0

  m for d sub shell =
  dxy dyz dz^2 dxz dx^2-y^2
  -2 -1 0 $+1$ $+2$
- **Spin Quantum Number (m_s or s)**
  Given by Uhlenback & Goudsmit
  Values of s = ±½
  Total value of spin in an atom = ±½ ×number of unpaired electrons
  Spin Angular momentum = $\sqrt{s(s+1)}\dfrac{h}{2\pi}$

RULES FOR FILLING OF ORBITALS

- **Aufbau principle :** The electrons are filled up in increasing order of the energy in subshells.
  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 5f^{14} 6d^{10}$
- **(n + ℓ) rule :** The subshell with lowest (n + ℓ) value is filled up first, but when two or more subshells have same (n + ℓ) value then the subshell with lowest value of n is filled up first.
- **Pauli exclusion principle :** Pauli stated that no two electrons in an atom can have same values of all four quantum numbers.
- **Hund's rule of maximum multiplicity :** Electrons are distributed among the orbitals of subshell in such a way as to give maximum number of unpaired electrons with parallel spin.