Date : ....

Unit-01 ([redacted]

Atomic Structure

10^{-9}

Rydberg's equation -

$$\boxed{\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)}$$

. R → rydberg constant

~~R = 1.097×~~

$R = 1.097 \times 10^{7}$

$= 10.97 \times 10^{6}$

S.I unit is m^{-1}.

for 3rd line of Brackett series ÷

↳ For 3rd series of Brackett,

Eqn is — $n_1 = 4$, $n_2 = 7$

$$\therefore \frac{1}{\lambda} = R_H\left(\frac{1}{4^2} - \frac{1}{7^2}\right)$$

Q. for a particular line in the Balmer's series, the wavelength is observed at 434 nm. Identify the line of the series.

Soln given, $\lambda = 434$ nm

$= 434 \times 10^{-9}$ m

& $n_1 = 2$, $n_2 = ?$

we have Rydberg's eqn -

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\Rightarrow \frac{1}{434 \times 10^{-9}} = 10.97 \times 10^{6}\left(\frac{1}{2^2} - \frac{1}{n_2^2}\right)$$

$$\Rightarrow \frac{10^{9}}{434 \times 10.97 \times 10^{6}} = \frac{1}{4} - \frac{1}{n_2^2}$$

$$\Rightarrow \frac{1000}{\cancel{4760.98}\ 4.76} \cdot 1 = \frac{1}{4} - \frac{1}{n_2^2}$$

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Rules for filling electrons in various orbitals :

1. Aufbau principle : (n+l) Rule

↳ In the ground state of the atoms, the orbitals are filled in order of their increasing energies.

- 1s 2s 2p 3s 3p 4s 3d 4p . . . . .

$\xrightarrow{\text{increasing order of energy}}$

2. Pauli Exclusion principle :

↳ No two electrons in an atom can have the same set of four quantum numbers. Thus only two electrons may exist in the same orbital and these electrons must have opposite spin.

$n = 1, l = 0(s), m_l = 0, m_s = \frac{1}{2}$ or $-\frac{1}{2}$

$\therefore$ 1st electron, $m_s = \frac{1}{2}$ &

2nd electron, $m_s = -\frac{1}{2}$

$\therefore$ 1s = 2 electron.

3. Hund's rule :

↳ According to Hund's rule, electron pairing will not take place in orbitals of same energy until each orbital is singly filled.

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4. Electronic configuration —

List

$_{1}H : 1s^1$ $\boxed{\uparrow}$

$_{2}He : 1s^2$ $\boxed{\uparrow\downarrow}$

$_{3}Li : 1s^2 2s^1$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow}$

$_{4}Be : 1s^2 2s^2$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$

$_{5}B : 1s^2 2s^2 2p^1$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow \quad \quad}$

$_{6}C : 1s^2 2s^2 2p^2$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\uparrow\quad}$

$_{7}N : 1s^2 2s^2 2p^3$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\uparrow\uparrow}$

$_{8}O : 1s^2 2s^2 2p^4 \rightarrow$ $\boxed{\uparrow\downarrow|\uparrow|\uparrow}$

$_{9}F : 1s^2 2s^2 2p^5 \rightarrow$ $\boxed{\uparrow\downarrow|\uparrow\downarrow|\uparrow}$

$_{10}Ne : 1s^2 2s^2 2p^6 \rightarrow$ $\boxed{\uparrow\downarrow|\uparrow\downarrow|\uparrow\downarrow}$

$_{11}Na : 1s^2 2s^2 2p^6 3s^1$ or $[Ne] 3s^1$

$_{12}Mg : [Ne] 3s^2$

$_{13}Al : [Ne] 3s^2 3p^1$

$_{14}Si : [Ne] 3s^2 3p^2$

$_{15}P : [Ne] 3s^2 3p^3$

$_{16}S : [Ne] 3s^2 3p^4$

$_{17}Cl : [Ne] 3s^2 3p^5$

$_{18}Ar : [Ne] 3s^2 3p^6$ or $1s^2 2s^2 2p^6 3s^2 3p^6$

$_{19}K : 1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ or $[Ar] 4s^1$

$_{20}Ca : [Ar] 4s^2$

$_{21}Sc : [Ar] 4s^2 3d^1$

$_{22}Ti : [Ar] 4s^2 3d^2$

$_{23}V : [Ar] 4s^2 3d^3$

$_{24}Cr : [Ar] 4s^1 3d^5$

$_{25}Mn : [Ar] 4s^2 3d^5$

$_{26}Fe : [Ar] 4s^2 3d^6$

$_{27}Co : [Ar] 4s^2 3d^7$

$_{28}Ni : [Ar] 4s^2 3d^8$

$_{29}Cu : [Ar] 4s^1 3d^{10}$

$_{30}Zn : [Ar] 4s^2 3d^{10}$

Teacher's Signature

$\Rightarrow 0.21 = \frac{1}{4} - \frac{1}{n_2^2}$

$\Rightarrow \frac{1}{n_2^2} + 0.21 = \frac{1}{4}$

$\Rightarrow \frac{1}{n_2^2} = \frac{1}{4} - 0.21$

~~$\Rightarrow \frac{1}{n_2^2} = \frac{1-0.8}{4}$~~

~~$\Rightarrow \frac{1}{n_2^2} = \frac{0.2}{4}$~~

~~$\Rightarrow \frac{1}{n_2^2} = \frac{2}{4\times 10}$~~

~~$\Rightarrow \frac{1}{n_2^2} = \frac{1}{20}$~~

~~$\Rightarrow n_2^2 = 20$~~

~~$\Rightarrow n_2 = 10$~~

$\Rightarrow \frac{1}{n_2^2} = 0.25 - 0.21$

$\Rightarrow \frac{1}{n_2^2} = 0.04$

$\Rightarrow n_2^2 = \frac{1}{0.04}$

$\Rightarrow n_2^2 = 25$

$\Rightarrow n_2 = 5$

Since $n_2 = 5$, hence it is 3rd line of Balmer's series.

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Series	n_1	n_2	Spectral Region
(1) Lyman	1	2,3,4,…	Ultraviolet (UV)
(2) Balmer	2	3,4,5,…	Visible Region
(3) Paschen	3	4,5,6,…	Infrared (IR)
(4) Brackett	4	5,6,7,…	Infrared (IR)
(5) Pfund	5	6,7,8,…	Infrared (IR)

Rutherford model of atom –

(1) Most of the space in the atom is empty as most of the α- particles passed through the foil undeflected.

(2) A few positively charged α-particles were deflected. The deflection must be due to enormous repulsive force showing that the positive charge of the atom is not spread throughout the atom.

(3) A very few particles (~1 in 20,000) bounced back ie, were deflected by nearly 180°. The positive charge has to be concentrated in a very small volume that repelled & deflected the positive charge α particles.

Drawbacks of Rutherford model –

(1) Rutherford model cannot explain the stability of an atom.

(2) It says nothing about distribution of the electrons around the nucleus and the energies of these electrons.

Note :-

Lyman series :- $n=2 \rightarrow n=1$ (shortest transition)
$n=\infty \rightarrow n=1$ (longest transition)

Now, in shortest transition ie, $n=2 \rightarrow n=1$. frequency (ν) is smallest and wavelength (λ) is longest, Whereas in $n=\infty \rightarrow n=1$ we have frequency (ν) is largest and wavelength (λ) is smalle

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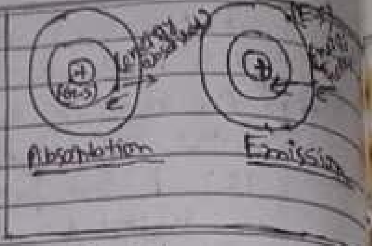
Bohr's model for H atom :-

postulates



(1) The electron in the hydrogen atom can move around the nucleus in a circular path called orbits. These orbits are arranged concentrically around the nucleus which are numbered as 1, 2, 3, 4 ... or designed as K, L, M, N ...

(2) The energy of an electron in the orbit does not change with time. However, the electron will move from a lower stationary state to a higher stationary state when required amount of energy is absorbed by the electron or energy is emitted when electron moves from higher stationary state to lower stationary state.

(3) An electron can move only in those orbits for which its angular momentum is some integral multiple of $h/2\pi$. That means angular momentum is quantised.

∴ Angular momentum $= n\frac{h}{2\pi}$, $n = 1, 2, 3, \ldots$

i.e. $\boxed{mvr = \frac{nh}{2\pi}}$, where m = mass

v = velocity

r = radius

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Bohr radius –

$\left[r_n = 52.9\, n^2\ \text{pm} \right.$ or $\left. r_n = 0.0529\, n^2\ \text{nm} \right]$

Bohr velocity –

$\left\{ v = \frac{2.19 \times 10^6}{n} \times Z\ \ \text{ms}^{-1} \right\}$

Bohr radius for Hydrogen like atom –

$r_n = \frac{52.9\, n^2}{Z}\ \text{pm}$

or $r_n = \frac{0.0529\, n^2}{Z}\ \text{nm}$

$\left[\text{nm} = 10^{-9} \times \text{m}, \ \text{pm} = 10^{-12} \times \text{m} \right]$

Note :- No. of spectral lines possible $= \frac{(n_2 - n_1)(n_2 - n_1 + 1)}{2}$

Limitations of Bohr's model :-

1. Bohr's model is unable to explain the spectrum of atoms other than hydrogen.

2. It could not explain the ability of atoms to form molecules by chemical bonds.

3. Bohr's theory was also unable to explain the splitting of spectral lines in the presence of magnetic field & electric field.

4. The main objection to the Bohr's theory came from the new principles i.e. Dual nature of matter and uncertainty principle.

Quantum number —

To describe electron in an atom we need the set of four numbers which are designated as n, l, m_l, m_s. This four number are called quantum numbers.

(1) Principal quantum no. (n) –

↳ 'n' is basically called the shell no.

It represents the energy and size of shell

$n = 1, 2, 3, 4$
(K, L, M, N)

(2) Azimuthal quantum no. (l) –

↳ 'l' represents the subshell of an electron.

It shows the angular momentum of electron.

$l = 0, 1, 2, 3, \ldots\ldots (n-1)$

if $n = 1$, then $l = 0$
$n = 2$, then $l = 0, 1$
$n = 3$, then $l = 0, 1, 2$
$n = 4$, then $l = 0, 1, 2, 3$
. . . .

- Subshell : 0 1 2 3 4

Designation : s p d f g

$s < p < d < f$
$\xrightarrow{\hspace{2cm}}$
energy increases

Notation

n	l	
1	0(s) $\longrightarrow$	1s
2	0(s) 1(p) $\longrightarrow$	2s 2p
3	0(s) 1(p) $\longrightarrow$ 2(d)	3s 3p 3d

(3) Magnetic quantum no. (m_l)

↳ m_l denotes the orbital.

$$\boxed{m_l = -l, \ldots\ldots, 0, \ldots\ldots, +l}$$

No. of orbitals

$l = 0$, $m_l = 0 \longrightarrow$ ①
$l = 1$, $m_l = -1, 0, 1 \longrightarrow$ ③
$l = 2$, $m_l = -2, -1, 0, 1, 2 \longrightarrow$ ⑤
$l = 3$, $m_l = -3, -2, -1, 0, 1, 2, 3 \longrightarrow$ ⑦

∴ $l \rightarrow (2l+1)$ values the m_l

or $n^2 = m_l$

Subshell :	s	p	d	f
orbitals :	1	3	5	7

(4) Spin quantum no. (m_s) :

'm_s' denotes the spin of electron.

Values are → $+\frac{1}{2}$ or $-\frac{1}{2}$.

Stability of half filled and completely filled orbitals :—

Half filled and completely filled orbitals are particularly stable due to the following reasons —

Half filled orbitals :

(i) Symmetry : Half filled orbitals have a symmetrical arrangement of electrons, which leads to greater stability.

(ii) Exchange energy : In half filled orbitals, electrons with parallel spins experience a favourable exchange energy, which increases stability.

(iii) Less repulsion : With fewer electrons, there is less repulsion between them, resulting in greater stability.

Example : (a) Half filled 3d orbital in Cr,
(b) Half filled 4d orbital in Mo (molybdenum)

Completely filled orbitals

(i) Maximum symmetry : Completely filled orbitals have the maximum possible symmetry, leading to enhanced stability.

(ii) Minimum energy : Completely filled orbitals have the lowest possible energy, making them more stable.

(iii) No unpaired electrons : With all electrons paired, there is no tendency to react and form bonds, increasing stability.

Example : (a) Completely filled 1s orbital of He.
(b) Completely filled 2p orbital of Ne.

Concept of exchange energy :—

↳ Exchange energy is the energy associated with the exchange of electrons between two or more orbitals. This energy arises from Pauli Exclusion Principle which states that two electrons with the same spin cannot occupy the same orbital.

How does exchange energy work?

↳ When two electrons with same spin occupy two different orbitals, they can exchanges places. This exchange process leads to a decrease in energy, known as the exchange energy.

Exchange energy plays a crucial role in :
(a) chemical bonding, (b) magnetic properties,
(c) electronic configurations.

Q. Why energy of an electron is negative?

Ans:- It is because when an electron is at infinite distance from the nucleus then the Kinetic energy of that electron cannot be calculated. So it is taken to be zero. When the electron come closer to the nucleus, the stability increases due to the loss of energy of electron and thus the energy of electron become less negative. That's why electronic energy is negative.

Dual behaviour of matter—

According to de Broglie, all material particles in motion possesses wave characteristics and the wavelength of particle is given by -

$$\boxed{\lambda = \frac{h}{mv} = \frac{h}{p}} \quad \left(\because \text{momentum, } p = mv\right)$$

Derivation

According to Planck, $E = h\nu$

According to Einstein, $E = mc^2$

$\therefore h\nu = mc^2$

$\Rightarrow h \cdot \frac{c}{\lambda} = mc^2 \quad \left(\because c = \lambda\nu \Rightarrow \nu = \frac{c}{\lambda}\right)$

$\Rightarrow \frac{h}{\lambda} = mc$

$\Rightarrow \lambda = \frac{h}{mc}$

$\Rightarrow \lambda = \frac{h}{mv}$ (∵ $c = v$, speed of light)

$\Rightarrow \boxed{\lambda = \frac{h}{p}}$

$\therefore \lambda \propto \frac{1}{p}$ i.e. wavelength of a particle is inversely proportional to momentum

Heisenberg's uncertainty principle:

It states that it is impossible to determine simultaneously, the exact position and exact momentum (or velocity) of an electron.

Mathematically,

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

Where, Δx = uncertainty in position
Δp = uncertainty in momentum

Relation between K.E and λ —

$$\boxed{\lambda = \frac{h}{\sqrt{2 K.E \times m}}}$$

Erwin Schrodinger equation—

$\boxed{\hat{H}\psi = E\psi}$, where $\hat{H}$ = mathematical operator
ψ = amplitude of wave
E = energy of the system

This eqn describes the spatial part of the wave function, ψ and its corresponding energy, E.

Examples :

↳ The exchange energy between the two electrons in the H_2 molecule leads to the formation of a covalent bond.

Anomalous electronic Configuration :

Anomalous electronic configurations refe to the electron configuration of certain ato that deviate from the expected or predicte configurations based on the Aufbau princip and Hund's rule .

Examples :-

(a) 'Cr' expected configuration is [Ar] $3d^4 4s^2$ but actual configuration is [Ar] $3d^5 4s^1$

(b) 'Cu' expected configuration is [Ar] $3d^9 4s$ but actual configuration is [Ar] $3d^{10} 4s^1$.

These anomalies occur due to -

(i) Exchange energy,
(ii) pairing energy,
(iii) Stability of half filled and complet filled orbitals.

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