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Inorg.-I (H/S)
Chapter - At. Structure.
Topics ⟶ (a) Schrodinger wave. Equation
(b) Physical. Significance.
(c) Atomic - Orbitals.

Schrodinger wave equation

Classical mechanics fails to explain the behaviour of electrons correctly due to uncertainty principle for electron.
Quantum - mechanics was developed by Schrodinger which describe the behaviour of electron around the nucleus by a mathematical equation known as Schrodinger wave. Equation.
On the basis of Quantum Mechanics a model of atom is proposed which consider electron as wave - particle duality of matter along with Heisenberg uncertainty principle.
The Schrodinger wave equation is expressed.

$$\nabla^2\psi + \frac{8\pi^2 m}{h^2}[E-V]\psi = 0.$$

or $$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

For a system such as an atom or molecule whose energy does not change with time, the Schrodinger wave equation is written as

$$\hat{H}\psi = E\psi$$

Where $\hat{H}$ = Mathematical Operator Called Hamiltonian Operator.
ψ = probability of finding electron in three dimensional space (amplitude function).
E = Total energy.
∇^2 = Laplacian Operator
V = Potential energy of electron.

Physical Significance

ψ gives the amplitude of wave function of electron. In case of light wave, the amplitude of wave at a point is proportional to the intensity of light. For electron ψ^2 may be taken as the intensity of the electron at any point.

ψ^2 means the probability of finding electrons in a given region also called probability density. Higher the value of ψ^2 greater probability of finding electrons.

Schrodinger wave equation is different equation of second order & solution of it provided several value of ψ including imaginary value (not-valid).

Only those values of ψ are acceptable which satisfy the following conditions:

(i) The wave function must be finite & continuous.
(ii) It must be single-valued.
(iii) The solution must be normalised & should satisfy

$$\int_0^\infty \psi \, d\tau = D$$

(iv) $\frac{d\psi}{dx}$, $\frac{d\psi}{dy}$ & $\frac{d\psi}{dz}$ must be continuous function of x, y & z. Respectively.

(c) Concept of Atomic Orbitals

According to Bohr, the electron revolves round in a well-defined Circular orbit. But the idea of uncertainty principle about its Position & velocity over ruled the Bohr's picture of fixed Circular Path. To explain

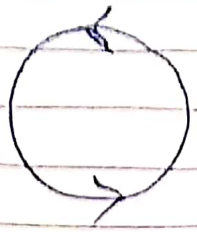
(i) Stability of atom
(ii) dual-behaviour
(iii) uncertainty principle.

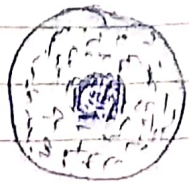
Thus the above Concept explained by wave mechanics.

The solution of Schrodinger wave equation led to the Concept of most-probable region in place of well-defined circular path as proposed by Bohr.

Definition of Orbitals:- It may be defined as the region in three dimensional space around the nucleus where the probability of finding electron is maximum.

A picture of orbitals,





(a) Orbit
Bohr orbit of
Circular path.

(b) Orbital
Electron cloud representation
of an orbital.

Difference b/w Orbit & Orbital.

Orbit	Orbital
(1) well-defined Circular Path around the nucleus.	(1) Represents region in three dimensional space in which probability of finding electron is maximum.
(2) It represents Planar motion of electron	(2) represents three dimensional motion around nucleus.
(3) It gives a definite path of an electron but it is contrary to uncertainty principle.	(3) Does not specify definite Path. It gives any where in space the electron.
(4) All the orbits must be Circular.	(4) Different orbitals have different shapes s-spherical, p-dumbbell
(5) Orbits have no directional characters.	(5) Orbitals (except s-) have directional character in space
(6) An orbit, the electrons filled by $2n^2$ Rule where n = principle q.N	(6) Any orbital can accommodate maximum two electrons.