

STUDY COURSE MATERIAL-6

CHEMISTRY

SESSION-2020-21

CLASS- XI

TOPIC:ATOMIC STRUCTURE

DAY-1

❖ TEACHING MATERIAL

QUANTUM MECHANICAL MODEL OF ATOM

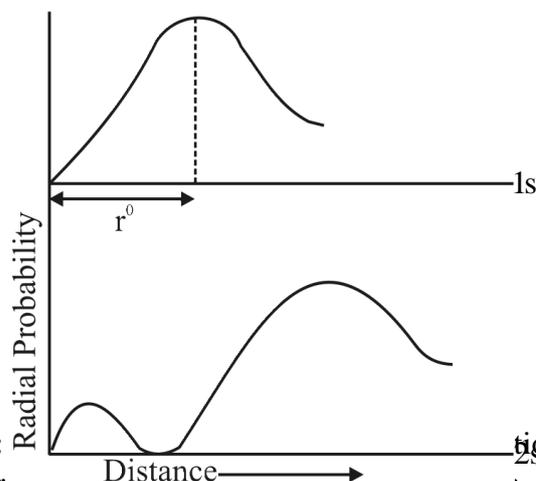
In 1920, a new model of atom was developed by **Ervin Schrodinger**. In the atomic model proposed by Schrodinger, idea of quantization and conclusions of de Broglie principle and Heisenberg uncertainty principle were incorporated. In this model the behaviour of the electron in an atom is described by the mathematical equation known as **Schrodinger Wave Equation**, given below:

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

Here, in this equation, x, y and z are the three space co-ordinates, m = mass of electron, h = Planck's constant, E = total energy, U = Potential energy, ψ = wave function of electron wave. The permitted solutions of **Schrodinger wave equation** are known as **wave functions** which correspond to a definite energy state of an electron known as **orbital**. Thus, the discrete Bohr orbits are replaced by orbitals, *i.e.*, "three dimensional region of definite shape about the nucleus where the electron density is maximum or where the probability of finding an electron is maximum or where the electron passes its maximum time."

The Schrodinger wave equation may simply be interpreted by stating that a particle or body of mass m , energy E and velocity v possesses wave like properties associated with it, with amplitude given by the wave function ψ (Psi).

- ★ ψ (Psi) gives the three dimensional amplitude of electron wave.
- ★ $\psi^2 dV$ is the probability of finding an electron in a volume dV about the nucleus of an atom.
- ★ The particular wave of ψ is called **eigen function** and the value of energy corresponding to this is called **eigen value**.
- ★ The eigen function of an electron is called atomic orbital.
- ★ The wave equation is applicable to atoms as well as molecules.
- ★ The solution of wave equation gives regions in space where ψ is +ve as well as -ve . But ψ^2 (probability of finding an electron) is always positive.



Probability Distribution : An atomic orbital is described by a wave function, ψ . ψ has no physical significance and refers to the amplitude of the electron wave. However, ψ^2 is a significant term and gives the probability of finding an electron or intensity of electron. An atomic orbital is a three-dimensional region of definite shape about the nucleus where there is more intensity of electrons. An atomic orbital is considered as a diffused electron cloud having more electron density close to the nucleus. The probability of finding an electron in a given volume about the nucleus is understood best in the form of radial probability distribution curves. The probability distribution curves for some orbitals are given below. The distance of maximum radial probability is the radius of an atom. The point at which radial probability becomes zero is known as *Nodal point*. In general, there are $(n - 1)$ nodal points for s-orbitals; $(n - 2)$ for p-orbitals; $(n - 3)$ for d-orbitals and $(n - 4)$ for f-orbitals ($n =$ principal quantum number).

- ✪ The radius of maximum probability of 1s electron is 0.53 \AA (Bohr radius).
- ✪ The number of regions of maximum probability for 1s, 2p, 3d, and 4f orbitals are one each.
- ✪ For 2s, 3p, 4d and 5f-atomic orbitals there are two regions of maximum probability.
- ✪ The small humps in the distribution curves show that the electron has a tendency to penetrate closer to the nucleus.
- ✪ In between the regions of maximum electron density, there is a region of zero electron density known as **nodal point**. Greater the number of nodal points, higher is the energy of an orbital.

❖ VIDEO-LINKS

LINK-1 : https://www.youtube.com/playlist?list=PLF_7kfnwLFCFnjki8KSeTQHyJ7OkdBdNA

DAY-2

❖ TEACHING MATERIAL

QUANTUM NUMBERS : In order to define the 'state' of an electron in an atom, a set of four numbers is required known as Quantum numbers. The term 'state' includes, the energy, position with respect to the nucleus, orientation in space and the interaction of the electron with other electrons.

- (i) **Principal Quantum Number (n) :** This quantum number was introduced by Bohr. It gives the average distance of the electron from the nucleus. It also indicates the average volume of the electron

cloud. It determines the main energy shell in which the electron is revolving round the nucleus. 'n' will have positive integral values only $n \neq 0$.

The main energy level (shell) corresponding to different values of n are:

Principal Quantum Number (n)	Main Energy Level
n = 1	K- shell
n = 2	L- shell
n = 3	M- shell
n = 4	N- shell

- ★ Energy of electron in 'n'th shell of hydrogen atom and like ions is $E_n = -\frac{13.6Z^2}{n^2}$ eV/ atom where 'Z' is the atomic number.
 - ★ As the distance of the electron from the nucleus increases, energy of electron also increases.
 - ★ Energy of electron increases with increasing values of "n".
 - ★ Energy of electron at infinite distance from the nucleus is zero.
 - ★ Total number of electrons in nth shell is $2n^2$.
 - ★ The angular momentum of an electron in an orbit depends upon its principal quantum number and is given by $mvr = \frac{nh}{2\pi}$ where 'n' is principal quantum number.
- (ii) **Azimuthal, Angular, Secondary, Subsidiary or Serial Quantum Number (l) :** It was given by Sommerfeld. It explains the fine spectrum of hydrogen atom. It gives the angular momentum of electron in elliptical orbit while in motion round the nucleus. It also gives the shape of the sub-shell in which the electron is located. It (l) may have any +ve integral value ranging from 0 to (n - 1).
- ★ The total values of l are equal to the Principle quantum number of 'n'.
 - ★ Principal Quantum number (n) and azimuthal Quantum number (l) can never have identical numerical values.
 - ★ The orbital angular momentum of an electron depends upon the azimuthal quantum number (l) and is given by:
 - ★ Orbital angular momentum = $\sqrt{l(l+1)} \cdot \frac{h}{2\pi} = \sqrt{l(l+1)} \cdot h$ (where h cross + $h = \frac{h}{2\pi}$).
 - ★ The total number of subshells (l) in a shell (n) is equal to shell number.
 - ★ The various sub shells corresponding to different values of 'l' are as follows:

Azimuthal Q. Number (l)	Sub-shell	Shape	Max. number of electrons
$l = 2$	s-	Symmetrically spherical shape	2
$l = 1$	p-	Dumb-bell	6
$l = 2$	d-	Double dumb-bell	10
$l = 3$	f-	Complicated shape	14
$l = 4$	g-	Highly complicated shape	18

The various shells are comprised of the following sub-shells:

(a)	$n = 1$	K-shell	Designation
	$l = 0$	s-sub-shell	1s
(b)	$n = 2,$	L-shell	
	$l = 0$	s-sub-shell	2s -
	$l = 1$	p-sub-shell	2p -
			not 2d
(c)	$n = 3$	M-shell	3s -
	$l = 0$	s-sub-shell	3p -
	$= 1$	p-sub-shell	3d -
	$= 2$	d-sub-shell	not 3f
(d)	$n = 4,$	N-shell	4s -
	$l = 0$	s-sub-shell	4p -
	$= 1$	p-sub-shell	4d -
	$= 2$	d-sub-shell	4f -
	$= 3$	f-sub-shell	

★ Increasing order of energy of subshells is :

$$s < p < d < f.$$

★ Decreasing order of screening effect :

$$s > p > d > f$$

❖ VIDEO-LINKS

LINK – 1 : https://www.youtube.com/playlist?list=PLF_7kfnwLFCFnjki8KSeTOHyJ7OkdBdNA

DAY-3

❖ TEACHING MATERIAL

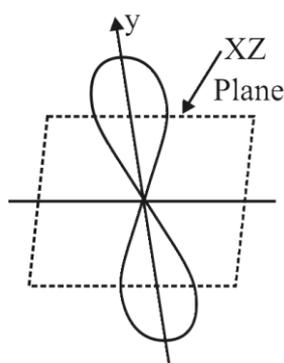
(iii) **Magnetic or Orientation Quantum Number (m):** It explains Zeeman effect. It gives the atomic orbital in which the electron is present. It specifies the orientations of atomic orbitals in a magnetic field. The values of 'm' vary from $-l$, through 0 to $+l$. Thus, the total values of m are $(2l + 1)$.

A subshell is made up of atomic orbitals which are described as follows:

Sub-shell (l)	Values of m (magnetic quantum number)	Atomic orbitals	Designations
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$l = 0$	$m = 0$	1	s
$l = 1$	$m = -1, 0, +1$	3	p_x, p_z, p_y
$l = 2$	$m = -2, -1, 0, +1, +2$	5	$d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_z^2$
$l = 3$	$m = 0, \pm 1, \pm 2, \pm 3$	7	Complicated

- ✪ The atomic orbitals p_x , p_y and p_z are dumb-bell shaped and possess equal energies but differ in their orientations in space. They are called degenerate orbitals.
- ✪ The plane where the electron density is almost zero is called nodal plane.
- ✪ Number of nodal plane for np orbital = 1.
- ✪ Pictorial representation of nodal plane:
- ✪ For p_y atomic orbital xz plane is the nodal plane :



Orbital	Designation of nodal plane
$2p_x$ or $3p_x$ etc.	yz
$2p_y$ or $3p_y$ etc.	xz
$2p_z$ or $3p_z$ etc.	xy

- ✪ The atomic orbitals d_{xy} , d_{xz} , d_{yz} , $d_{x^2-y^2}$ and d_z^2 are also degenerate (possess equal energies).
- ✪ The probability of finding the electron in the xy plane in the atomic orbital, $d_{x^2-y^2}$ is not zero.
- ✪ The atomic orbital having doughnut or a belly band or baby soother like shape is d_z^2 . It is dumb-bell shaped with a collar of high electron density in the xy plane.
- ✪ Nodal planes for d_{xy} , d_{yz} and d_{xz} orbitals are 2 each.
- ✪ Orbital Nodal plane
- d_{xy} xz and yz planes
- d_{xz} xy and yz planes
- d_{yz} xy and xz planes
- ✪ f -orbitals are seven in number designated as,

$$f_{x^3}, f_{y^3}, f_{z^3}, f_{x^2-y^2}, f_{x^2-z^2}, f_{z^2-x^2}, f_{xyz}$$

Spin quantum Number (s) : While in motion around the nucleus, the electron spins about its own axis. The spin may be clockwise or anticlockwise. The spinning electron would add to the angular momentum of the electron and therefore changes the energy associated with the electron. Assuming

the spin to be quantized, there are two possible values of s , i.e. $s = +\frac{1}{2}$ and $-\frac{1}{2}$ depending upon whether the electron spins clockwise or anticlockwise. As a convention, the clockwise and anticlockwise spins are represented by an arrow (\uparrow) and (\downarrow) respectively. Two electrons having the same direction of spin are said to have parallel spins while the two having different direction of spins are said to have anti-parallel spins.

For each value of 'm' there are two values of spin quantum number, $s = +\frac{1}{2}$ and $-\frac{1}{2}$ i.e. in any atomic orbital only two electrons can be accommodated having anti-parallel ($\uparrow\downarrow$) spin.

- ✪ The solution of Schrodinger wave equation gives the principal (n), azimuthal (l) and magnetic quantum numbers (m) but not the spin quantum number (s). It was introduced on account of the spin of revolving electron.

Significance of Quantum Numbers. The four quantum numbers are of physical significance. They give the address of an electron i.e. they are capable of indicating the probable position (shell, sub-shell, atomic orbital) and energy of an electron in the atom. For example, if for an electron.

$n = 3, l = 1, m = -1$, and $s = +\frac{1}{2}$, then it indicates that the electron is:

- present in the third shell (M-shell)
- present in the 3p sub-shell (since for p, $l = 1$)
- present in the $3p_x$ or $3p_y$ atomic orbital
- spinning in clockwise direction

❖ VIDEO-LINKS

LINK-1: https://www.youtube.com/playlist?list=PLF_7kfnwLFCFnji8KSeTQHyJ7OkdBdNA

DAY-4

❖ TEACHING MATERIAL

Pauli's Exclusion Principle: This principle states, "No two electrons in an atom can have an identical set of all the four quantum numbers". If three quantum numbers are the same, the fourth will definitely be different. This principle shows that an atomic orbital cannot have more than two electrons and if there are two electrons in any atomic orbital, they will have anti parallel spins. This principle is very helpful in determining the maximum number of electrons in a shell or a sub-shell. For example:

For First Energy Level (K-Shell):

$n = 1, l = 0$, (1 s-sub-shell), $m = 0$ (1 s -atomic orbital) $s = \pm\frac{1}{2}$ (Two electrons having opposite spins)

These electrons are designated as $1s^2$

For Second Energy Level (L-Shell):

Principal Q. number(n)	Azimuthal Q. number (l)	Magnetic Q. number (m)	spin Q. number(s)	Designation
$n = 2$	$l = 0$ (2s)	$m = 0$ (2s)	$\pm \frac{1}{2}$	$2s^2$
	l (2p)	$m = -1$ (2p _x)	$\pm \frac{1}{2}$	$2p^6$
		$m = 0$ (2p _z)	$\pm \frac{1}{2}$	
		$m = 1$ (2p _y)	$\pm \frac{1}{2}$	

- ✪ Total electrons in second shell are eight.
- ✪ Similarly, it can be shown that d-sub-shell ($l = 2$) can accommodate 10 and f-subshell can have a maximum of fourteen (14) electrons.

Shielding or Screening Effect: According to the screening rule, “the electrons in the completely filled inner shells screen the outer electrons against the attraction by the nucleus”, i.e. the outer electrons are not attracted by the nucleus so effectively as they would have been attracted had the inner shell electrons not been present. This is known as **Shielding or Screening Effect**. Due to this effect, the ns orbitals are filled with electrons earlier than the $(n - 1)$ d -orbitals. In a similar way the 5s, 5p and 6s-orbitals are occupied by electrons before the 4f-orbitals.

- ✪ In a given shell, the decreasing order of screening effect is : $s > p > d > f$.

❖ VIDEO-LINKS

LINK – 1 : https://www.youtube.com/playlist?list=PLF_7kfnwLFCFnjki8KSeTQHjYJ7OkdBdNA

DAY-5

❖ TEACHING MATERIAL

ELECTRONIC CONFIGURATION OF ELEMENTS:

The distribution of electrons in various shells and sub-shells is called electronic configuration of elements. This arrangement of electrons in the atom decides the properties of an element. The following rules are used for writing the electronic configuration:

1. **Aufbau’s Principle:** Aufbau is not the name of any Scientist. It is a German word which means ‘building up’ or ‘construction’. According to this principle, “sub-shells are filled with electrons in the increasing order of their energies”, i.e. Sub-shell of lower energy will be filled first with electrons.
 - ✪ Sub-shell having lower value of $(n + l)$ will be of lower energy, where n is the principal and l , the azimuthal quantum number for the sub-shell.
 - ✪ When the values of $(n + l)$ for two or more sub-shells available for electrons, are the same, then that having lower value of ‘ n ’ will be of lower energy and hence will be occupied by the electrons first.
2. **Hund’s Rule of Maximum Multiplicity:** According to this rule, “pairing of electrons in a sub-shell starts after all the available atomic orbitals of that sub-shell are singly filled (half-filled) with

electrons having parallel spins” or pairing of electrons in a sub-shell is impossible in the presence of vacant atomic orbitals in that sub-shell”.

- ✪ In p-sub shell, the fourth electron starts pairing, and the sixth electron starts pairing in d-sub-shell.
 - ✪ In f-sub-shell, pairing starts with eight electron.
 - ✪ This rule gives the number of unpaired electrons in an atom, ion or molecule.
3. Exactly half-filled sub-shells have lesser energy and thus assume more stability than any other arrangement. Thus, p^3 is more stable arrangement than p^2 , p^4 or p^5 .
 4. When the electronic configuration ns^2np^6 is attained in the outermost shell of an atom, the next incoming electron enters the $(n + 1)$ s-sub-shell. The nd and nf -sub- shells will be vacant.

Electronic configuration of the Elements

Element	Symbol	At. No.	Electronic Configuration
Hydrogen	H	1	$1s^2$
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^2, 2s^1$
Beryllium	Be	4	$1s^2, 2s^2$
Boron	B	5	$1s^2, 2s^2, 2p^1$
Carbon	C	6	$1s^2, 2s^2, 2p^2$
Nitrogen	N	7	$1s^2, 2s^2, 2p^3$
Oxygen	O	8	$1s^2, 2s^2, 2p^4$
Fluorine	F	9	$1s^2, 2s^2, 2p^5$
Neon	Ne	10	$1s^2, 2s^2, 2p^6$
Sodium	Na	11	$1s^2, 2s^2, p^6, 3s^1$
Magnesium	Mg	12	$1s^2, 2s^2, p^6, 3s^2$
Aluminium	Al	13	$1s^2, 2s^2, p^6, 3s^2, 3p^1$
Silicon	Si	14	$1s^2, 2s^2, p^6, 3s^2, 3p^2$
Phosphorus	P	15	$1s^2, 2s^2, p^6, 3s^2, 3p^3$
Sulphur	S	16	$1s^2, 2s^2, p^6, 3s^2, 3p^4$
Chlorine	Cl	17	$1s^2, 2s^2, p^6, 3s^2, 3p^5$
Argon	Ar	18	$1s^2, 2s^2, p^6, 3s^2, 3p^6$
Potassium	K	19	$1s^2, 2s^2, p^6, 3s^2, p^6, 4s^1$
Calcium	Ca	20	$1s^2, 2s^2, p^6, 3s^2, p^6, 4s^2$
Scandium	Sc	21	$1s^2, 2s^2, p^6, 3s^2, p^6, d^1, 4s^2$
Titanium	Ti	22	$1s^2, 2s^2, p^6, 3s^2, p^6, d^2, 4s^2$
Vanadium	V	23	$1s^2, 2s^2, p^6, 3s^2, p^6, d^3, 4s^2$
Chromium	Cr	24	$1s^2, 2s^2, p^6, 3s^2, p^6, d^5, 4s^1$
Manganese	Mn	25	$1s^2, 2s^2, p^6, 3s^2, p^6, d^5, 4s^2$
Iron	Fe	26	$1s^2, 2s^2, p^6, 3s^2, p^6, d^6, 4s^2$
Cobalt	Co	27	$1s^2, 2s^2, p^6, 3s^2, p^6, d^7, 4s^2$
Nickel	Ni	28	$1s^2, 2s^2, p^6, 3s^2, p^6, d^8, 4s^2$
Copper	Cu	29	$1s^2, 2s^2, p^6, 3s^2, p^6, d^{10}, 4s^1$
Zinc	Zn	30	$1s^2, 2s^2, p^6, 3s^2, p^6, d^{10}, 4s^2$
Gallium	Ga	31	$1s^2, 2s^2, p^6, 3s^2, p^6, d^{10}, 4s^2, p^1$
Germanium	Ge	32	$1s^2, 2s^2, p^6, 3s^2, p^6, d^{10}, 4s^2, p^2$
Arsenic	As	33	$1s^2, 2s^2, p^6, 3s^2, p^6, d^{10}, 4s^2, p^3$
Selenium	Se	34	$1s^2, 2s^2, p^6, 3s^2, p^6, d^{10}, 4s^2, p^4$

- Example 17** (a) A compound of vanadium has a magnetic moment of 1.73 BM. Find the electronic configuration of vanadium ion in the compound
 (b) Name the orbitals corresponding to given set of quantum numbers

- (a) $n = 3, l = 2, m = \pm 2$ (b) $n = 4, l = 0, m = 0$
 (c) $n = 2, l = 1, m = \pm 1$ (d) $n = 2, l = 1, m = 2$

Solution

(a) Magnetic moment = $\sqrt{n(n+2)}$ where n = number of unpaired electrons

$$\therefore \sqrt{n(n+2)} = 1.73 \Rightarrow n^2 + 2n = (1.73)^2 \therefore n = 1$$

Therefore vanadium atom must have one unpaired electron and thus its electronic configuration ${}_{23}\text{V}^{4+} : 1s^2 2s^2 2p^6 3s^2 3p^6 3d^1$

- (b) (a) $3dx^2 - y^2$ or $3dxy$ (b) $4s$ (c) $2p_x$ or $2p_y$ (d) no such orbital

Example 18

(a) Find the orbital angular momentum of an electron in the following orbital

- (i) $3p$ (ii) $3d$ (iii) $3s$

(b) Arrange the electrons represented by the following sets of quantum number in decreasing order of energy

- (i) $n = 4, l = 0, m = 0, m_s = \pm 1/2$ (ii) $n = 3, l = 2, m = 0, m_s = \pm 1/2$
 (iii) $n = 3, l = 0, m = 0, m_s = -1/2$ (vi) $n = 3, l = 0, m = 0, m_s = -1/2$

Solution

(a) $u = \sqrt{l(l+1)} \frac{h}{2\pi} = \sqrt{l(l+1)} h$ (i) For $3p, l = 1 \mu_l = \sqrt{l(l+1)} = \sqrt{2} h$

(ii) For $3d, l = 2 \mu_l = \sqrt{2(2+1)} = \sqrt{6} h$ (iii) For $3s, l = 0, \mu_l = 0$

(b) Higher is the value of $(n+l)$ higher is the energy; if $(n+l)$ are same, higher the n values, higher the energy

For (i) $(n+l) = 4$ $4s$ orbital **For (ii)** $(n+l) = 5$ $3d$ orbital

For (iii) $(n+l) = 4$ $3p$ orbital **For (iv),** $(n+l) = 3$ $3s$ orbital

Decreasing order of energy = (i) > (ii) > (iii) > (iv)

Example 19

Why electron cannot exist inside the nucleus according to Heisenberg's uncertainty principle?

Solution

Diameter of the atomic nucleus is of the order of $10^{-15} m$. The maximum uncertainty in the position of electron is $10^{-15} m$. Mass of electron = $9.1 \times 10^{-31} kg$.

$$\Delta x \cdot \Delta p = \frac{h}{4\pi} \quad \Delta x \times (m \cdot \Delta v) = h/4\pi \quad \Delta v = \frac{h}{4\pi} \times \frac{1}{\Delta x \cdot m} = \frac{6.63 \times 10^{-34}}{4 \times \frac{22}{7}} \times \frac{1}{10^{-15} \times 9.1 \times 10^{-31}}$$

$$\Delta v = 5.80 \times 10^{10} ms^{-1}$$

This value is much higher than the velocity of light and hence not possible.

Example 20

How many 7s electron are there in an atom with Z = 104?

Solution

The electronic configuration of the said element is:

$$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^2, 4p^6, \\ 4d^{10}, 4f^{14}, 5s^2, 5p^6, 5d^{10}, 5f^{14}, 6s^2, 6p^6, 6d^2, 7s^2$$

Hence, there are two 7s electrons.

Classroom Practice Paper

1. (True/False): A single photon excites only a single electron.
2. According de Broglie the wavelength of a particle is given by $\lambda =$ _____.
3. The minimum value of the product of uncertainty in position and momentum is _____.
4. The shape of p-orbital is _____.
5. (True/False) The energy of s-orbital is lower than the energy of p-orbital.

❖ VIDEO-LINKS

LINK -1 : https://www.youtube.com/playlist?list=PLF_7kfnwLFCFnjki8KSeTQHjJ7OkdBdNA