Unit 2

Quantum Mechanical Model of Atom

Erwin Schrödinger
(1887 - 1961)

Erwin Schrödinger was awarded the Nobel Prize in physics in 1933 for "the discovery of new productive forms of atomic theory". Schrödinger had wide interests starting from chemistry, physics, maths and botany. He was not satisfied with the quantum condition in Bohr's orbit theory and believed that atomic spectra should really be determined by some kind of eigenvalue problem and proposed the wave equation, now named after him.

Learning Objectives:

After studying this unit, students will be able to

- Recognise various atomic models
- Explain the dual behaviour of matter
- Derive de Broglie equation and solve numerical problems
- Explain Heisenberg's uncertainty principle and solve related problems
- Appreciate the significance of quantum numbers
- Summarise important features of quantum mechanical model of atom
- Draw the shapes of various atomic orbitals
- Explain the Aufbau principle
- Describe Hund's rule and Pauli's exclusion principle
- Apply the relevant rules for filling electrons in atoms and write the electronic configuration of various atoms

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2.1 Introduction to atom models:

Let us recall the history of the development of atomic models from the previous classes. We know that all things are made of matter. The basic unit that makes up all matter is atom. The word 'atom' has been derived from the Greek word '*a-tomio*' meaning non-divisible. Atom was considered as non-divisible until the discovery of sub-atomic particles such as electron, proton and neutron. J. J. Thomson's cathode ray experiment revealed that atoms consist of negatively charged particles called electrons. He proposed that atom is a positively charged sphere in which the electrons are embedded like the seeds in the watermelon. Later, Rutherford's α-ray scattering experiment results proved that Thomson's model was wrong. Rutherford bombarded a thin gold foil with a stream of fast moving α–particles. It was observed that

(i) most of the α–particles passed through the foil

(ii) some of them were deflected through a small angle and

(iii) very few α–particles were reflected back by 180°

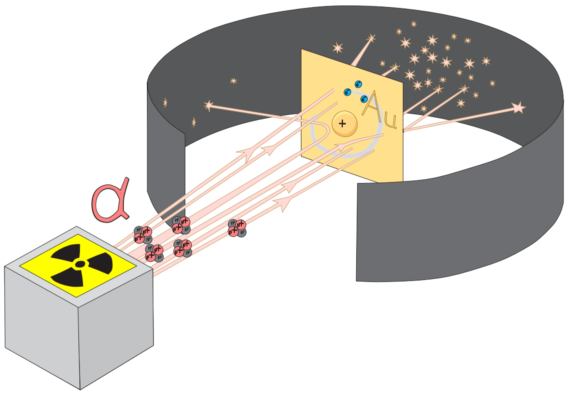


Figure. 2.1 Rutherford's α-ray scattering experiment

Based on these observations, he proposed that in an atom there is a tiny positively charged nucleus and the electrons are moving around the nucleus with high speed. The theory of electromagnetic radiation states that a moving charged particle should continuously loose its energy in the form of radiation. Therefore, the moving electron in an atom should continuously loose its energy and finally collide with nucleus resulting in the collapse of the atom. However, this doesn't happen and the atoms are stable. Moreover, this model does not explain the distribution of electrons around the nucleus and their energies.

2.1.1 Bohr atom model:

The work of Planck and Einstein showed that the energy of electromagnetic radiation is quantised in units of $h\nu$ (where ν is the frequency of radiation and h is Planck's constant 6.626×10^{-34} Js). Extending Planck's quantum hypothesis to the energies of atoms, Niels Bohr proposed a new atomic model for the hydrogen atom. This model is based on the following assumptions:

1. The energies of electrons in an atom are quantised.
2. The electron is revolving around the nucleus in a certain circular path of fixed energy called stationary orbit.
3. Electron can revolve only in those orbits in which the angular momentum (mvr) of the electron must be equal to an integral multiple of $h/2\pi$.

i.e. $mvr = nh/2\pi$ -------- (2.1)

where n = 1,2,3,...etc.,

4. As long as an electron revolves in the fixed stationary orbit, it doesn't lose its energy. However, when an electron jumps from higher energy state (E_2) to a lower energy state (E_1), the excess energy is emitted as radiation. The frequency of the emitted radiation is

$$E_2 - E_1 = h\nu$$

and

$$\nu = \frac{(E_2 - E_1)}{h} \text{ -------- } (2.2)$$

Conversely, when suitable energy is supplied to an electron, it will jump from lower energy orbit to a higher energy orbit.

Applying Bohr's postulates to a hydrogen like atom (one electron species such as H, He^+ and Li^{2+} etc..) the radius of the nth orbit and the energy of the electron revolving in the nth orbit were derived. The results are as follows:

$$r_n = \frac{(0.529)n^2}{Z} \text{Å} \text{ ---------------- } (2.3)$$

$$E_n = \frac{(-13.6)\,Z^2}{n^2} \text{eV atom}^{-1} \text{ --------}(2.4)$$

(or)

$$E_n = \frac{(-1312.8)\,Z^2}{n^2} \text{kJ mol}^{-1} \text{ --------}(2.5)$$

The detailed derivation of r_n and E_n will be discussed in 12th standard atomic physics unit.

2.1.2 Limitation of Bohr's atom model:

The Bohr's atom model is applicable only to species having one electron such as hydrogen, Li^{2+} etc... and not applicable to multi electron atoms. It was unable to explain the splitting of spectral lines in the presence of magnetic field (Zeeman effect) or an electric field (Stark effect). Bohr's theory was unable to explain why the electron is restricted to revolve around the nucleus in a fixed orbit in which the angular momentum of the electron is equal to $nh/2\pi$ and a logical answer for this, was provided by Louis de Broglie.

2.2 Wave particle duality of matter

Albert Einstein proposed that light has dual nature. i.e. light photons behave both like a particle and as a wave. Louis de Broglie extended this concept and proposed that all forms of matter showed dual character. To quantify this relation, he derived an equation for the wavelength of a matter wave. He combined the following two equations of energy of which one represents wave character ($h\upsilon$) and the other represents the particle nature (mc^2).

(i) Planck's quantum hypothesis:

$$E = h\nu \text{ -------- } (2.6)$$

(ii) Einstein's mass-energy relationship

$$E = mc^2 \text{ ---------}(2.7)$$

From (2.6) and (2.7)

$$h\nu = mc^2$$

$$hc/\lambda = mc^2$$

$$\lambda = h / mc \text{ ------------}(2.8)$$

The equation 2.8 represents the wavelength of photons whose momentum is given by mc (Photons have zero rest mass)

For a particle of matter with mass m and moving with a velocity v, the equation 2.8 can be written as

$$\lambda = h / mv \text{ ------------ } (2.9)$$

This is valid only when the particle travels at speeds much less than the speed of Light.

This equation implies that a moving particle can be considered as a wave and a wave can exhibit the properties (i.e momentum) of a particle. For a particle with high linear momentum (mv) the wavelength will be so small and cannot be observed. For a microscopic particle such as an electron, the mass is of the order of 10^{-31} kg, hence the wavelength is much larger than the size of atom and it becomes significant.

Let us understand this by calculating de Broglie wavelength in the following two cases:

(i) A 6.626 kg iron ball moving at10 ms^{-1}

(ii) An electron moving at 72.73 ms^{-1}

$\lambda_{\text{iron ball}} = h/mv$

$$= \frac{6.626 \times 10^{-34}\,kgm^2s^{-1}}{6.626\,kg \times 10\,ms^{-1}} = 1 \times 10^{-35}\text{ m}$$

$\lambda_{\text{electron}} = h/mv$

$$= \frac{6.626 \times 10^{-34}\,kgm^2s^{-1}}{9.11 \times 10^{-31}\,kg \times 72.73\,ms^{-1}}$$

$$= \frac{6.626}{662.6} \times 10^{-3}\text{ m} = 1 \times 10^{-5}\text{m}$$

For the electron, the de Broglie wavelength is significant and measurable while for the iron ball it is too small to measure, hence it becomes insignificant.

Evaluate Yourself

1. Calculate the de-Broglie wavelength of an electron that has been accelerated from rest through a potential difference of 1 keV.

2.2.1 Quantisation of angular momentum and de Broglie concept:

According to the de Broglie concept, the electron that revolves around the nucleus exhibits both particle and wave character. In order for the electron wave to exist in phase, the circumference of the orbit should be an integral multiple of the wavelength of the electron wave. Otherwise, the electron wave is out of phase.

Circumference of the orbit $= n\lambda$

$$2\pi r = n\lambda \text{ ------------}(2.10)$$

$$2\pi r = nh/mv$$

Rearranging,

$$mvr = nh/2\pi \text{ ----------}(2.11)$$

Angular momentum $= nh/2\pi$

The above equation was already predicted by Bohr. Hence, De Broglie and Bohr's concepts are in agreement with each other.

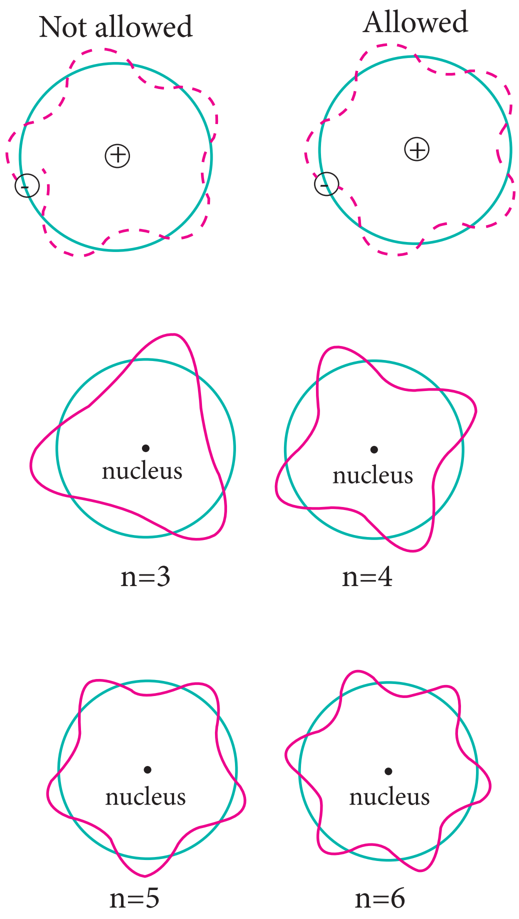


Figure. 2.2 Wave nature of electrons in allowed Bohr orbits

Davison and Germer experiment :

The wave nature of electron was experimentally confirmed by Davisson and Germer. They allowed the accelerated beam of electrons to fall on a nickel crystal and recorded the diffraction pattern. The resultant diffraction pattern is similar to the x-ray diffraction pattern. The finding of wave nature of electron leads to the development of various experimental techniques such as electron microscope, low energy electron diffraction etc…

2.3 Heisenberg's uncertainty principle

The dual nature of matter imposes a limitation on the simultaneous determination of position and momentum of a microscopic particle. Based on this, Heisenberg arrived at his uncertainty principle, which states that 'It is impossible to **accurately** determine both the position and the momentum of a microscopic particle **simultaneously**'. The product of uncertainty (error) in the measurement is expressed as follows.

$$\Delta x.\Delta p \geq h/4\pi \text{ -------- } (2.11)$$

where, Δx and Δp are uncertainties in determining the position and momentum, respectively.

The uncertainty principle has negligible effect for macroscopic objects and becomes significant only for microscopic particles such as electrons. Let us understand this by calculating the uncertainty in the velocity of the electron in hydrogen atom. (Bohr radius of 1st orbit is 0.529 Å) Assuming that the position of the electron in this orbit is determined with the accuracy of 0.5 % of the radius.

Uncertainity in position = Δx

$$= \frac{0.5\,\%}{100\,\%} \text{ x } 0.529 \text{ Å}$$

$$= \frac{0.5}{100} \text{ x } 0.529 \text{ x } 10^{-10} \text{ m}$$

$$\Delta x = 2.645 \text{ x } 10^{-13} \text{ m}$$

From the Heisenberg's uncertainity principle,

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

$$\Delta x.(m.\Delta v) \geq \frac{h}{4\pi}$$

$$\Delta v \geq \frac{h}{4\pi.\,m\,.\,\Delta x}$$

$$\Delta v \geq \frac{6.626 \text{ x } 10^{-34} \text{ kg } m^2 s^{-1}}{4 \text{x } 3.14 \text{ x } 9.11 \text{ x} 10^{-31} \text{ kg x } 2.645 \text{ x } 10^{-13} \text{ m}}$$

$$\Delta v \geq 2.189 \text{ x } 10^8 \text{ ms}^{-1}$$

Therefore, the uncertainty in the velocity of the electron is comparable with the velocity of light. At this high level of uncertainty it is very difficult to find out the exact velocity.

Evaluate Yourself

2. Calculate the uncertainty in the position of an electron, if the uncertainty in its velocity is 5.7×10^5 ms^{-1}.

2.4 Quantum mechanical model of atom – Schrödinger Equation:

The motion of objects that we come across in our daily life can be well described using classical mechanics which is based on the Newton's laws of motion. In classical mechanics the physical state of the particle is defined by its position and momentum. If we know both these properties, we can predict the future state of the system based on the force acting on it using classical mechanics. However, according to Heisenberg's uncertainty principle both these properties cannot be measured simultaneously with absolute accuracy for a microscopic particle such as an electron. The classical mechanics does not consider the dual nature of the matter which is significant for microscopic particles. As a consequence, it fails to explain the motion of microscopic particles. Based on the Heisenberg's principle and the dual nature of the microscopic particles, a new mechanics called quantum mechanics was developed.

Erwin Schrödinger expressed the wave nature of electron in terms of a differential equation. This equation determines the change of wave function in space depending on the field of force in which the electron moves. The time independent Schrödinger equation can be expressed as,

$$\hat{H}\Psi = E\Psi \text{-------} (2.12)$$

Where $\hat{H}$ is called Hamiltonian operator, Ψ is the wave function and is a funciton of position co-ordinates of the particle and is denoted as $\Psi(x,y,z)$ E is the energy of the system

$$\hat{H} = \left[\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V\right]$$

(2.12) can be written as,

$$\left[\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+V\psi\right]=E\psi$$

Multiply by $-\frac{8\pi^2 m}{h^2}$ and rearranging

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

$$\text{------} (2.13)$$

The above schrödinger wave equation does not contain time as a variable and is referred to as time independent Schrödinger wave equation. This equation can be solved only for certain values of E, the total energy. i.e. the energy of the system is quantised. The permitted total energy values are called eigen values and corresponding wave functions represent the atomic orbitals.

2.4.1 Main features of the quantum mechanical model of atom

1. The energy of electrons in atoms is quantised

2. The existence of quantized electronic energy levels is a direct result of the wave like properties of electrons. The solutions of Schrödinger wave equation gives the allowed energy levels (orbits).

3. According to Heisenberg uncertainty principle, the exact position and momentum of an electron can not be determined with absolute accuracy. As a consequence, quantum mechanics introduced the concept of orbital. Orbital is a three dimensional space in which the probability of finding the electron is maximum.

4. The solution of Schrödinger wave equation for the allowed energies of an atom gives the wave function ψ, which represents an atomic orbital. The wave nature of electron present in an orbital can be well defined by the wave function ψ.

5. The wave function ψ itself has no physical meaning. However, the probability of finding the electron in a small volume dxdydz around a point (x,y,z) is proportional to $|\psi(x,y,z)|^2$ dxdydz $|\psi(x,y,z)|^2$ is known as probability density and is always positive.

2.5 Quantum numbers

The electron in an atom can be characterised by a set of four quantum numbers, namely principal quantum number (n), azimuthal quantum number (l), magnetic quantum number (m) and spin quantum number (s). When Schrödinger equation is solved for a wave function Ψ, the solution contains the first three quantum numbers n, l and m. The fourth quantum number arises due to the spinning of the electron about its own axis. However, classical pictures of species spinning around themselves are incorrect.

Principal quantum number (n):

This quantum number represents the energy level in which electron revolves around the nucleus and is denoted by the symbol 'n'.

1. The 'n' can have the values 1, 2, 3,… n=1 represents K shell; n=2 represents L shell and n = 3, 4, 5 represent the M, N, O shells, respectively.

2. The maximum number of electrons that can be accommodated in a given shell is $2n^2$.

3. 'n' gives the energy of the electron, $E_n = \frac{(-1312.8)\,Z^2}{n^2}\,\text{kJ mol}^{-1}$ and the distance of the electron from the nucleus is given by $r_n = \frac{(0.529)n^2}{Z}\,\text{Å}$

Azimuthal Quantum number (*l*) or subsidiary quantum number :

1. It is represented by the letter '*l*', and can take integral values from zero to n-1, where n is the principal quantum number

2. Each *l* value represents a subshell (orbital). *l* = 0, 1, 2, 3 and 4 represents the s, p, d, f and g orbitals respectively.

3. The maximum number of electrons that can be accommodated in a given subshell (orbital) is 2(2*l*+1).

4. It is used to calculate the orbital angular momentum using the expression

$$Angular\ momentum = \sqrt{l(l+1)}\,\frac{h}{2\pi} ----(2.14)$$

Magnetic quantum number (m_l):

1. It is denoted by the letter 'm_l'. It takes integral values ranging from -*l* to +*l* through 0. i.e. if *l*=1; m = -1, 0 and +1
2. Different values of m for a given l value, represent different orientation of orbitals in space.
3. The Zeeman Effect (the splitting of spectral lines in a magnetic field) provides the experimental justification for this quantum number.
4. The magnitude of the angular momentum is determined by the quantum number *l* while its direction is given by magnetic quantum number.

Spin quantum number (m_s):

1. The spin quantum number represents the spin of the electron and is denoted by the letter 'm_s'
2. The electron in an atom revolves not only around the nucleus but also spins. It is usual to write this as electron spins about its own axis either in a clockwise direction or in anti-clockwise direction. The visualisation is not true. However spin is to be understood as representing a property that revealed itself in magnetic fields.
3. Corresponding to the clockwise and anti-clockwise spinning of the electron, maximum two values are possible for this quantum number.
4. The values of 'm_s' is equal to -½ and + ½

Table 2.1 Quantum numbers and its significance

Shell	Principal quantum number (n)	maximum number of electron in a shell (orbital) $2n^2$	Azimuthal quantum number (l) = 0,1.... (n-1)	Maximum no. of electron in a orbital 2 (2*l*+1)	Magnetic quantum number (m) different possible orientation of orbital	Designation of orbitals in a given shell
K	1	$2(1)^2 = 2$	0	2[2(0)+1] = 2	0	1s
L	2	$2(2)^2 = 8$	0	2	0	2s
			1	2[2(1)+1] =6	-1, 0, +1	$2p_y$, $2p_z$, $2p_x$

Shell	Principal quantum number (n)	maximum number of electron in a shell (orbital) $2n^2$	Azimuthal quantum number (l) = 0,1.... (n-1)	Maximum no. of electron in a orbital $2(2l+1)$	Magnetic quantum number (m) different possible orientation of orbital	Designation of orbitals in a given shell
M	3	$2(3)^2 = 18$	0	2	0	3s
			1	6	-1, 0, +1	$3p_y$, $3p_z$,$3p_x$,
			2	2[2(2)+1] = 10	-2, -1, 0, +1, +2	$3d_{x^2-y^2}$, $3d_{yz}$, $3d_{z^2}$, $3d_{zx}$, $3d_{xy}$
N	4	$2(4)^2 = 32$	0	2	0	4s
			1	6	-1, 0, +1	$4p_y$, $4p_z$, $4p_x$
			2	10	-2, -1, 0, +1, +2	$4d_{x^2-y^2}$, $4d_{xy}$, $4d_{z^2}$, $4d_{yz}$, $4d_{zx}$
			3	2[2(3)+1] = 14	-3, -2, -1, 0, +1, +2, +3	$f_{y(3x^2-y^2)}$, $f_{z(x^2-y^2)}$, f_{yz^2}, f_{z^3}, f_{xz^2}, f_{xyz}, $f_{x(x^2-3y^2)}$,

The labels on the orbitals, such as p_x, d_{z^2}, f_{xyz} etc. are not associated with specific 'm' values

Evaluate Yourself

3. How many orbitals are possible in the 4th energy level? (n=4)

2.5.1 Shapes of atomic orbitals:

The solution to Schrödinger equation gives the permitted energy values called eigen values and the wave functions corresponding to the eigen values are called atomic orbitals. The solution (Ψ) of the Schrödinger wave equation for one electron system like hydrogen can be represented in the following form in spherical polar coordinates r, θ, φ as,

$$\Psi(r, \theta, \varphi) = R(r).f(\theta).g(\varphi) \text{ ------ } (2.15)$$

(where R(r) is called radial wave function, other two functions are called angular wave functions)

As we know, the Ψ itself has no physical meaning and the square of the wave function $|\Psi|^2$ is related to the probability of finding the electrons within a given volume of space. Let us analyse how $|\Psi|^2$ varies with the distance from nucleus (radial distribution of the probability) and the direction from the nucleus (angular distribution of the probability).

Radial distribution function:

Consider a single electron of hydrogen atom in the ground state for which the quantum numbers are n=1 and l=0. i.e. it occupies 1s orbital. The plot of $R(r)^2$ versus r for 1s orbital is given in Figure 2.3

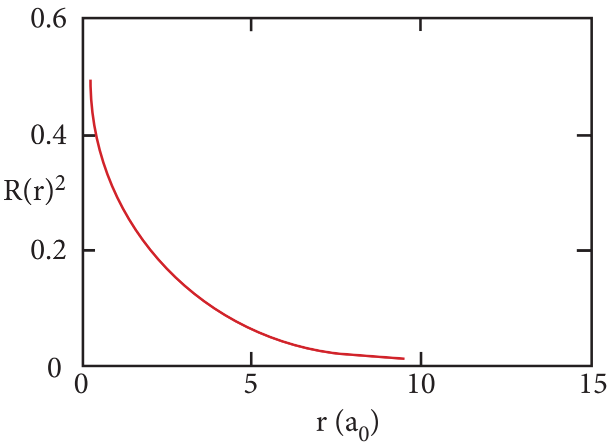


Figure. 2.3 Plot of $R(r)^2$ versus r for 1s orbital of hydrogen

The graph shows that as the distance between the electron and the nucleus decreases, the probability of finding the electron increases. At r=0, the quantity $R(r)^2$ is maximum i.e. The maximum value for $|\Psi|^2$ is at the nucleus. However, probability of finding the electron in a given spherical shell around the nucleus is important. Let us consider the volume (dV) bounded by two spheres of radii r and r+dr.

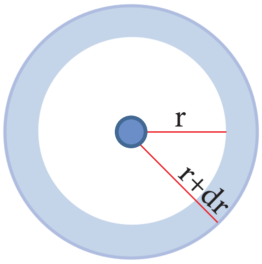


Figure 2.4

Volume of the sphere, $V = \frac{4}{3}\pi r^3$

$$\frac{dV}{dr} = \frac{4}{3}\pi(3r^2)$$

$$dV = 4\pi r^2 dr$$

$$\Psi^2 dV = 4\pi r^2 \Psi^2 dr \quad ---------- (2.16)$$

The plot of $4\pi r^2 . R(r)^2$ versus r is given below.

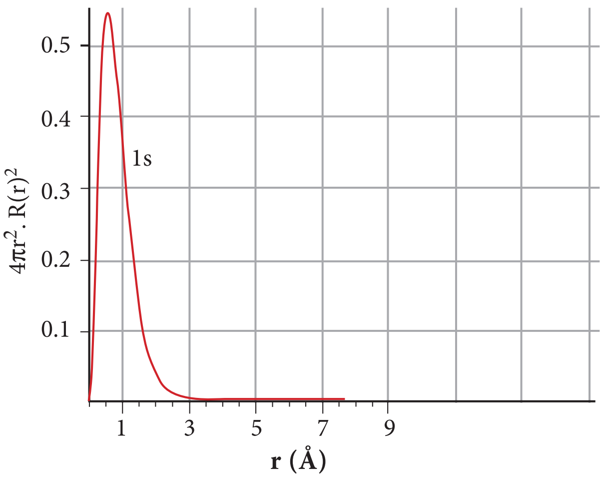


Figure 2.5 Plot of $4\pi r^2 . R(r)^2$ versus r for 1s orbital of hydrogen

The above plot shows that the maximum probability occurs at distance of 0.52 **Å** from the nucleus. This is equal to the Bohr radius. It indicates that the maximum probability of finding the electron around the nucleus is at this distance. However, there is a probability to find the electron at other distances also. The radial distribution function of 2s, 3s, 3p and 3d orbitals of the hydrogen atom are represented as follows.

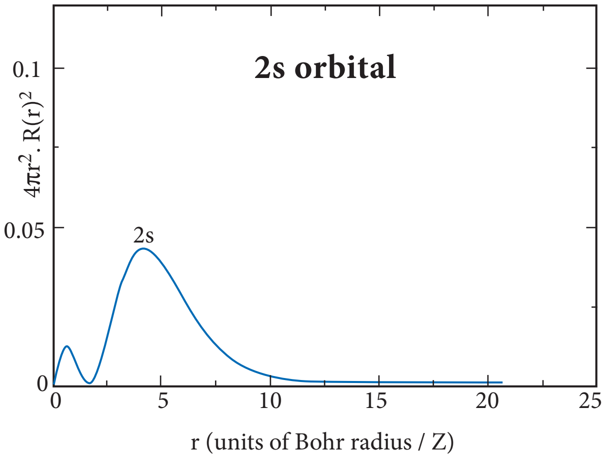


Figure 2.6 (a) - Plot of $4\pi r^2 . R(r)^2$ versus r for 2s orbitals of hydrogen

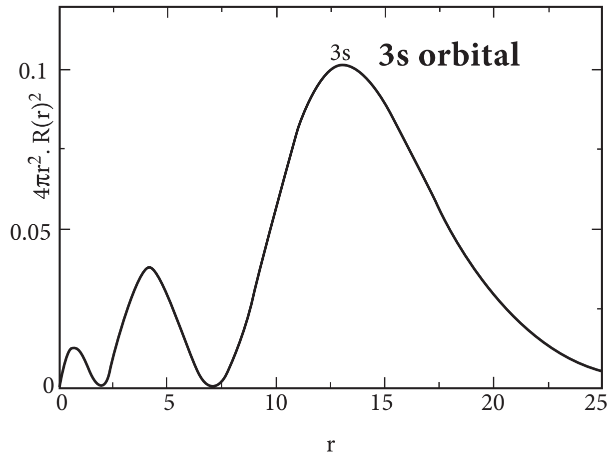


Figure 2.6 (b) - Plot of $4\pi r^2$. $R(r)^2$ versus r for 3s orbitals of hydrogen

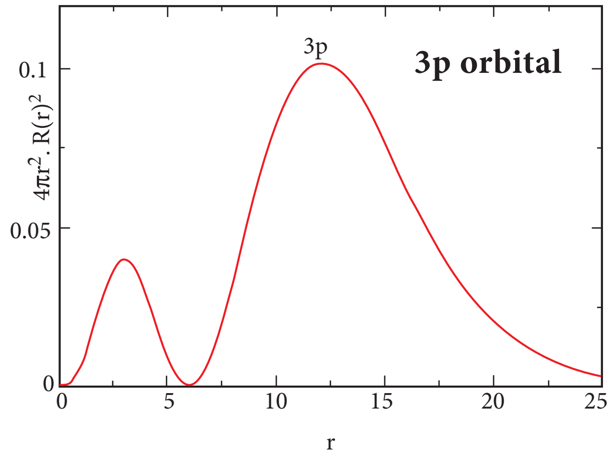


Figure 2.6 (c) - Plot of $4\pi r^2$. $R(r)^2$ versus r for 3p orbitals of hydrogen

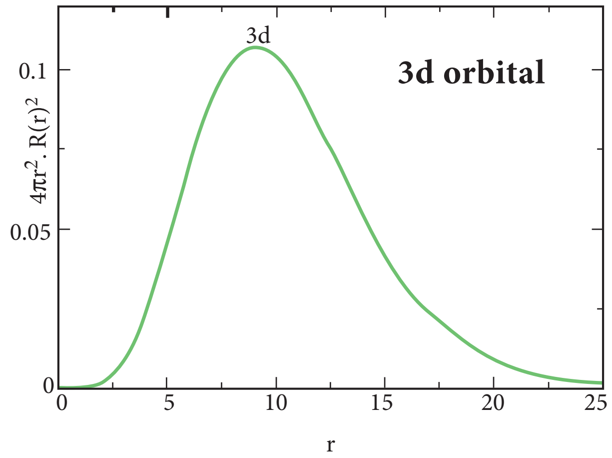


Figure 2.6 (d) - Plot of $4\pi r^2$. $R(r)^2$ versus r for 3d orbitals of hydrogen

For 2s orbital, as the distance from nucleus r increases, the probability density first increases, reaches a small maximum followed by a sharp decrease to zero and then increases to another maximum, after that decreases to zero. The region where this probability density function reduces to zero is called nodal surface or a radial node. In general, it has been found that ns-orbital has (n–1) nodes. In other words, number of radial nodes for 2s orbital is one, for 3s orbital it is two and so on. The plot of $4\pi r^2$. $R(r)^2$ versus r for 3p and 3d orbitals shows similar pattern but the number of radial nodes are equal to($n-l-1$) (where n is principal quantum number and l is azimuthal quantum number of the orbital).

Angular distribution function:

The variation of the probability of locating the electron on a sphere with nucleus at its centre depends on the azimuthal quantum number of the orbital in which the electron is present. For 1s orbital, l=0 and m=0. $f(\theta) = 1/\sqrt{2}$ and $g(\varphi) = 1/\sqrt{2}\pi$. Therefore, the angular distribution function is equal to $1/2\sqrt{\pi}$. i.e. it is independent of the angle θ and φ. Hence, the probability of finding the electron is independent of the direction from the nucleus. The shape of the s orbital is spherical as shown in the figure 2.7

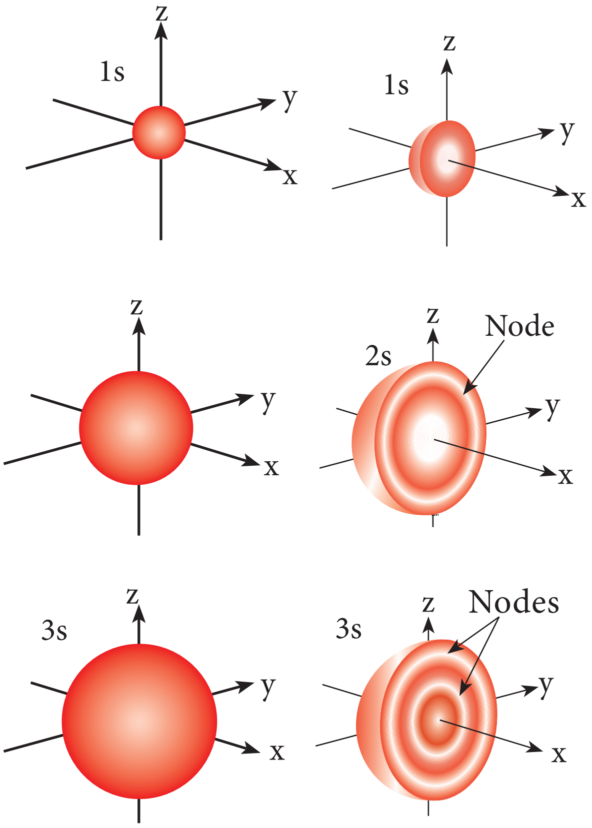
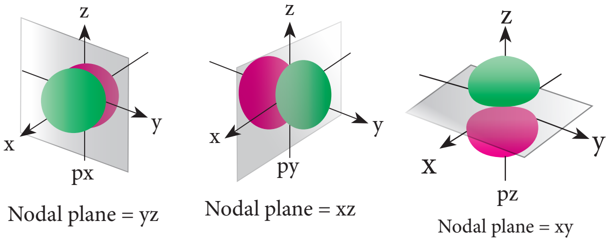


Figure 2.7 Shapes of 1s, 2s and 3s orbitals

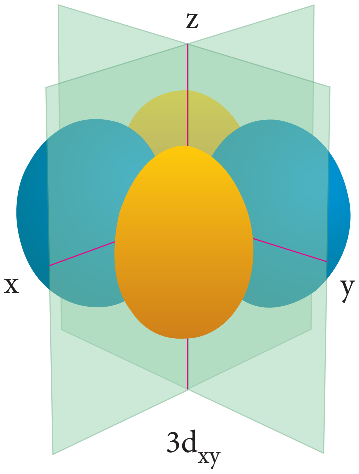
For p orbitals l=1 and the corresponding m values are -1, 0 and +1. The angular distribution functions are quite complex and are not discussed here. The shape of the p orbital is shown in Figure 2.8. The three different m values indicates that there are three different orientations possible for p orbitals. These orbitals are designated as p_x, p_y and p_z and the angular distribution for these orbitals shows that the lobes are along the x, y and z axis respectively. As seen in the Figure 2.8 the 2p orbitals have one nodal plane.

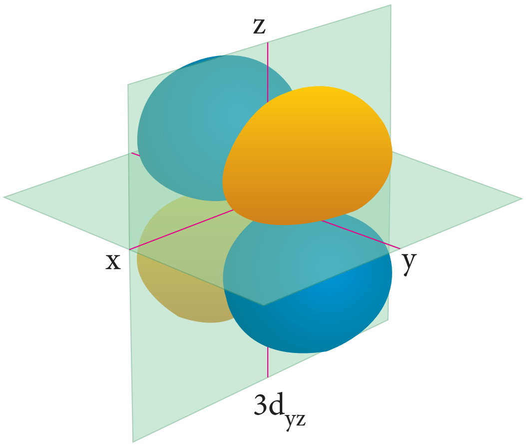


(b) Cartoon representations of 2p orbitals

Figure 2.8 Shapes of 2p orbitals

For 'd' orbital l = 2 and the corresponding m values are -2, -1, 0 +1,+2. The shape of the d orbital looks like a 'clover leaf'. The five m values give rise to five d orbitals namely d_{xy} , d_{yz}, d_{zx}, $d_{x^2-y^2}$ and d_{z^2}. The 3d orbitals contain two nodal planes as shown in Figure 2.9.





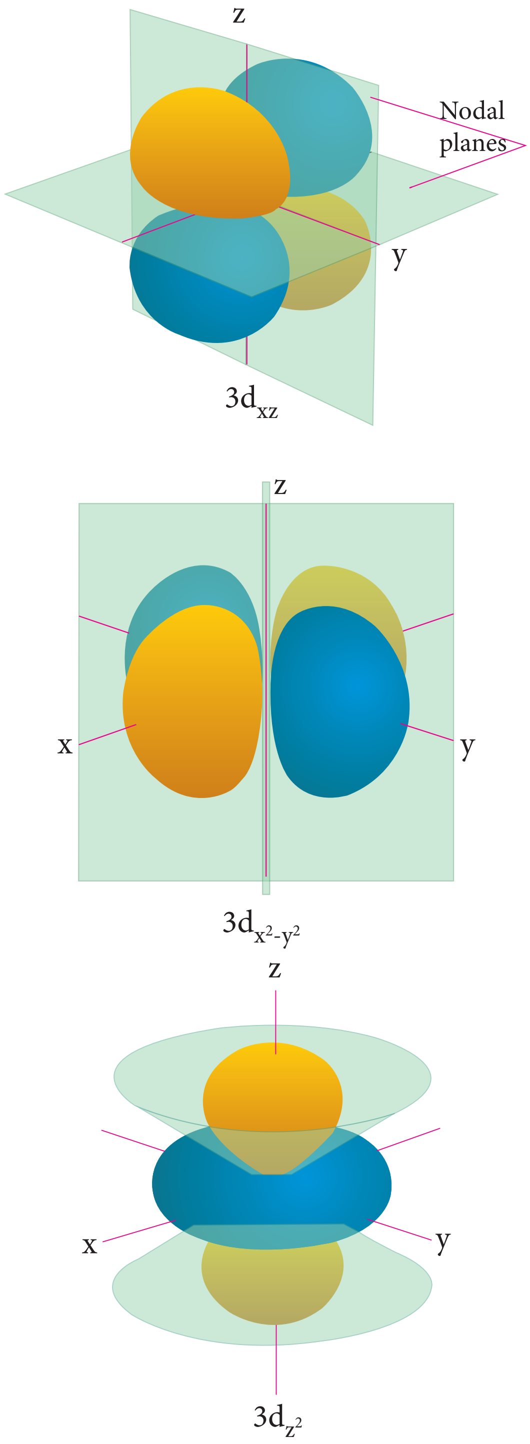


Figure 2.9 shapes of d orbitals

For 'f' orbital, $l = 3$ and the m values are -3, -2,-1, 0, +1, +2, +3 corresponding to seven f orbitals f_{z^3}, f_{xz^2}, f_{yz^2}, f_{xyz}, $f_{z(x^2-y^2)}$, $f_{x(x^2-3y^2)}$, $f_{y(3x^2-y^2)}$, which are shown in Figure 2.10. There are 3 nodal planes in the f-orbitals.

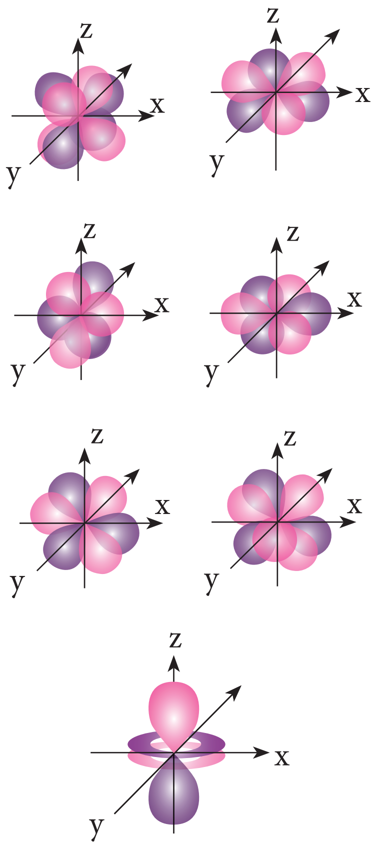


Figure 2.10 shapes of f-orbitals

Evaluate Yourself

4. Calculate the total number of angular nodes and radial nodes present in 3d and 4f orbitals.

2.5.2 Energies of orbitals

In hydrogen atom, only one electron is present. For such one electron system, the energy of the electron in the n^{th} orbit is given by the expression

$$E_n = \frac{(-1312.8)\, Z^2}{n^2} \text{ kJ mol}^{-1}$$

From this equation, we know that the energy depends only on the value of principal quantum number. As the n value increases the energy of the orbital also increases. The energies of various orbitals will be in the following order:

1s < 2s = 2p < 3s = 3p = 3d <4s = 4p = 4d = 4f < 5s = 5p = 5d = 5f < 6s = 6p = 6d = 6f < 7s

The electron in the hydrogen atom occupies the 1s orbital that has the lowest energy. This state is called ground state. When this electron gains some energy, it moves to the higher energy orbitals such as 2s, 2p etc… These states are called excited states.

However, the above order is not true for atoms other than hydrogen (multi-electron systems). For such systems the Schrödinger equation is quite complex. For these systems the relative order of energies of various orbitals is given approximately by the (n+l) rule. It states that, the lower the value of (n + l) for an orbital, the lower is its energy. If two orbitals have the same value of (n + l), the orbital with lower value of n will have the lower energy. Using this rule the order of energies of various orbitals can be expressed as follows.

Table 2.2 n+*l* values of different orbitals

Orbital	n	*l*	n+*l*
1s	1	0	1
2s	2	0	2
2p	2	1	3
3s	3	0	3
3p	3	1	4
3d	3	2	5
4s	4	0	4
4p	4	1	5
4d	4	2	6
4f	4	3	7
5s	5	0	5
5p	5	1	6
5d	5	2	7
5f	5	3	8
6s	6	0	6
6p	6	1	7
6d	6	2	8
7s	7	0	7

Based on the (n+*l*) rule, the increasing order of energies of orbitals is as follows:

1s < 2s < 2p < 3s < 3p < 4s <3d <4p <5s<4d < 5p < 6s<4f< 5d < 6p < 7s < 5f < 6d

As we know there are three different orientations in space that are possible for a p orbital. All the three p orbitals, namely, p_x, p_y and p_z have same energies and are called degenerate orbitals. However, in the presence of magnetic or electric field the degeneracy is lost.

In a multi-electron atom, in addition to the electrostatic attractive force between the electron and nucleus, there exists a repulsive force among the electrons. These two forces are operating in the opposite direction. This results in the decrease in the nuclear force of attraction on electron. The net charge experienced by the electron is called effective nuclear charge. The effective nuclear charge depends on the shape of the orbitals and it decreases with increase in azimuthal quantum number *l*. The order of the effective nuclear charge felt by a electron in an orbital within the given shell is s > p > d > f. Greater the effective nuclear charge, greater is the stability of the orbital. Hence, within a given energy level, the energy of the orbitals are in the following order. s < p < d < f.

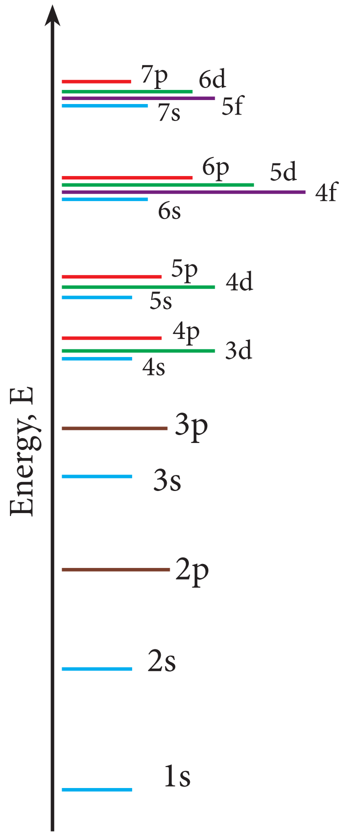


Figure. 2.11 Energy levels of atomic orbitals

The energies of same orbital decrease with an increase in the atomic number. For example, the energy of the 2s orbital of hydrogen atom is greater than that of 2s orbital of lithium and that of lithium is greater than that of sodium and so on, that is, $E_{2s}(H) > E_{2s}(Li) > E_{2s}(Na) > E_{2s}(K)$.

Evaluate Yourself

5. Energy of an electron in hydrogen atom in ground state is -13.6 eV. What is the energy of the electron in the second excited state?

2.6 Filling of orbitals:

In an atom, the electrons are filled in various orbitals according to aufbau principle, Pauli exclusion principle and Hund's rule. These rules are described below.

2.6.1 Aufbau principle:

The word Aufbau in German means 'building up'. In the ground state of the atoms, the orbitals are filled in the order of their increasing energies. That is the electrons first occupy the lowest energy orbital available to them.

Once the lower energy orbitals are completely filled, then the electrons enter the next higher energy orbitals. The order of filling of various orbitals as per the Aufbau principle is given in the figure 2.12 which is in accordance with (n+*l*) rule.

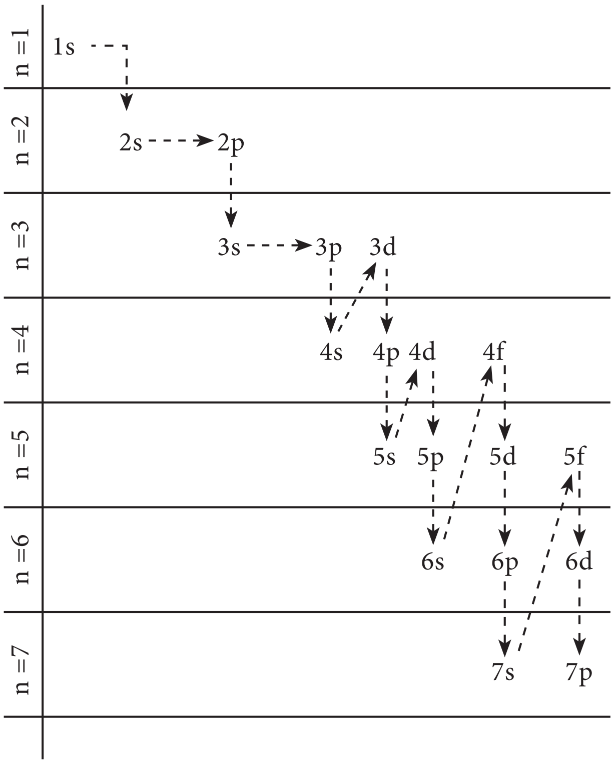


Figure. 2.12 Aufbau principle

2.6.2 Pauli Exclusion Principle :

Pauli formulated the exclusion principle which states that "No two electrons in an atom can have the same set of values of all four quantum numbers." It means that, each electron must have unique values for the four quantum numbers (n, *l*, m and s).

For the lone electron present in hydrogen atom, the four quantum numbers are: n = 1; l = 0; m = 0 and s = +½. For the two electrons present in helium, one electron has the quantum numbers same as the electron of hydrogen atom, n = 1, *l* = 0, m = 0 and s = +½. For other electron, the fourth quantum number is different i.e., n = 1, *l* = 0, m = 0 and s = –½.

As we know that the spin quantum number can have only two values +½ and –½, only two electrons can be accommodated in a given orbital in accordance with Pauli exclusion principle. Let us understand this by writing all the four quantum numbers for the eight electron in L shell.

Table 2.3 Quantum numbers of electrons in L shell

Electron	n	*l*	m	s
1st	2	0	0	+½
2nd	2	0	0	-½
3rd	2	1	-1	+½
4th	2	1	0	+½
5th	2	1	+1	+½
6th	2	1	-1	-½
7th	2	1	0	- ½
8th	2	1	+1	-½

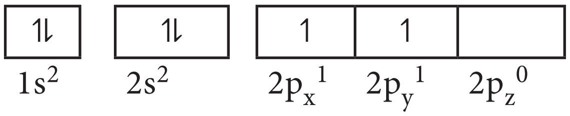
2.6.3 Hund's rule of maximum multiplicity

The Aufbau principle describes how the electrons are filled in various orbitals. But the rule does not deal with the filling of electrons in the degenerate orbitals (i.e. orbitals having same energy) such as p_x, p_y and p_z. In what order these orbitals to be filled? The answer is provided by the Hund's rule of maximum multiplicity. It states that electron pairing in the degenerate orbitals does not take place until all the available orbitals contains one electron each.

We know that there are three p orbitals, five d orbitals and seven f orbitals. According to this rule, pairing of electrons in these orbitals starts only when the 4th, 6th and 8th electron enters the p, d and f orbitals respectively.

For example, consider the carbon atom which has six electrons. According to Aufbau principle, the electronic configuration is $1s^2$, $2s^2$, $2p^2$

It can be represented as below,



In this case, in order to minimise the electron-electron repulsion, the sixth electron enters the unoccupied $2p_y$ orbital as per Hunds rule. i.e. it does not get paired with the fifth electron already present in the $2p_x$ orbital.

Evaluate Yourself

6. How many unpaired electrons are present in the ground state of Fe^{3+} (z=26), Mn^{2+} (z=25) and argon (z=18)?

2.6.4 Electronic configuration of atoms

The distribution of electrons into various orbitals of an atom is called its electronic configuration. It can be written by applying the aufbau principle, Pauli exclusion principle and Hund's rule. The electronic configuration is written as nl^x , where n represents the principle of quantum number, '*l*' represents the letter designation of the orbital [s(*l*=0), p (*l*=1), d(*l*=2) and f(*l*=3)] and 'x' represents the number of electron present in that orbital.

Let us consider the hydrogen atom which has only one electron and it occupies the lowest energy orbital i.e. 1s according to aufbau principle. In this case n=1; *l*=s; x=1.

Hence the electronic configuration is $1s^1$. (read as one-ess-one).

The orbital diagram for this configuration is,

$$\boxed{\upharpoonleft}$$
$$1s^1$$

The electronic configuration and orbital diagram for the elements upto atomic number 10 are given below :

Table 2. 4 Electronic configuration and orbital diagrams for first 10 elements

Element	Electronic Configuration	Orbital diagram
H^1	$1s^1$	$\boxed{\upharpoonleft}$ $1s^1$
He^2	$1s^2$	$\boxed{\upharpoonleft\downharpoonright}$ $1s^2$
Li^3	$1s^2\ 2s^1$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft}$ $1s^2\ \ 2s^1$
Be^4	$1s^2\ 2s^2$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}$ $1s^2\ \ 2s^2$
B^5	$1s^2\ 2s^2\ 2p^1$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft}\boxed{\ }\boxed{\ }$ $1s^2\ \ 2s^2\ \ 2p_x{}^1\ \ 2p_y\ \ 2p_z$
C^6	$1s^2\ 2s^2\ 2p^2$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft}\boxed{\upharpoonleft}\boxed{\ }$ $1s^2\ \ 2s^2\ \ 2p_x{}^1\ \ 2p_y{}^1\ \ 2p_z$
N^7	$1s^2\ 2s^2\ 2p^3$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft}\boxed{\upharpoonleft}\boxed{\upharpoonleft}$ $1s^2\ \ 2s^2\ \ 2p_x{}^1\ \ 2p_y{}^1\ \ 2p_z{}^1$
O^8	$1s^2\ 2s^2\ 2p^4$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\boxed{\upharpoonleft}\boxed{\upharpoonleft}$ $1s^2\ \ 2s^2\ \ 2p_x{}^2\ \ 2p_y{}^1\ \ 2p_z{}^1$
F^9	$1s^2\ 2s^2\ 2p^5$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\boxed{\upharpoonleft\downharpoonright}\boxed{\upharpoonleft}$ $1s^2\ \ 2s^2\ \ 2p_x{}^2\ \ 2p_y{}^2\ \ 2p_z{}^1$
Ne^{10}	$1s^2\ 2s^2\ 2p^6$	$\boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\ \boxed{\upharpoonleft\downharpoonright}\boxed{\upharpoonleft\downharpoonright}\boxed{\upharpoonleft\downharpoonright}$ $1s^2\ \ 2s^2\ \ 2p_x{}^2\ \ 2p_y{}^2\ \ 2p_z{}^2$

The actual electronic configuration of some elements such as chromium and copper slightly differ from the expected electronic configuration in accordance with the Aufbau principle.

For chromium - 24

Expected configuration :

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^4\ 4s^2$

Actual configuration :

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5\ 4s^1$

For copper - 29

Expected configuration :

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^9\ 4s^2$

Actual configuration :

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$

The reason for above observed configuration is that fully filled orbitals and half filled orbitals have been found to have extra stability. In other words, p^3, p^6, d^5, d^{10}, f^7 and f^{14} configurations are more stable than p^2, p^5, d^4, d^9, f^6 and f^{13}. Due to this stability, one of the 4s electrons occupies the 3d orbital in chromium and copper to attain the half filled and the completely filled configurations respectively.

Evaluate Yourself

7. Explain the meaning of the symbol $4f^2$. Write all the four quantum numbers for these electrons.

2.6.5 Stability of half filled and completely filled orbitals:

The exactly half filled and completely filled orbitals have greater stability than other partially filled configurations in degenerate orbitals. This can be explained on the basis of symmetry and exchange energy. For example chromium has the electronic configuration of $[Ar]3d^5\ 4s^1$ and not $[Ar]3d^4\ 4s^2$ due to the symmetrical distribution and exchange energies of d electrons.

Symmetrical distribution of electron:

Symmetry leads to stability. The half filled and fully filled configurations have symmetrical distribution of electrons (Figure 2.13) and hence they are more stable than the unsymmetrical configurations.

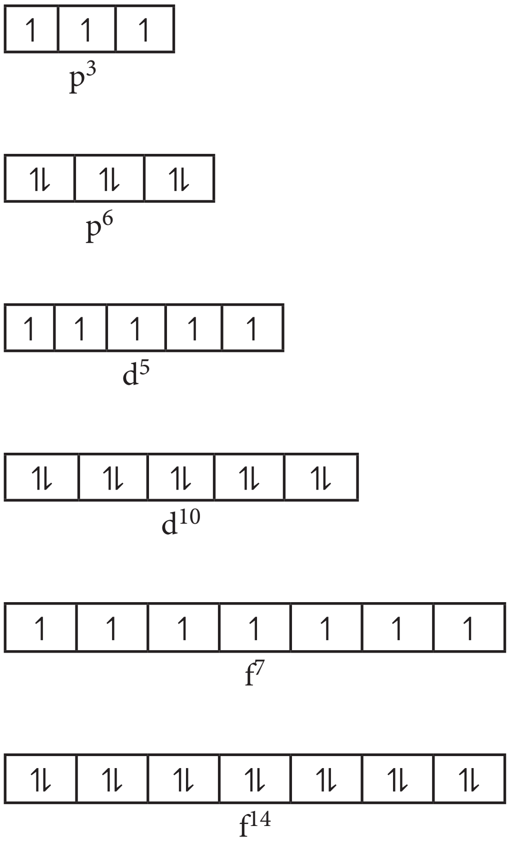


Figure 2.13 Half filled and fully filled p, d and f orbitals

The degenerate orbitals such as p_x, p_y and p_z have equal energies and their orientation in space are different as shown in Figure 2.14. Due to this symmetrical distribution, the shielding of one electron on the other is relatively small and hence the electrons are attracted more strongly by the nucleus and it increases the stability.

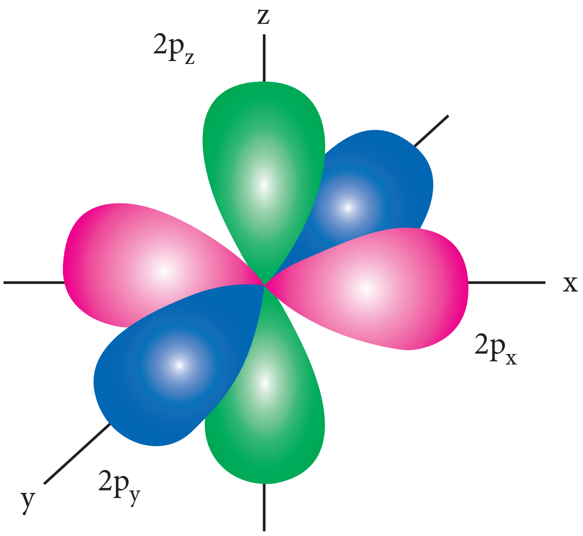


Figure 2.14 Shape of the degenerate p orbitals.

Exchange energy:

If two or more electrons with the same spin are present in degenerate orbitals, there is a possibility for exchanging their positions. During exchange process the energy is released and the released energy is called exchange energy. If more number of exchanges are possible, more exchange energy is released. More number of exchanges are possible only in case of half filled and fully filled configurations.

For example, in chromium the electronic configuration is $[Ar]3d^5\ 4s^1$. The 3d orbital is half filled and there are ten possible exchanges as shown in Figure 2.15. On the other hand only six exchanges are possible for $[Ar]3d^4\ 4s^2$ configuration. Hence, exchange energy for the half filled configuration is more. This increases the stability of half filled 3d orbitals.

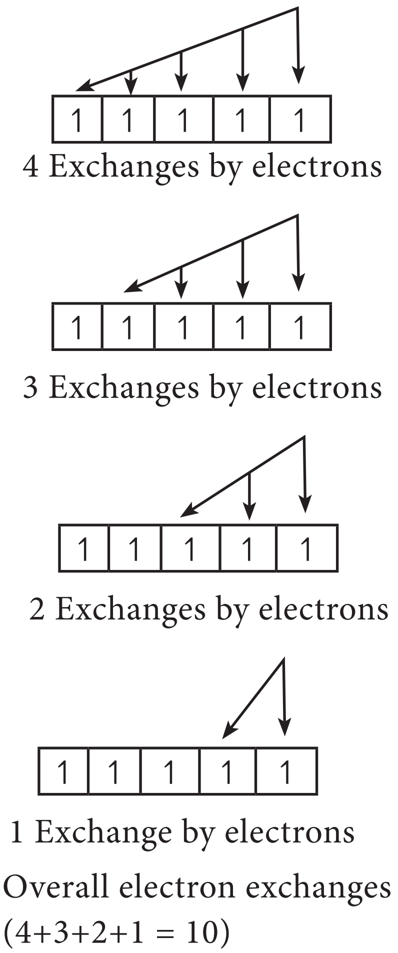


Figure 2.15 (a)

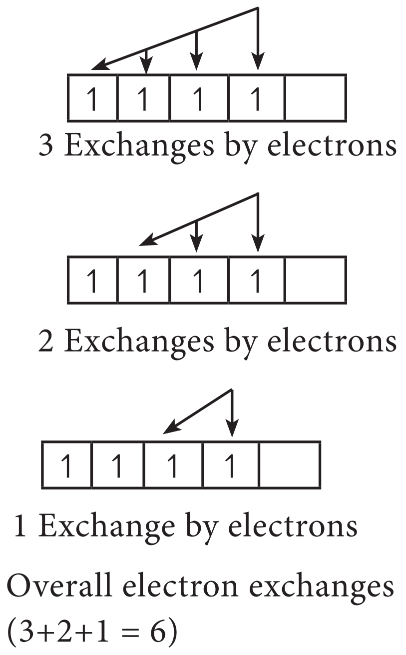


Figure 2.15 (b)

Figure 2.15 Possible exchanges in chromium d orbitals: a) for d^5 configuration b) for d^4 configuration

The exchange energy is the basis for Hund's rule, which allows maximum multiplicity, that is electron pairing is possible only when all the degenerate orbitals contain one electron each.

Evaluate Yourself

8. Which ion has the stable electronic configuration? Ni^{2+} or Fe^{3+}.

SUMMARY

The atoms were believed to be non -divisible until the discovery of subatomic particles. J. J. Thomson proposed that the atom is a positively charged sphere in which the electrons are embedded. However, it fails to explain the stability of atoms. Rutherford, based on his α-rays scattering experiment, introduced the term nucleus which is a positively charged one and the negatively charged electrons are revolving around it, at high speeds. Bohr modified the Rutherford theory and introduced stationary orbits by taking into account the quantisation of energy. Louis de Broglie proposed that all matter possess dual nature. i.e. they behave both as a wave and a particle. De Broglie wavelength $\lambda = h/mv = h/\sqrt{2mev}$ is significant for a microscopic particle such as an electron. The wave nature of electron is also proved by Davisson and Germer through electron diffraction. For a microscopic particle such as an electron, the simultaneous measurement of the conjugate variables such as position and momentum involves uncertainty which is known as Heisenberg's uncertainty principle and it is expressed as $\Delta x.\Delta p \geq h/4\pi$.

De Broglie's concept and Heisenberg's uncertainty principle lead to the development of quantum mechanical model of atom. Erwin Schrodinger, developed an equation for an electron wave which is expressed as $\hat{H}\psi = E\psi$. This second order differential equation is exactly solvable for one electron system such as H, He^+ etc... but it is quite complex for multi-electron systems. The Schrödinger wave equation is solvable for certain energy values called eigen values. The wave functions corresponding to these eigen values are called atomic orbitals. The wave function ψ itself has no physical meaning. However, $|\psi|^2$ is related to the probability of finding electron around the nucleus. Thus the quantum mechanical model introduced us the term orbital which is the three dimensional space in which the probability of finding the electron is maximum. The electron in an orbital can be described by a set of four quantum numbers namely, principal quantum number (n) representing the principal energy level, azimuthal quantum number (*l*) representing the sub shell (orbital), magnetic quantum number (m) representing the different orientation of orbitals in space and spin quantum number (s) representing the spinning of electron about its own axis.

The general solution of Schrodinger for a one electron system can be expressed in spherical polar coordinates (r, θ, φ)

$$\Psi(r, \theta, \varphi) = R(r).f(\theta).g(\varphi)$$

(where R(r) is called radial wave function, other two functions are called angular wave functions).

The plot of $4\pi r^2. R(r)^2$ versus r gives the radial distribution curves. The number of radial nodes is given by$(n-l-1)$ whereas the angular nodes is equal to *l*. The angular distribution curve gives the boundary space diagram of orbital.

s orbital is spherical in nature and the d orbital has clover leaf shape.

Electrons are filled in various orbitals in the increasing order of their energies which is known as Aufbau principle. The relative energies of various orbitals are given by (n+*l*) rule which states that, the lower the value of (n + *l*) for an orbital, the lower is its energy. If two orbitals have the same value of (n + *l*), the orbital with lower value of n will have the lower energy. As per Pauli's exclusion principle, the maximum number of electrons that can be accommodated in an orbital is two. In the case of degenerate orbitals electron pairing does not take place until all the available degenerate orbitals contain one electron each. This is known as Hund's rule. Based on these principles, electronic configurations of atoms can be written. In degenerate orbitals, the completely filled and half filled configurations are more stable than the partially filled configurations. This is due to the symmetry and exchange energies.

EVALUATION :

Choose the best answer

1. Electronic configuration of species M^{2+} is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^6$ and its atomic weight is 56. The number of neutrons in the nucleus of species M is

   a) 26 b) 22 c) 30 d) 24

2. The energy of light of wavelength 45 nm is

   a) 6.67×10^{15}J b) 6.67×10^{11}J

   c) 4.42×10^{-18}J d) 4.42×10^{-15}J

3. The energies E_1 and E_2 of two radiations are 25 eV and 50 eV respectively. The relation between their wavelengths ie λ_1 and λ_2 will be

   a) $\frac{\lambda_1}{\lambda_2} = 1$ b) $\lambda_1 = 2\lambda_2$ c) $\lambda_1 = \sqrt{25 \times 50}\ \lambda_2$ d) $2\lambda_1 = \lambda_2$

4. Splitting of spectral lines in an electric field is called

   a) Zeeman effect b) Shielding effect

   c) Compton effect d) Stark effect

5. Based on equation $E = -\ 2.178 \times 10^{-18}\ J \left(\frac{z^2}{n^2}\right)$, certain conclusions are written. Which of them is not correct ? (NEET)

   a) Equation can be used to calculate the change in energy when the electron changes orbit

   b) For n = 1, the electron has a more negative energy than it does for n = 6 which means that the electron is more loosely bound in the smallest allowed orbit

   c) The negative sign in equation simply means that the energy of electron bound to the nucleus is lower than it would be if the electrons were at the infinite distance from the nucleus.

   d) Larger the value of n, the larger is the orbit radius.

6. According to the Bohr Theory, which of the following transitions in the hydrogen atom will give rise to the least energetic photon ?

   a) n = 6 to n = 1 b) n = 5 to n = 4

   c) n = 5 to n = 3 d) n = 6 to n = 5

7. Assertion : The spectrum of He^+ is expected to be similar to that of hydrogen

Reason : He^+ is also one electron system.

(a) If both assertion and reason are true and reason is the correct explanation of assertion.

(b) If both assertion and reason are true but reason is not the correct explanation of assertion.

(c) If assertion is true but reason is false

(d) If both assertion and reason are false

8. Which of the following pairs of d-orbitals will have electron density along the axes ? (NEET Phase - II)

a) d_{z^2}, d_{xz} b) d_{xz}, d_{yz} c) $d_{z^2}, d_{x^2-y^2}$ d) $d_{xy}, d_{x^2-y^2}$

9. Two electrons occupying the same orbital are distinguished by

a) azimuthal quantum number b) spin quantum number

c) magnetic quantum number d) orbital quantum number

10. The electronic configuration of Eu (Atomic no. 63) Gd (Atomic no. 64) and Tb (Atomic no. 65) are (NEET - Phase II)

a) [Xe] $4f^6\ 5d^1\ 6s^2$, [Xe] $4f^7\ 5d^1\ 6s^2$ and [Xe] $4f^8\ 5d^1\ 6s^2$

b) [Xe] $4f^7$, $6s^2$, [Xe] $4f^7\ 5d^1\ 6s^2$ and [Xe] $4f^9\ 6s^2$

c) [Xe] $4f^7$, $6s^2$, [Xe] $4f^8\ 6s^2$ and [Xe] $4f^8\ 5d^1\ 6s^2$

d) [Xe] $4f^6\ 5d^1\ 6s^2$, [Xe] $4f^7\ 5d^1\ 6s^2$ and [Xe] $4f^9\ 6s^2$

11. The maximum number of electrons in a sub shell is given by the expression

a) $2n^2$ b) $2l + 1$ c) $4l + 2$ d) none of these

12. For d-electron, the orbital angular momentum is

a) $\frac{\sqrt{2h}}{2\pi}$ b) $\frac{\sqrt{2h}}{2\pi}$ c) $\frac{\sqrt{2\times 4}\,h}{2\pi}$ d) $\frac{\sqrt{6}\,h}{2\pi}$

13. What is the maximum numbers of electrons that can be associated with the following set of quantum numbers ? n = 3, l = 1 and m = –1

a) 4 b) 6 c) 2 d) = 10

14. Assertion : Number of radial and angular nodes for 3p orbital are 1, 1 respectively.

Reason : Number of radial and angular nodes depends only on principal quantum number.

(a) both assertion and reason are true and reason is the correct explanation of assertion.

(b) both assertion and reason are true but reason is not the correct explanation of assertion.

(c) assertion is true but reason is false

(d) both assertion and reason are false

15. The total number of orbitals associated with the principal quantum number n = 3 is

a) 9 b) 8 c) 5 d) 7

16. If n = 6, the correct sequence for filling of electrons will be,

a) ns → (n – 2) f → (n – 1)d → np b) ns → (n – 1) d → (n – 2) f → np

c) ns → (n – 2) f → np → (n – 1) d d) none of these are correct

17. Consider the following sets of quantum numbers :

	n	*l*	m	s
(i)	3	0	0	$+\frac{1}{2}$
(ii)	2	2	1	$-\frac{1}{2}$
(iii)	4	3	–2	$+\frac{1}{2}$
(iv)	1	0	–1	$+\frac{1}{2}$
(v)	3	4	3	$-\frac{1}{2}$

Which of the following sets of quantum number is not possible ?

a) (i), (ii), (iii) and (iv)   b) (ii), (iv) and (v)

c) (i) and (iii)   d) (ii), (iii) and (iv)

18. How many electrons in an atom with atomic number 105 can have (n + l) = 8 ?

a) 30   b) 17   c) 15   d) unpredictable

19. Electron density in the yz plane of $3d_{xy}$ orbital is

a) zero   b) 0.50   c) 0.75   d) 0.90

20. If uncertainty in position and momentum are equal, then minimum uncertainty in velocity is

a) $\frac{1}{m}\sqrt{\frac{h}{\pi}}$ d) $\sqrt{\frac{h}{\pi}}$ c) $\frac{1}{2m}\sqrt{\frac{h}{\pi}}$ d) $\frac{h}{4\pi}$

21. A macroscopic particle of mass 100 g and moving at a velocity of 100 cm s^{-1} will have a de Broglie wavelength of

a) 6.6×10^{-29} cm   b) 6.6×10^{-30} cm   c) 6.6×10^{-31} cm   d) 6.6×10^{-32} cm

22. The ratio of de Broglie wavelengths of a deuterium atom to that of an α - particle, when the velocity of the former is five times greater than that of later, is

a) 4   b) 0.2   c) 2.5   d) 0.4

23. The energy of an electron in the 3rd orbit of hydrogen atom is –E. The energy of an electron in the first orbit will be

a) $-3E$ b) ${}^{-E}\!/_{3}$ c) ${}^{-E}\!/_{9}$ d) $-9E$

24. Time independent Schnodinger wave equation is

a) $\hat{H}\psi = E\psi$ b) $\nabla^2\psi + \frac{8\pi^2 m}{h^2}(E+V)\,\psi = 0$

c) $\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{h^2}(E-V)\,\psi = 0$ d) all of these

25. Which of the following does not represent the mathematical expression for the Heisenberg uncertainty principle ?

a) $\Delta x \,.\, \Delta p \geq {}^{h}\!/_{4\pi}$ b) $\Delta x \,.\, \Delta v \geq {}^{h}\!/_{4\pi m}$

c) $\Delta E \,.\, \Delta t \geq {}^{h}\!/_{4\pi}$ d) $\Delta E \,.\, \Delta x \geq {}^{h}\!/_{4\pi}$

Write brief answer to the following questions

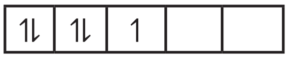
26. Which quantum number reveal information about the shape, energy, orientation and size of orbitals?

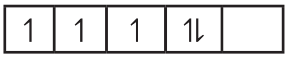
27. How many orbitals are possible for n =4?

28. How many radial nodes for 2s, 4p, 5d and 4f orbitals exhibit? How many angular nodes?

29. The stabilisation of a half filled d - orbital is more pronounced than that of the p-orbital why?

30. Consider the following electronic arrangements for the d^5 configuration.


(a)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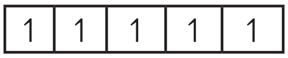

(c)

(i) which of these represents the ground state

(ii) which configuration has the maximum exchange energy.

31. State and explain pauli exclusion principle.

32. Define orbital? what are the n and l values for $3p_x$ and $4d_{x^2-y^2}$ electron?

33. Explain briefly the time independent schrodinger wave equation?

34. Calculate the uncertainty in position of an electron, if $\Delta v = 0.1\%$ and $\upsilon = 2.2 \text{ x} 10^6$ ms^{-1}

35. Determine the values of all the four quantum numbers of the 8th electron in O- atom and 15th electron in Cl atom.

36. The quantum mechanical treatment of the hydrogen atom gives the energy value:

$$E_n = \frac{-13.6}{n^2} \text{ ev atom}^{-1}$$

i) use this expression to find ΔE between n = 3 and n=4

ii) Calculate the wavelength corresponding to the above transition.

37. How fast must a 54g tennis ball travel in order to have a de Broglie wavelength that is equal to that of a photon of green light 5400Å?

38. For each of the following, give the sub level designation, the allowable m values and the number of orbitals

i) $n = 4, l = 2$, ii) $n = 5, l = 3$ iii) $n=7, l=0$

39. Give the electronic configuration of Mn^{2+} and Cr^{3+}

40. Describe the Aufbau principle

41. An atom of an element contains 35 electrons and 45 neutrons. Deduce

i) the number of protons

ii) the electronic configuration for the element

iii) All the four quantum numbers for the last electron

42. Show that the circumference of the Bohr orbit for the hydrogen atom is an integral multiple of the de Broglie wave length associated with the electron revolving arround the nucleus.

43. Calculate the energy required for the process.

$$He^{+}_{(g)} \rightarrow He^{2+}_{(g)} + e^{-}$$

The ionisation energy for the H atom in its ground state is - 13.6 ev atom^{-1}.

44. An ion with mass number 37 possesses unit negative charge. If the ion contains 11.1% more neutrons than electrons. Find the symbol of the ion.

45. The Li^{2+} ion is a hydrogen like ion that can be described by the Bohr model. Calculate the Bohr radius of the third orbit and calculate the energy of an electron in 4th orbit.

46. Protons can be accelerated in particle accelerators. Calculate the wavelength (in Å) of such accelerated proton moving at 2.85×10^{8} ms^{-1} (the mass of proton is 1.673×10^{-27} Kg).

47. What is the de Broglie wavelength (in cm) of a 160g cricket ball travelling at 140 Km hr^{-1}.

48. Suppose that the uncertainty in determining the position of an electron in an orbit is 0.6 Å. What is the uncertainty in its momentum?

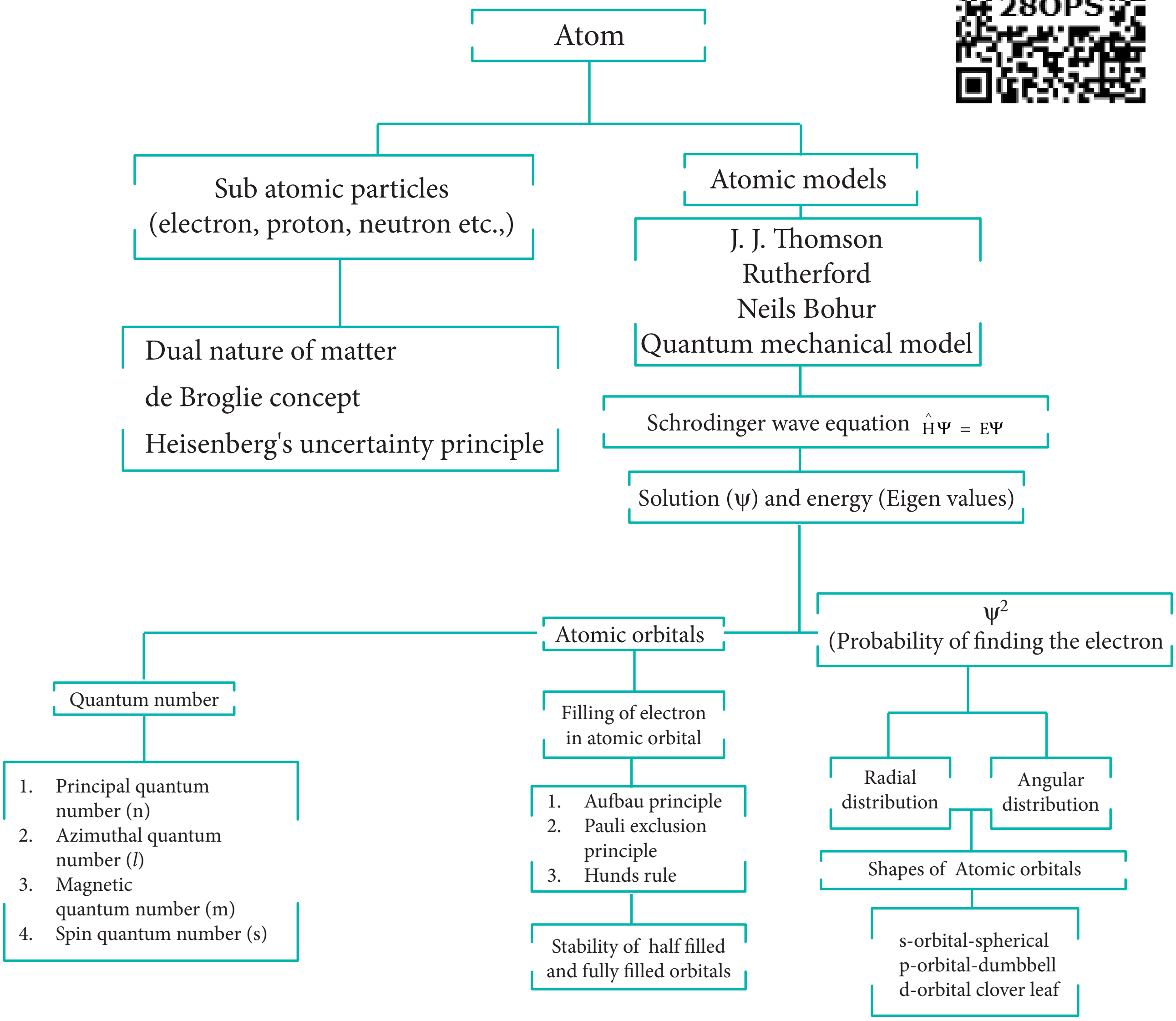
49. Show that if the measurement of the uncertainty in the location of the particle is equal to its de Broglie wavelength, the minimum uncertainty in its velocity (ΔV)is equal to 1/ 4π of its velocity(V)

50. What is the de Broglie wave length of an electron, which is accelerated from the rest, through a potential difference of 100V?

51. Identify the missing quantum numbers and the sub energy level

n	l	m	Sub energy level
?	?	0	4d
3	1	0	?
?	?	?	5p
?	?	-2	3d

CONCEPT MAP


Atom
Sub atomic particles (electron, proton, neutron etc.,)
Atomic models
J. J. Thomson
Rutherford
Neils Bohur
Quantum mechanical model
Dual nature of matter
de Broglie concept
Heisenberg's uncertainty principle
Schrodinger wave equation $\hat{H}\Psi = E\Psi$
Solution (ψ) and energy (Eigen values)
Atomic orbitals
ψ^2
(Probability of finding the electron
Quantum number
1. Principal quantum number (n)
2. Azimuthal quantum number (*l*)
3. Magnetic quantum number (m)
4. Spin quantum number (s)
Filling of electron in atomic orbital
1. Aufbau principle
2. Pauli exclusion principle
3. Hunds rule
Stability of half filled and fully filled orbitals
Radial distribution
Angular distribution
Shapes of Atomic orbitals
s-orbital-spherical
p-orbital-dumbbell
d-orbital clover leaf