



Atomic and Molecular Structure

Module I

Syllabus

Atomic orbitals (s,p,d,f) orbital shapes, Electronic Configuration, Molecular orbital theory (MOT), bonding and anti-bonding orbitals, Molecular orbital diagrams of Homonuclear and Heteronuclear diatomic molecules- Be₂, O₂, CO, NO their bond order and magnetic properties.

1.1 Introduction

1.1.1 Atomic and Molecular Structure

In 1803, an English chemist John Dalton put forth "Dalton's Atomic Theory", involving 'atom' as a smallest particle of an element.

According to Dalton's theory, the following postulates had been put forth.

- All elements are made up of small tiny particles called as "atoms".
- In an element, all 'atoms' are always of same masses and sizes, and the properties of all atoms also same whereas, atoms of different elements have all varying mass, size and properties. In short, "No two elements are same".
- This smallest particle 'atom' cannot be divided or formed or destroyed.
- During chemical reaction between different elements, the respective atoms combine in simple whole number resulting into a chemical compound. Thus during such reactions, atoms have capacity to get separated/rearranged from parent element and also combined with other atoms to form compound.

Thus, the smallest particle named atom (Greek word atom meaning cannot be broken/cut) gave insight to scientists about the matter and its inner structure. However, the further work by other scientists like Thompson, Rutherford, Bohr give more detailed picture about atom. It was concluded that the nature of matter is more complex and it cannot be only one type of atom.

1.1.2 Scientific History of Work

- ★ Scientific history of work is as,
- 1803 = Dalton's atomic theory
- 1897-98 = Cathode rays - stream of electrons - negatively charged particles in an element, but atom is electrically neutral. Therefore a positive charge must be present as a counter part in an element.
- 1907 = Sir J.J. Thompson's cathode rays experiment - electrons.
- 1911 = Lord Rutherford performed series of experiments, and emerged with suggestions on the structure of an atom.



1.2 Rutherford's Atomic Model

In 1911 Lord Rutherford performed an experiment popularly known as “ α -particle scattering experiment”.

Construction

- (a) Source of α -particles - A radioactive element, e.g. Radium.
- (b) Lead block - to embed radioactive element safely.
- (c) Thin gold foil - placed in path of beam of α -particles from radioactive elements (source).
- (d) Circular fluorescent screen - To detect the direction of α -particles after striking gold foil.

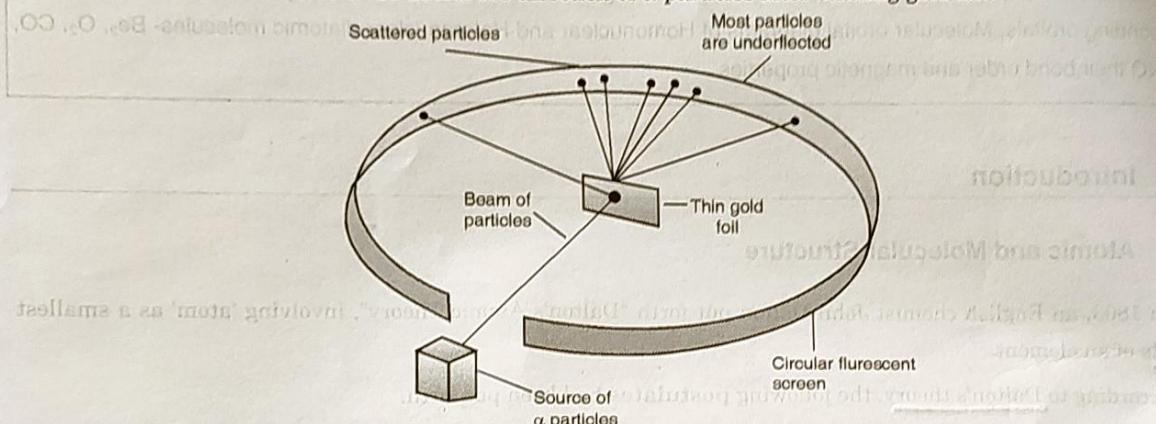


Fig. 1.2.1 : Rutherford scattering experiment

- Structurally Rutherford's model symbolises electrons revolving around nucleus in an atom similar to planets around 'Sun' in solar system.
- The mass of an atom is total of masses of protons and neutrons in its nucleus.
- The nucleus of atom is very small as compared to that of an atom itself. Thus there is empty space/hollow area surrounding to nucleus i.e. within an atom.

Experimental details

All components of scattering experiment were arranged in place and the beam of α -particles was released from source. This beam was made to strike the thin gold foil and the direction in which deflected rays struck the screen were observed.

Observations

The following observations were noted – on striking the α -particles on thin gold foil :

(a)	Majority of α -particles passed through gold foil with no deflection from their original path.	It is due to large empty space around nucleus, which probably allows the α -particles to pass through the foil without getting deflected.
(b)	Some α -particles got deflected back through 'small' angles and other few deflected through 'large' angles.	The atom has positive centre – nucleus – which repels positive particles thus deflecting them back with varying severity depending upon the rate of collision.

1.2.1 Conclusions by Rutherford

- Every atom possesses a nucleus at centre. Such nucleus is rigid, positively charged and dense in nature. The positive charge is due to "protons" – positively charged particles. It also has neutral particles known as "neutrons".
- Every atom is a neutral particle because its positive charge is equally compensated by 'electrons', i.e. negatively charged particles which are revolving around the nucleus in circular orbits.
- "The number of protons = The number of electrons".
- The mass of atom is entirely concentrated at centre of nucleus- which is due to protons and neutrons.
- Electrons strictly revolve around nucleus in circular path, i.e. orbit.
- The magnitude of positive charge is approximately half of the mass of nucleus.
- On continuing the work, Rutherford also had conclusions about mass of positively charged particle being same as that of hydrogen atom carrying positive charge. Therefore in 1914, the positive particle was named as "proton" and represented as, ${}_1^P$ where, P is proton, mass and charge = 1, i.e. unity.

1.2.2 Definition of Proton

- A proton is defined as "a hydrogen atom converted in hydrogen ion with positive charge due to loss of one electron having only nucleus with a positive charge".
 - In 1932 Neutrons were discovered by Chadwick, during radioactive disintegration of Beryllium with alpha rays.
- $${}_4^9\text{Be} + {}_2^4\text{He} \rightarrow {}_6^{12}\text{C} + {}_0^1\text{n}$$
- He concluded that neutron does not carry charge and its mass is almost same as proton.
Symbolically represented as ${}_0^1\text{n}$
Where, n = neutron charge = 0 (zero) mass = 1 (one) i.e. unity

Moseley's X-ray spectra studies of elements helped to conclude that, "atomic number of an element is same as nuclear charge" i.e. equal to number of protons (to also electrons).

Atomic mass = Total of protons and neutrons.

Nucleons = The particles inside nucleus are known as nucleons.

E.g. Protons and neutrons

1.2.3 Drawbacks of Rutherford's Atomic Model

The following are major drawbacks of Rutherford's nuclear atomic model :

- (i) **Behavior of electrons :** It fails to explain behavior of electrons in an atom.
- (ii) **Stability of atom :** It fails to explain the stable nature of an atom because, according to electromagnetic theory, if an electron i.e. a charged particle is in fast motion, it tends to release light radiations and hence it fails to maintain its rotation along a specific path, i.e. orbit. Hence, the curvature of spiral path would go on decreasing and ultimately the particle i.e. electron would also come closer to nucleus and fall into it. Thus atom would be unstable. But in reality atom is absolutely stable, which is unexplained by Rutherford.



1.3 Bohr's Atomic Theory

Niels Bohr put forth an atomic model with following objectives :

- To overcome the entire drawback in Rutherford's nuclear atomic model.
- To explain the spectrum of hydrogen or hydrogen like molecules.

Bohr's atomic model is based on Planck's quantum theory of radiation.

The Bohr model

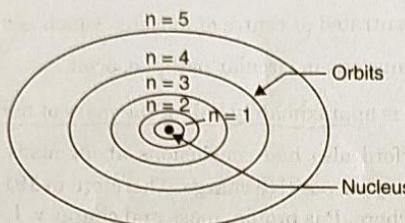


Fig. 1.3.1

Postulates of Bohr's atomic model

The following are the main postulates of Bohr's atomic model :

- In any atom, the electron represents as a tiny particle.
- It revolves round the centre known as nucleus in fixed concentric circular paths called as orbits or energy shells or energy levels.
- The electron revolves in these orbits maintaining fixed distance from the nucleus.
- These energy levels are represented by capital letters: K, L, M, N etc in succession starting from the nucleus. The values of n (principle quantum number) are assigned for these levels as: for K shell (1^{st} shell) $n = 1$, for L shell (2^{nd} shell) $n = 2$ etc. and so on.
- According to Bohr, an electron revolving in particular orbit if maintains its path, it neither absorbs nor emits energy.
- Hence, these energy levels are also called as stationary states.

With these basic postulates, the following two cases become evident,

- Electron at lower energy level Electron at higher energy level

$$n = 1 \text{ energy} = E_1 \xrightarrow[\text{absorbed(photon)}]{\text{Energy}} n = 2 \text{ energy} = E_2$$

$$\therefore E_2 - E_1 = \Delta E \quad \dots \text{Absorbed energy}$$

$$\therefore \Delta E = h\nu \quad \dots \text{(According to Planck's quantum theory)}$$

Where, $h = \text{Planck's constant}$

$\nu = \text{Frequency of radiation that electron absorbs}$



- (b) Similarly when electron emits energy/radiations

$$\Delta E = E_2 - E_1 = h\nu$$

The spectral line in the emission spectrum is due to energy released i.e. ΔE . The angular momentum of the revolving electron is given as,

$$mvr = n \frac{h}{2\pi}$$

Where,

m = Mass of an electron,

v = Velocity of the electron,

r = Radius of the orbit in which the electron is moving,

n = An integral (the principle quantum number) which denotes the number of the orbit in which the electrons are revolving and

h = Planck's constant.

This equation refers that the angular momentum of the revolving electron is quantized i.e., the magnitude of the angular momentum is always a whole number. This is known as the "Principle quantization of Angular Momentum".

1.3.1 Significance/Advantages of Bohr's Atomic Model

- The above expression could give,
 - (i) The radius of n^{th} orbit,
 - (ii) Velocity and energy of an electron revolving in the n^{th} orbit.
- Bohr's model also led to an expression for the frequency and wavelength (λ) of the spectral line in emission spectrum when an electron falls from n_2 orbit (higher orbit) to n_1 orbit (lower orbit).

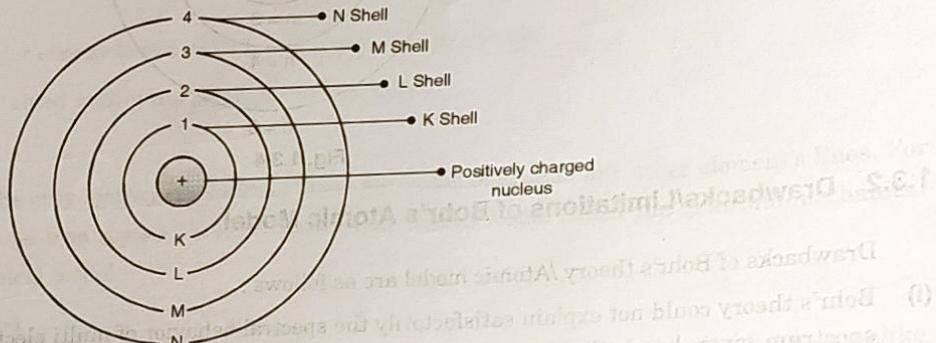


Fig. 1.3.2

According to Bohr's, the stability of an atom is explained as,

- The electron revolves with constant energy, as long as it is in a particular orbit. Hence atom is stable. When the solution of a substance faces an electromagnetic radiation some selective wavelength of it are absorbed by the dissolved substance.



- The wavelengths thus absorbed indicate the specific characteristics of that substance. The electrons get excited.
- The absorbed photons from the electromagnetic radiation by the substance now appear as dark lines in the spectrum. The appearance of dark lines proves absorption of photons/energy by the substance in solution. Thus the Bohr atomic model explains the absorption.
- The lowest allowable energy state of an atom is called its **ground state**.
- When an atom gains energy, it is in an excited state.
- Bohr suggested that an electron moves around the nucleus only in certain allowed circular orbits.

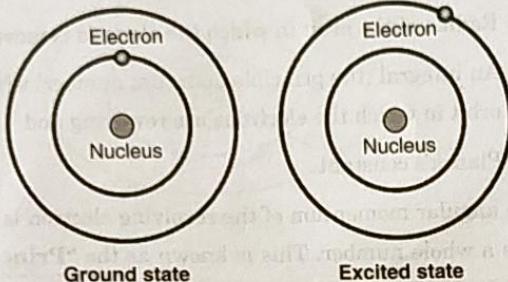


Fig. 1.3.3

- The electron releases energy as it falls back towards the ground state.

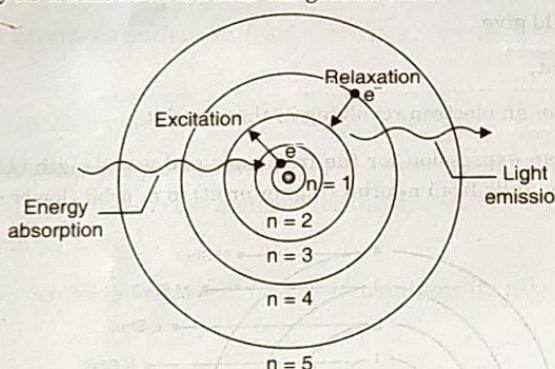


Fig. 1.3.4

1.3.2 Drawbacks/Limitations of Bohr's Atomic Model

Drawbacks of Bohr's theory /Atomic model are as follows :

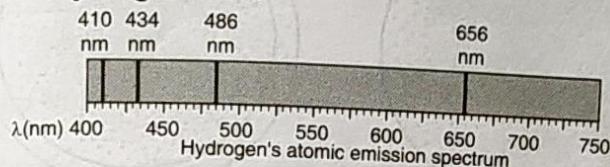
- (i) Bohr's theory could not explain satisfactorily the spectral behavior of multi electron species. The origin of the spectrum given by single electron species like H, He⁺, Li⁺, etc. are only explained on the basis of Bohr's model.
- (ii) According to Bohr's theory, the circular orbits are planar in nature, in which the electrons keep revolving. But this is not supported by modern theory, which suggests that an electron moves around the nucleus in the three dimensional space.

(iii) Zeeman effect

- According to modern theories, when an excited atom of a substance giving the line emission spectrum, if exposed to magnetic field, its spectrum is further split into more thinner lines which are very closely spaced.
- Such splitting of a line emission spectrum into numerous closely spaced lines under the influence of magnetic field is called as "Zeeman effect".

(iv) Stark effect

- Similar to Zeeman effects the excited atom shows lines on splitting when exposed to "electrical field".
- Bohr's model does not explain the "Zeeman effect" and "Stark effect".

1.3.3 Atomic Spectrum of Hydrogen Atom**Fig. 1.3.5 : Hydrogen's atomic emission spectrum**

- In 1913, Niels Bohr, a Danish physicist working in Rutherford's laboratory, proposed a quantum model for the hydrogen atom that seemed to answer this question.
- This model correctly predicted the frequency lines in hydrogen's atomic emission spectrum as shown in Fig. 1.3.5.

1.3.4 Structure of Hydrogen Atom

- Hydrogen has only one electron in s orbital ; $n = 1$
- The number is called the Principal quantum number (n) and it indicates the relative size and energy of atomic orbitals.
- n specifies the atom's major energy levels, called the principal energy levels.
- Energy sublevels are contained within the principal energy levels.

Failure of Bohr's model

- Bohr's model explained the only hydrogen's spectral lines, but failed to explain any other element's lines. For this reason, the Bohr model was replaced with a more sophisticated model called the quantum-mechanical approach or wave-mechanical model.

Quantum Mechanical Model

- Louis de Broglie (1892–1987) hypothesized that particles, including electrons' could also have wavelike behaviors.
- Electrons do not behave like particles flying through space.
- We cannot, in general, describe their exact paths.



Schrodinger's wave equation

- Schrodinger treated electrons as waves in a model called the quantum mechanical model of the atom.
- Schrodinger's equation applied equally well to elements other than hydrogen (unlike Bohr's model).
- The quantum mechanical model makes no attempt to predict the path of an electron around the nucleus.
- Hence then Bohr's orbits were replaced with quantum-mechanical orbitals.
- Orbitals are different from orbits in that they represent probability maps that show a statistical distribution of where the electron is likely to be found.

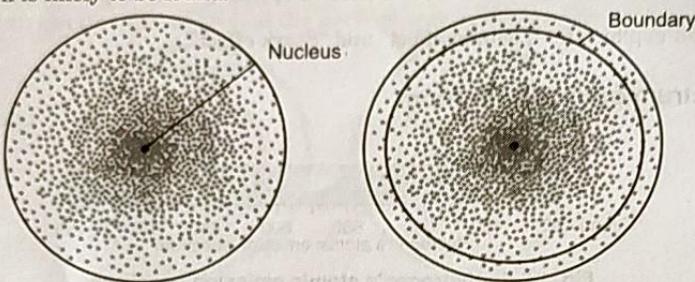


Fig. 1.3.6 : Density map

- The lowest-energy orbital in the quantum-mechanical model, is a number and a letter which specify orbital.
- The lowest-energy orbital is called the 1s orbital.
- It is specified by the number 1 and the letter 's'.

1.4 Quantum Numbers

The wave equation for hydrogen atom, when solved, which gave rise to idea of "quantum numbers".

The four quantum numbers and their notations are,

- Principal quantum number (n)
- Azimuthal quantum number (l)
- Magnetic quantum number (m)
- Spin quantum number (s)

Quantum numbers helped to explain the energy level of an electron in an atom.

1.4.1 Principal Quantum Number (n)

This quantum number indicates,

- The "most probable" position where an electron revolves / can be found from nucleus of the atom.
- The energy level/shell number to which the electron belongs.

The value of 'n' is always a positive integral as, 1, 2, 3 etc. starting from nearest to the nucleus.

E.g. Presently with respect to the number of elements known, the value of $n = 7$ is the maximum value i.e. 7th shell to which the electron is being found.

The notations of main energy levels are as,

Where,
 $n = 1 \dots K$ shell
 $n = 2 \dots L$ shell
 $n = 3 \dots M$ shell
 $n = 4 \dots N$ shell

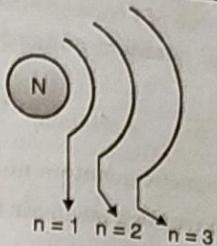


Fig. 1.4.1

1.4.2 Azimuthal Quantum Number (l)

This quantum number signifies the sub-level /sub-shell in which an electron enters and revolves. The value of l is $(n - 1)$, and subshells are s, p, d, f. i.e.,

- When $n = 1, l = 0$ means, when $n = 1$, and $l = 0$, there is only one subshell 's'
- When $n = 2, l = 0$ means, when $n = 1$, and $l = 0$, there are two subshells 's' and p and so on.

1.4.3 Magnetic Quantum Number (M)

This quantum number indicates magnetic property of an electron which owes to its rotation. The value of m ranges between $-l$ to $+l$ i.e. it will be $(2l + 1)$ values. E.g. When $l = 0$, m will have one value, and $l = 1$, then $m = 3$ values i.e. $(-1, 0, +1)$ and so on.

1.4.4 Spin Quantum Number (s)

This quantum number indicates 'spin' of the electron i.e. every electron rotates around nucleus and same time rotates around its own axis.

$$s = +\frac{1}{2} \text{ or } -\frac{1}{2}$$

1.5 Atomic orbitals (s, p, d, f) orbital shapes

- Wavefunctions of electrons in the atoms are called atomic orbitals, which have a dependence on position. Square of the wavefunction - probability density of electron.
- The wavefunction of an electron in a hydrogen atom is specified by three quantum numbers, specifying energy and probability of finding an electron.

1. Principal quantum number, n - specifies energy of the orbitals. In a hydrogen atom, all atomic orbitals with the same value of n have the same energy and are said to belong to the same SHELL of the atom.
2. Orbital angular momentum quantum number, l .

$$l = 0, 1, 2, \dots, n - 1$$



Each value of l corresponds to a different type of orbital with a different shape. The orbitals of a shell with principal quantum number n fall into n groups, called subshells; each subshell is identified by a different l value.

$l = 0$ s-orbitals, $l = 1$ p-orbitals, $l = 2$ d-orbitals, $l = 3$ f-orbitals.

3. Magnetic quantum number, m_l : distinguishes the orbitals within a subshell. Determines how the atom behaves in a magnetic field.

$m_l = l, l-1, \dots, -l$ $2l+1$ m_l values for each l , $l = 1; m_l = +1, 0, -1$

Where, n is related to the size of the orbital,

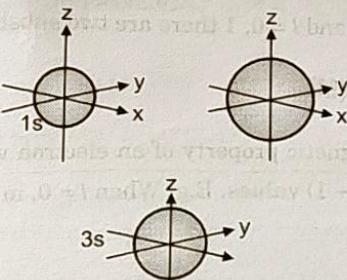
l is related to its shape, and

m_l is related to its orientation in space.

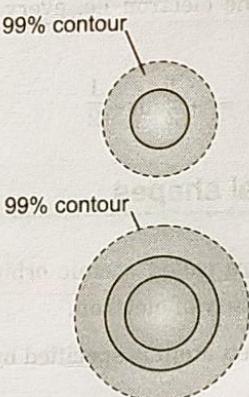
1.5.1 Atomic Orbital Shapes

- An s orbital is spherical.
- A p orbital has two lobes along a straight line through the nucleus, with one lobe on either side.
- A d orbital has a more complicated shape.

1. S sublevel



- All s orbitals are spherical, and their size increases with increasing principle quantum number.

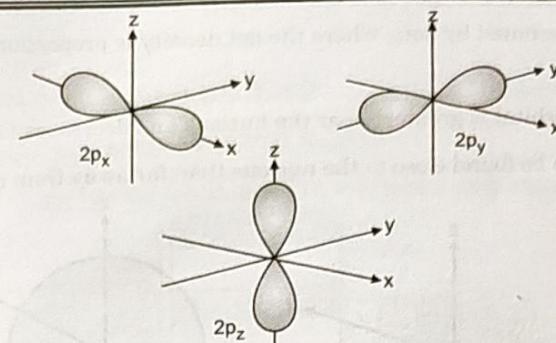


2s orbital

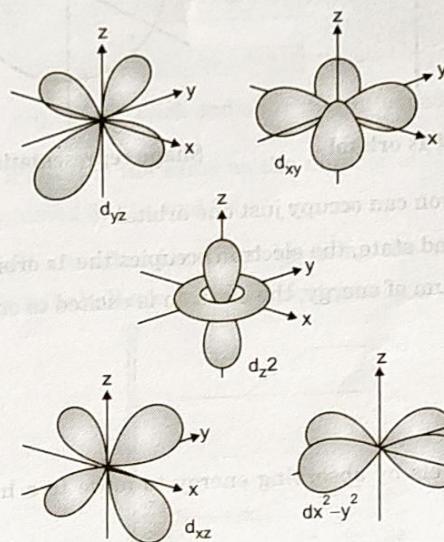
- The cross-sectional view of a 1s orbital and a 2s orbital highlights the difference in the two orbitals' sizes.

2. P sublevel

The three p orbitals are dumbbell shaped and are oriented along the three perpendicular x, y and z axes.

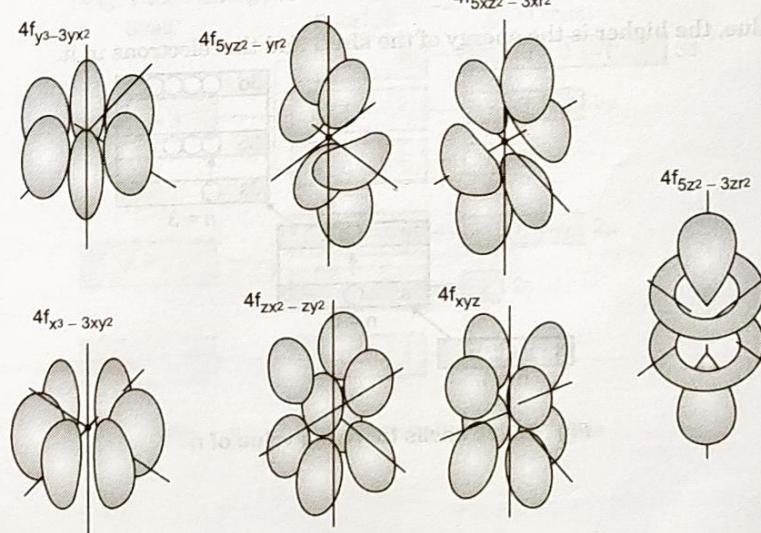


3. d sublevel



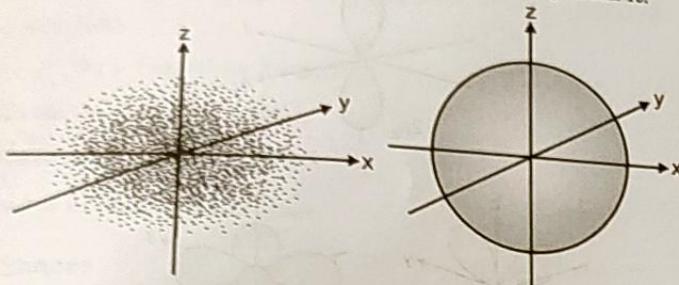
Four of the five d orbitals have the same shape but lie in different planes. The d_{z^2} orbital has its own unique shape.

4. f sublevel





- Orbitals are sometimes represented by dots, where the dot density is proportional to the probability of finding the electron.
- The **dot density** for the 1s orbital is greatest near the nucleus and decreases farther away from the nucleus.
- The electron is more likely to be found close to the nucleus than far away from it.



Dot representation of 1s orbital

Shape representation of 1s orbital

- At any given time, hydrogen's electron can occupy just one orbital.
 - o When hydrogen is in the ground state, the electron occupies the 1s orbital.
 - o When the atom gains a quantum of energy, the electron is excited to one of the unoccupied orbitals.

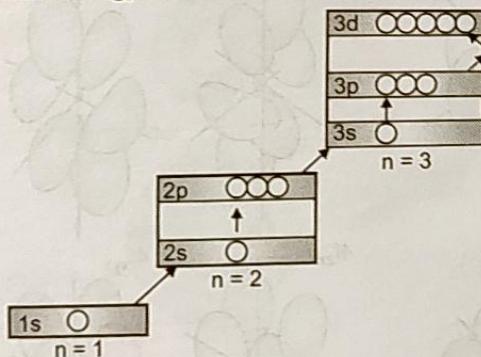
1.5.2 Hydrogenic Energy Levels

Transitions Between Energy Levels

An electron can change energy levels by absorbing energy to move to a higher energy level or by emitting energy to move to a lower energy level.

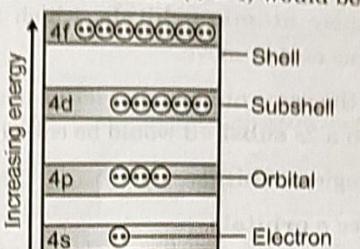
Shells

- The location of a **shell** and the electrons in it is indicated by a number n assigned to the **shell**.
- The value of n is as 1, 2, 3, 4, etc.
- The higher the n value, the higher is the energy of the **shell** and the electrons in it.

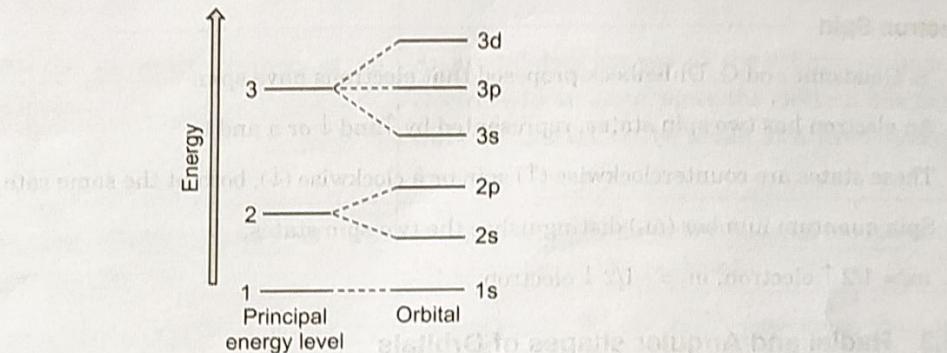
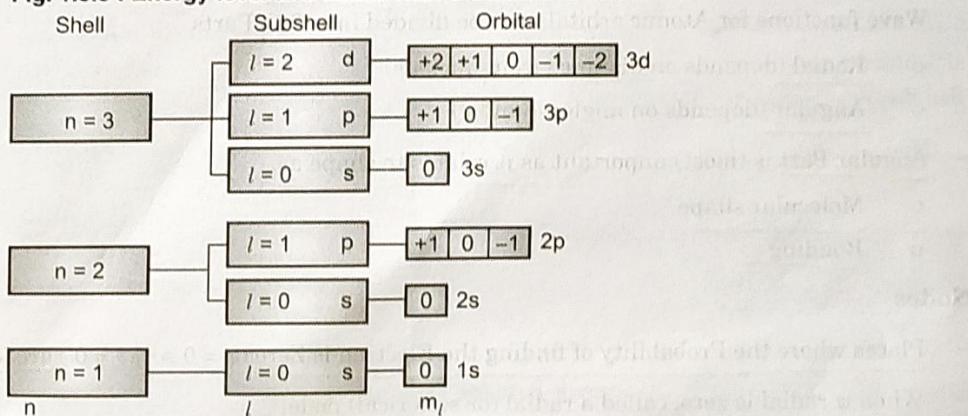
Fig. 1.5.1 : shells for rising value of n

Subshells

- Each **shell** is made up of one or more **subshells** that are designated by a letter as *s*, *p*, *d*, or *f*. The number of the **shell** to which a **subshell** belongs is given as,
- For example, a *p* **subshell** located in the fourth **shell** ($n = 4$) would be designated as a ***4p subshell***.

**Fig. 1.5.2 : Shell and subshell representation**

- The number of **subshells** in a **shell** is the same as the number of the **shell**. Thus, **shell number 3** ($n = 3$) contains three **subshells**, designated *3s*, *3p*, and *3d*.
- Electrons located in a **subshell** are often identified by using the same designation as the **subshell** they occupy. Thus, electrons in a *3d* **subshell** are called *3d* electrons.

**Fig. 1.5.3 : Energy level and shells with orbitals/subshells****Fig. 1.5.4 : Shells, subshells and orbitals**



Orbitals

s orbitals - correspond to $l = 0$ and $m = 0$

For Hydrogen atom the ground state is $n = 0$ and $m = 0$; a s orbital

- Thus the atomic orbitals surround the nucleus in which the electron is located.
- Each **subshell** consists of one or more **atomic orbitals**, which are specific volumes of space around the nucleus in which electrons of the same energy move.
- **Atomic orbitals** are designated by the same number and letter used to designate the **subshell** to which they belong. Thus, an s orbital located in a 2s subshell would be called a **2s orbital**.
 - o All s **subshells** consist of a single s orbital.
 - o All p **subshells** consist of three p orbitals.
 - o All d **subshells** consist of five d orbitals.
 - o All f **subshells** consist of seven f orbitals.
- According to the quantum mechanical model, **all types of atomic orbitals can contain a maximum of two electrons**.
- Thus, a single d **orbital** can contain a maximum of 2 electrons, and a d **subshell** that contains five orbitals can contain a maximum of 10 electrons.

Electron Spin

S. Goudsmit and G. Uhlenbeck proposed that electrons have spin.

- An electron has two spin states, represented by \uparrow and \downarrow or a and b.
- These states are counterclockwise (\uparrow) spin or a clockwise (\downarrow), both at the same rate.
- Spin quantum number (m_s) distinguishes the two spin states,
 $m_s = 1/2 \uparrow$ electron, $m_s = -1/2 \downarrow$ electron

1.5.3 Radial and Angular shapes of Orbitals

- Wave functions for Atomic orbitals can be divided into Two Parts
 - o Radial (depends on distance from nucleus)
 - o Angular (depends on angles ϕ and θ)
- Angular Part is (most) important as it relates to shape as,
 - o Molecular shape
 - o Bonding

Nodes

- Places where the Probability of finding the Electron is Zero ($\psi = 0$ so $\psi^2 = 0$) are known as nodes.
- When ψ radial is zero, called a radial (or spherical) node,
There are $n - l - 1$ radial nodes.
- When ψ angular is zero, called an angular node (or a nodal plane),
There are l angular nodes.



1.5.4 Radial Distribution Function

- The wave function ψ^2 , over estimates Probability of an electron Close to Nucleus and under estimates it Further Out.
- Hence it is Corrected by multiplying ψ^2 by $4\pi r^2$
 - o Takes into account that a wedge is smaller toward the center than end.
 - o This correction only works for s orbitals.

Table 1.5.1 : Difference between an orbit and an orbitals

Sr. No.	Orbit	Orbital
1.	Orbit is defined as "a definite circular path at a definite distance from the nucleus in which the electron revolves round the nucleus".	An orbital is defined as "a three-dimensional region or space around the nucleus where the probability of finding an electron with certain energy is maximum".
2.	Orbits are numbered as 1, 2, 3, 4... from the nucleus and are designated by the letters K, L, M, N, etc.	No numbering or notations for atomic orbitals.
3.	An orbit indicates an exact position of an electron in an atom.	An orbital does not specify the definite position of electrons in an atom, since the electron due to its wave nature cannot be found at a fixed distance from the nucleus.
4.	It represents the planar motion of the electron, around the nucleus.	It represents the three dimensional motion of the electron around the nucleus.
5.	The maximum number of electrons in an orbit is equal to $2n^2$ where n is the number of the orbit.	An orbital cannot accommodate more than two electron and these two electrons must have opposite spins.
6.	Orbits are circular in shape.	Orbitals have different shapes, e.g. s-orbital is spherically symmetrical, p-orbitals are dumb-bell shaped etc.

1.6 Electronic Configuration

Concept of electron charge cloud and an atomic orbital

1. Electron charge cloud

In an atom, nucleus at centre is "fixed", but the electrons revolve around it. Thus the electron can be positioned at variable positions around the 'nucleus'. The maximum probability of finding an electron lies near the nucleus and goes on decreasing as distance from nucleus wideness/increases in all directions.



2. Atomic orbital

The region / three dimensional space surrounding the nucleus of atom, where highest probability of finding an electron exists is known as, "Atomic orbital".

1.6.1 Pauli's Exclusion Principle

- Pauli's exclusion principle states that, "No two electron in an atom can have identical set of all four quantum numbers".
- This principle indicates that in any atom only two electrons can be placed in one single orbital with set of values as $n = l = m \neq s$.
- When two electrons with same 's' value come together, they get repelled, and hence switch to other orbital. Thus for two electrons to be in 'same' orbital must have 'opposite' spins.

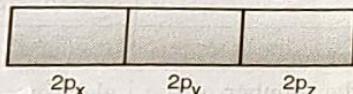
1.6.2 Hund's Rule of Maximum Multiplicity

This rule defines :

- (i) Maximum number of electrons in an orbital with specified set of quantum numbers with opposite spins must be only '2'.
- (ii) If $n = l = m = s$, then in an orbital only '1' electron gets place and it remains unpaired.
- (iii) In any subshell, the electrons always enter in empty orbital first.

E.g. Suppose $2p$ subshell, Here $n = 2$, $\therefore l = 1 \therefore$ orbitals $= (2l + 1) = 3$, represented as,

The entering electron will enter into $2p_x$, $2p_y$ and $2p_z$ in succession with same spin. The 4th electron in same shell shall enter in $2p_x$, pairing with the existing one, with opposite spin.



Many electron atoms

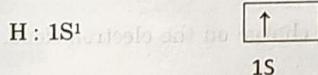
- The atoms other than hydrogen come in this category. From Helium all the known elements show various different effects on periodic properties. The orbitals have penetrating power depending on the energy, shielding / screening effect depending on forces of attractions between nucleus and outer most electrons in shell. These effects govern Effective Nuclear Charge of the atom.
- In case of hydrogen, the Electronic Structure of H atom ($Z = 1$) can be explained as,
- Electron in the lowest energy level - ground state of the atom, $n = 1 \Rightarrow 1s$ orbital
- Quantum numbers of this $1s$ electron
 $n = 1, \quad l = 0, \quad ml = 0, \quad ms = +1/2 \text{ or } -1/2$
- In other elements, where many electrons present,
- If the electron acquires energy, the electron can undergo a transition to the $n = 2$ shell and,
- Can occupy the $2s$ or one of the three $2p$ orbitals (for H-atom all have the same energy)



- Hence, The state of an electron in a H atom is defined by the four quantum numbers n, l, m_l, m_s .
- But as the value of n increases, the size of the atom increases.
- Many-electron atoms ($Z > 1$)
- Electrons occupy orbitals like those of H atom.
- Energies of orbitals of many electron atoms are not the same as those for the H atom.
- Nuclear attraction for electrons is greater as Z increases lowering the electrons' energy; also have to account for electron-electron repulsion.
- In the Schrodinger equation, $V(r)$ has to account for both the nuclear-electron attraction and the electron-electron repulsion.
- For example for He ($Z = 2$), $V(r)$ contains three terms
- Thus for many-electron atoms,
- The electron density of an isolated many-electron atom is sum of the electron densities of each electron taken individually
- Every electron in an atom has a set of four quantum numbers, n, l, m_l and m_s .
- The electron-electron repulsion opposes electron-nuclear attraction.
- The repulsion "shields" the electron from the full attraction of the nucleus.
- Electrons feel an "effective" nuclear charge which is less than the full nuclear charge.
 - o s orbitals have a non-zero probability density at the nucleus, penetrate through inner shells
 - o s electrons feel stronger nuclear attraction; are tightly bound and hence lower in energy
 - o p orbitals have zero probability density at the nucleus; less penetrating than s and hence p electrons are higher in energy.
 - o d orbitals less penetrating than p and hence d electrons are higher in energy than p
- In many electron atoms, because of shielding and penetration effects, order of the energy of orbitals in a given shell is typically $s < p < d < f$.
- Energies of orbitals depend on both n and l (not just n as in the H atom)

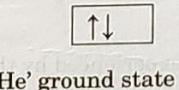
Orbital Diagram

- Hydrogen has its one electron in the 1s orbital:

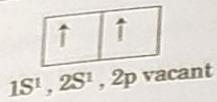


- Helium has two electrons : $\text{He} - 1\text{S}^2$

Both occupy the 1s orbital with opposite spins.



- Helium can also exist in an excited state such as:



- The process continues as atomic number goes on increasing and every new electron enters in next energy level orbital following the same pattern.

1. Penetration and shielding

(A) Penetration Power/effect of orbital

- Penetration Power is defined as "the ability of an orbital to attract an electron".
- This process of pulling or attracting an electron is accompanied with release of energy.
- It is also governed by the distance between the orbital and the nucleus i.e. atomic radius.
- Electrons are negatively charged and are pulled pretty close to each other by their natural attraction to the positive charge of a nucleus.
- The orbital number (n) and subshell (ml) define how close an electron can approach the nucleus.
- The Penetration effect of 's' orbital is the maximum because of the closeness to the nucleus than are the "p, d and f" orbitals.
- Thus penetration power is inversely proportional to the atomic radius.
- Penetration can be defined as "The ability of an electron to get close to the nucleus".
- Different orbitals have greater nuclear penetration than others.
- The electron probability density for s-orbitals is highest in the center of the orbital, or at the nucleus. The s orbital has $l=0$, p has $l=1$. The angular momentum being higher, the energy also is. Because of the penetration, that is, because the 2s electron can spend time near the nucleus, it is less effectively shielded by the core electrons than a 2p electron. d orbital is double dumb-bell shaped and comes after p orbital. f orbital has diffused shape and exists next to d orbital.

(B) Shielding effect

- The shielding effect describes the attraction between an electron and the nucleus in any atom with more than one electron shell.

Definition

- Shielding effect can be defined as " a reduction in the effective nuclear charge on the electron cloud, due to difference in the forces of attraction of the electrons on the nucleus".
- The shielding effect is prominent in "many electron atoms".
- It describes the decrease in attraction between an electron and the nucleus in any atom with more than one electron shell.
- More the electron shells in an atom, the greater the shielding effect experienced by the outermost electrons.
- It Increases down the group because more electron shells are being added.

- Decreases left to right across the period because of bigger positive nuclear charges pulling more on the electron clouds.
- With fewer electrons, there is less repulsion and the electrons are pulled closer to the nucleus.

For example

- 3d elements - Shielding effect is pronounced more in the 3d elements. The general trend of elements in the same period is that the atomic radii decrease from left to right. In case of 3d elements, as we move from left to right, electrons are added to the inner 3d orbital which pushes the outer 4s orbital.

Effect of shielding on Ionization Energies

- The higher the shielding affects the lower the ionization energy because, the more electrons shielding the outer electron shell from the nucleus, the less energy required to expel an electron from said atom.

Atomic Radius

- Atomic radius increases from top to bottom within a group because, shielding effect increases down the group because of the increase in the number of protons and electrons across a period. One proton has a greater effect than one electron; thus, electrons are pulled towards the nucleus, resulting in a smaller radius. This is caused by electron shielding.

Factors governing shielding effect

It depends on many factors like;

- Size of atom ,
- Charge density ,
- Orbitals involved ,
- Effective nucleus charge

2. Effective nuclear charge**Definition**

- It is defined as "the attractive positive charge of nuclear protons acting on valence electrons".
- The effective nuclear charge is always less than the total number of protons present in a nucleus due to shielding effect.
- Effective nuclear charge is behind all other periodic table tendencies.

For example

- In carbon the 4 valence electrons in the outermost shell feel a +6 charge surrounded by two shielding electrons for a +4 effective nuclear charge.
- Or silicon it would also be a +4 effective nuclear charge because the 14 protons in the nucleus are surrounded by 10 shielding electrons.
- Hydrogen atom contains one proton and one electron. The effective nuclear charge on electron is equal to 1 in hydrogen atom.

- Helium contains two protons and two electrons. Hence ENC is +2.
- Shielding effect reduces the effective nuclear charge on electron cloud due to differences in attraction between electrons and nucleus.

1.6.3 Aufbau Principle

- The rule states that, "when an atom is in ground state, the electrons tend to occupy the lowest energy orbital available". Conversely, "the electrons enter the orbitals successively in order of increasing energies".
- The orbital energy is given by quantum numbers n and l and orbitals accommodate the electrons in increasing value of $(n+l)$.
- E.g. Consider shell $4s$ (here $n = 4$, hence $l = 0(s)$),
 $n+l = 4+0=4$
 Whereas $3d$ (here $n = 3$, and $l = 2(d) = 5$)
 $\therefore 4s$ has lower energy than $3d$.
- Electrons enter $4s$ before $3d$. The following order is observed according to this principle for entering electrons.
 $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s$

The electronic configuration of elements from Hydrogen ($Z = 1$) to Uuo ($Z = 118$) is given below in Table 1.6.1.

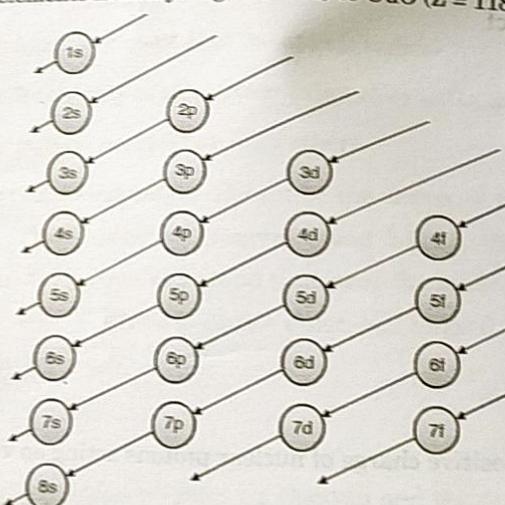


Fig. 1.6.1 : Order of filling of electrons as per Aufbau principle

Table 1.6.1 : Ground state electronic configuration of atoms in gaseous state

Z	Symbol	Configuration as (core) plus "Outermost" orbitals
1	H	$1s^1$
2	He	$1s^2$, or [He]
3	Li	[He] $2s^1$

Z	Symbol	Configuration as (core) plus "Outermost" orbitals
4	Be	[He]2s ²
5	B	[He]2s ² 2p ¹
6	C	[He]2s ² 2p ²
7	N	[He]2s ² 2p ³
8	O	[He]2s ² 2p ⁴
9	F	[He]2s ² 2p ⁵
10	Ne	[He]2s ² 2p ⁶ or [Ne]
11	Na	[He]3s ¹
12	Mg	[Ne]3s ²
13	Al	[Ne]3s ¹ 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 ⁵ or [Ar]
19	K	[Ar] 4s ¹
20	Ca	[Ar] 4s ²
21	Sc	[Ar] 3d ¹ 4s ²
22	Ti	[Ar] 3d ² 4s ²
23	V	[Ar] 3d ³ 4s ²
24	Cr	[Ar] 3d ⁵ 4s ¹
25	Mn	[Ar] 3d ⁵ 4s ²
26	Fe	[Ar] 3d ⁶ 4s ²
27	Co	[Ar] 3d ⁷ 4s ²
28	Ni	[Ar] 3d ⁸ 4s ²

Z	Symbol	Configuration as (core) plus "Outermost" orbitals
29	Cu	[Ar] 3d ¹⁰ 4s ¹
30	Zn	[Ar] 3d ¹⁰ 4s ²
31	Ga	[Ar] 3d ¹⁰ 4s ² 4p ¹
32	Ge	[Ar] 3d ¹⁰ 4s ² 4p ²
33	As	[Ar] 3d ¹⁰ 4s ² 4p ³
34	Se	[Ar] 3d ¹⁰ 4s ² 4p ⁴
35	Br	[Ar] 3d ¹⁰ 4s ² 4p ⁵
36	Kr	[Ar] 3d ¹⁰ 4s ² 4p ⁶ or [Kr]
37	Rb	[Kr] 5s ¹
38	Sr	[Kr] 5s ²
39	Y	[Kr] 4d ¹ 5s ²
40	Zr	[Kr] 4d ² 5s ²
41	Nb	[Kr] 4d ⁴ 5s ¹
42	Mo	[Kr] 4d ⁵ 5s ¹
43	Tc	[Kr] 4d ⁶ 5s ¹
44	Ru	[Kr] 4d ⁷ 5s ¹
45	Rh	[Kr] 4d ⁸ 5s ¹
46	Pd	[Kr] 4d ¹⁰
47	Ag	[Kr] 4d ¹⁰ 5s ¹
48	Cd	[Kr] 4d ¹⁰ 5s ²
49	In	[Kr] 4d ¹⁰ 5s ² 5p ¹
50	Sn	[Kr] 4d ¹⁰ 5s ² 5p ²
51	Sb	[Kr] 4d ¹⁰ 5s ² 5p ³
52	Te	[Kr] 4d ¹⁰ 5s ² 5p ⁴
53	I	[Kr] 4d ¹⁰ 5s ² 5p ⁵

Z	Symbol	Configuration as (core) plus "Outermost" orbitals
54	Xe	[Kr] 4d ¹⁰ 5s ² 5p ⁶ or [Xe]
55	Cs	[Xe] 6s ¹
56	Ba	[Xe] 6s ²
57	La	[Xe] 5d ¹ 6s ²
58	Ce	[Xe] 4f ² 5d ¹⁰ 6s ²
59	Pr	[Xe] 4f ² 6s ²
60	Nd	[Xe] 4f ⁴ 6s ²
61	Pm	[Xe] 4f ⁵ 6s ²
62	Sm	[Xe] 4f ⁶ 6s ²
63	Eu	[Xe] 4f ⁷ 6s ²
64	Gd	[Xe] 4f ⁷ 5d ¹ 6s ²
65	Tb	[Xe] 4f ⁹ 6s ²
66	Dy	[Xe] 4f ¹⁰ 6s ²
67	Ho	[Xe] 4f ¹¹ 6s ²
68	Er	[Xe] 4f ¹² 6s ²
69	Tm	[Xe] 4f ¹³ 6s ²
70	Yb	[Xe] 4f ¹⁴ 6s ²
71	Lu	[Xe] 4f ¹⁴ 5d ¹ 6s ²
72	Hf	[Xe] 4f ¹⁴ 5d ² 6s ²
73	Ta	[Xe] 4f ¹⁴ 5d ³ 6s ²
74	W	[Xe] 4f ¹⁴ 5d ⁴ 6s ²
75	Re	[Xe] 4f ¹⁴ 5d ⁵ 6s ²
76	Os	[Xe] 4f ¹⁴ 5d ⁶ 6s ²
77	Ir	[Xe] 4f ¹⁴ 5d ⁷ 6s ²
78	Pt	[Xe] 4f ¹⁴ 5d ⁹ 6s ¹

Z	Symbol	Configuration as (core) plus "Outermost" orbitals
79	Au	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ¹
80	Hg	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ²
81	Tl	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ¹ 6p ¹
82	Pb	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ² 6p ²
83	Bi	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ² 6p ³
84	Po	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁴
85	At	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁵
86	Rn	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁶ or [Rn]
87	Fr	[Rn] 7s ¹
88	Ra	[Rn] 7s ²
89	Ac	[Rn] 6d ¹ 7s ²
90	Th	[Rn] 6d ² 7s ²
91	Pa	[Rn] 5f ² 6d ¹ 7s ²
92	U	[Rn] 5f ³ 6d ¹ 7s ²
93	Np	[Rn] 5f ⁵ 6d ⁰ 7s ²
94	Pu	[Rn] 5f ⁶ 7s ²
95	Am	[Rn] 5f ⁷ 7s ²
96	Cm	[Rn] 5f ⁷ 6d ¹ 7s ²
97	Bk	[Rn] 5f ⁸ 6d ¹ 7s ²
98	Cf	[Rn] 5f ¹⁰ 7s ²
99	Es	[Rn] 5f ¹¹ 7s ²
100	Fm	[Rn] 5f ¹² 7s ²
101	Md	[Rn] 5f ¹³ 7s ²
102	No	[Rn] 5f ¹⁴ 7s ²
103	Lr	[Rn] 5f ¹⁴ 6d ¹ 7s ²

Z	Symbol	Configuration as (core) plus "Outermost" orbitals
104	Rf	[Rn] 5f ¹⁴ 6d ² 7s ²
105	Ha	[Rn] 5f ¹⁴ 6d ³ 7s ²
106	Sg	[Rn] 5f ¹⁴ 6d ⁴ 7s ²
107	Bh	[Rn] 5f ¹⁴ 6d ⁵ 7s ²
108	Hs	[Rn] 5f ¹⁴ 6d ⁶ 7s ²
109	Mt	[Rn] 5f ¹⁴ 6d ⁷ 7s ²
110	Ds	[Rn] 5f ¹⁴ 6d ⁸ 7s ²
111	Rg	[Rn] 5f ¹⁴ 6d ⁹ 7s ²
112	Cn	[Rn] 5f ¹⁴ 6d ⁹ 7s ²
113	Uut	[Rn] 5f ¹⁴ 6d ¹⁰ 7s ² 7p ¹
114	Fl	[Rn] 5f ¹⁴ 6d ¹⁰ 7s ² 7p ²
115	Uup	[Rn] 5f ¹⁴ 6d ¹⁰ 7s ² 7p ³
116	Lv	[Rn] 5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁴
117	UuS	[Rn] 5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁵
118	UuO	[Rn] 5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁶

1.6.4 Anomalies in Electronic Configurations

- Explain few anomalies present in elements in,
- (i) Transition series 1 with suitable examples
- (ii) Inner transition series - Lanthanons with examples".
- All the elements known are arranged in long form of periodic table in increasing order of atomic numbers - i.e. as per modern periodic law "the physical and chemical properties of elements are periodic functions of their atomic numbers."

(i) Transition series 1

The following anomalies are observed/shown in electronic configuration of certain elements in transition series 1 are considered as examples :

1. Chromium : Atomic number 24 : Transition series 1

3p⁶ 3d⁵ 4s¹ ...outer observed configuration



$3p^6 3d^4 4s^2$...outer observed configuration

2. Copper : Atomic number 29 : Transition series 1

$3p^6 3d^{10} 4s^1$...outer observed configuration

$3p^6 3d^9 4s^2$...outer expected configuration

Explanation

For such an anomaly is based on half filled and completely filled d-orbital, which an atom prefers.

3. Iron (Fe) : Atomic Number 26 : Transition series 1

$3p^6 3d^6 4s^0$...outer observed configuration

$3p^6 3d^4 4s^2$...outer expected configuration

Explanation

The observed electronic configuration is proved by experimental study, which is accounted for the ionization energy needed for the 4s and 3d electron.

(ii) In inner transition elements

The following anomalies observed.

1. Lanthanum : La Atomic number 57

$4d^{10}, 5s^2, 4p^6, 5d^1, 6s^2$...observed electronic configuration

$4d^{10}, 5s^2, 4p^6, 4f^1, 5d^0, 6s^2$...expected configuration

2. Palladium : Pd Atomic number 46

$5s^0, 4d^{10}$...observed electronic configuration

$5s^2, 4d^8$...expected electronic configuration

3. Silver : Ag : Atomic number 47

$5s^1, 4d^{10}$...observed electronic configuration

$5s^2, 4d^9$...expected electronic configuration

Explanation is based on half filled and completely filled d orbital.



1.7 The Molecular Orbital Theory

- The Molecular Orbital Theory was put forth in the 1930s by F Hund and R.S. Mulliken and later it was developed by J.E. Lennard-Jones and Charles Coulson.
- Earlier to this valence bond theory was also proposed by Linus Pauling. The two theories reflect distinctly different conceptual approaches to the basic structural model of a molecule. For example, according to VBT only the half filled atomic orbitals of one atom overlaps with the half filled atomic orbital of the other atom resulting in the formation of a covalent bond. Their completely filled atomic orbitals remain intact. But in MOT, the nuclei of the two atoms lie at appropriate distance so that all the atomic orbitals of one atom overlap with all the atomic orbital of the other atom provided the overlapping orbitals are of the same symmetry.



$$\text{Bond order} = \frac{1}{2}(8 - 4) = 2$$

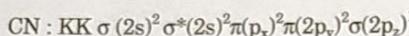
Evidently, the species NO^+ has the highest bond order and thus has the shortest bond length.

Ex. 1.8.3 : Compare the bond energy, bond length and magnetic character of CN and CN^- species with the help of molecular orbital theory.

Soln. : In order to compare bond energy and bond length,

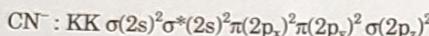
We shall first calculate bond orders for these species from their electronic configurations.

CN has 13 electrons and its electronic configuration is



$$\text{Bond order} = \frac{1}{2}(7 - 2) = 2 \frac{1}{2}$$

CN^- : In this case, one electron is added to $\sigma(2p_z)$ MO so that its electronic configuration is



$$\text{Bond order} = \frac{1}{2}(8 - 2) = 3$$

Since CN^- has a higher bond order, it has larger bond energy and smaller bond length than CN . Further since there is one unpaired electron in $\sigma(2p_z)$ MO of CN , it will be paramagnetic. But CN^- is evidently diamagnetic.

Summary

Atomic and Molecular Structure

According to Dalton's theory, the following postulates had been put forth.

- All elements are made up of small tiny particles called as "atoms".
- In an element, all 'atoms' are always of same masses and sizes, and the properties of all atoms also same whereas, atoms of different elements have all varying mass, size and properties. In short, "No two elements are same".
- This smallest particle 'atom' cannot be divided or formed or destroyed.

Rutherford's Atomic Model

In 1911 Lord Rutherford performed an experiment popularly known as " α -particle scattering experiment".

Experimental details

All components of scattering experiment were arranged in place and the beam of α -particles was released from source. This beam was made to strike the thin gold foil and the direction in which deflected rays struck the screen were observed.

Conclusions by Rutherford

- Every atom possesses a nucleus at centre. Such nucleus is rigid, positively charged and dense in nature. The positive charge is due to "protons" - positively charged particles. It also has neutral particles known as "neutrons".
 - Every atom is a neutral particle because its positive charge is equally compensated by 'electrons', i.e. negatively charged particles which are revolving around the nucleus in circular orbits.
- "The number of protons = The number of electrons".



Definition of Proton

- A proton is defined as "a hydrogen atom converted in hydrogen ion with positive charge due to loss of one electron having only nucleus with a positive charge".

Drawbacks of Rutherford's Atomic Model

The following are major drawbacks of Rutherford's nuclear atomic model :

- Behavior of electrons :** It fails to explain behavior of electrons in an atom.
- Stability of atom :** It fails to explain the stable nature of an atom because, according to electromagnetic theory, if an electron i.e. a charged particle is in fast motion, it tends to release light radiations and hence it fails to maintain its rotation along a specific path. i.e. orbit. Hence, the curvature of spiral path would go on decreasing and ultimately the particle i.e. electron would also come closer to nucleus and fall into it. Thus atom would be unstable. But in reality atom is absolutely stable, which is unexplained by Rutherford.

Bohr's Atomic Theory

Niels Bohr put forth an atomic model with following objectives :

- To overcome the entire drawback in Rutherford's nuclear atomic model.
- To explain the spectrum of hydrogen or hydrogen like molecules.
- Postulates of Bohr's atomic model
- Significance/Advantages of Bohr's Atomic Model
- The above expression could give,
 - The radius of n^{th} orbit,
 - Velocity and energy of an electron revolving in the n^{th} orbit.
- Drawbacks/Limitations of Bohr's Atomic Model

- Zeeman effect
- Stark effect
- Atomic Spectrum of Hydrogen Atom
- Structure of Hydrogen Atom
- Quantum Mechanical Model
- Schrödinger's wave equation

Quantum Numbers

The wave equation for hydrogen atom, when solved, which gave rise to idea of "quantum numbers".

The four quantum numbers and their notations are,

- Principal quantum number (n)
- Azimuthal quantum number (l)
- Magnetic quantum number (m)
- Spin quantum number (s)

Atomic orbitals (s,p,d,f) orbital shapes

Hydrogenic Energy Levels

Transitions Between Energy Levels

An electron can change energy levels by absorbing energy to move to a higher energy level or by emitting energy to move to a lower energy level.

Shells

- The location of a **shell** and the electrons in it is indicated by a number n assigned to the **shell**.
- The value of n is as 1, 2, 3, 4, etc.

Subshells

- Each **shell** is made up of one or more **subshells** that are designated by a letter as *s*, *p*, *d*, or *f*.
- The number of the **shell** to which a **subshell** belongs is given as :
- For example, a *p* **subshell** located in the fourth **shell** ($n = 4$) would be designated as a *4p subshell*.
- The number of **subshells** in a **shell** is the same as the number of the **shell**. Thus, **shell** number 3 ($n = 3$) has three **subshells** designated as *3s*, *3p*, and *3d*.



= 3) contains three subshells, designated 3s, 3p, and 3d.

- Electrons located in a subshell are often identified by using the same designation as the subshell they occupy. Thus, electrons in a 3d subshell are called 3d electrons

Orbitals

s orbitals: correspond to $l = 0$ and $ml = 0$

- All s subshells consist of a single s orbital.
- All p subshells consist of three p orbitals.
- All d subshells consist of five d orbitals.
- All f subshells consist of seven f orbitals.

Electron Spin

Electronic Configuration

Pauli's exclusion principle

- Pauli's exclusion principle states that, "No two electron in an atom can have identical set of all four quantum numbers".
- This principle indicates that in any atom only two electrons can be placed in one single orbital with set of values as $n = l = m \neq s$.
- When two electrons with same 's' value come together, they get repelled, and hence switch to other orbital. Thus for two electrons to be in 'same' orbital must have 'opposite' spins.

Hund's rule of maximum multiplicity

This rule defines :

- (i) Maximum number of electrons in an orbital with specified set of quantum numbers with opposite spins must be only '2'.
- (ii) If $n = l = m = s$, then in an orbital only '1' electron gets place and it remains unpaired.
- (iii) In any subshell, the electrons always enter in empty orbital first.

E.g. Suppose 2p subshell, Here $n = 2$, $\therefore l = 1$:

orbitals = $(2l + 1) = 3$,

Penetration Power/effect of orbital

- Penetration Power is defined as "the ability of orbital to attract an electron".

Shielding effect

- The shielding effect describes the attraction between an electron and the nucleus in any atom with more than one electron shell.
- Shielding effect can be defined as "a reduction in the effective nuclear charge on the electron cloud, due to a difference in the forces of attraction of the electrons on the nucleus".
- The shielding effect, is prominent in "many electron atoms".

Aufbau principle

- The rule states that, "when an atom is in ground state, the electrons tend to occupy the lowest energy orbital available". Conversely, "the electrons enter the orbitals successively in order of increasing energies".

Anomalies in electronic configurations

- Explain few anomalies present in elements in
 - (i) Transition series 1 with suitable examples
 - (ii) Inner transition series - Lanthanons with examples".
- All the elements known are arranged in long form of periodic table in increasing order of atomic numbers - i.e. as per modern periodic law "the physical and chemical properties of elements are periodic functions of their atomic numbers."

The Molecular Orbital Theory

- The Molecular Orbital Theory was put forth in the 1930s by F Hund and R.S. Mulliken and later it was developed by J.E. Lennard-Jones and Charles Coulson.

**Review Questions**

- Q. 1 What is Rutherford's atomic model ?
- Q. 2 Explain Rutherford's atomic model, giving the experimental details. What were major conclusions by Rutherford?
- Q. 3 Give limitations of Rutherford's atomic model.
- Q. 4 Define proton.
- Q. 5 Discuss Bohr's modification of Rutherford's atomic model.
- Q. 6 Explain Bohr's atomic model.
- Q. 7 Describe Bohr's atomic theory for hydrogen atom.
- Q. 8 What are the advantages of Bohr's Atomic Model ?
- Q. 9 Discuss limitations of Bohr's atomic model.
- Q. 10 List different quantum numbers with their notations.
- Q. 11 Compare and contrast an orbit and an orbital.
- Q. 12 What is the concept of electron charge cloud and an atomic orbital?
- Q. 13 State "Hund's rule of maximum multiplicity" of electrons in an orbital. Explain with one example.
- Q. 14 State "Aufbau principle / $(n + l)$ rule. Give series of orbitals in order of energy level. Give schematic diagram of energy levels.

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