ATOMIC STRUCTURE

B.Sc.-I Chemistry(H/S)
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Paper-I(B)
Lecture-03

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ATOMIC STRUCTURE

Shapes of orbitals in chemistry

Orbitals

- **Orbits** are the energy level where electron move while the **orbital** is the path where electron move around the central nucleus .
- A large number of orbitals are possible in an atom
- An orbital cann be distinguished by their shape,size and orientation
- K,L,M, and N etc are the shell and s,p,d,f are the **subshells**.

An atomic orbital is a mathematical function that describes the wave-like behavior of electron (one electron or a pair of electrons) in an atom in atomic theory and quantum mechanics

This mathematical function can be used to calculate the probability of finding any electron(which is maximum).

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Orbitals	Value of n	Value of l	Value of (n+l)	
1s	1	0	1+0=1	
2s	2	0	2+0=2	
2p	2	1	2+1=3	2p(n=2)
3s	3	0	3+0=3	3s(n=3)
3p	3	1	3+1=4	3p(n=3) has lower energythan
4s	4	0	4+0=4	4s(n=4)
3d	3	2	3+2=5	3d(n=3)has lower energythan
4p	4	1	4+1=5	4p(n=4)

Arragements of orbitals with icreasing energy(n+l) value

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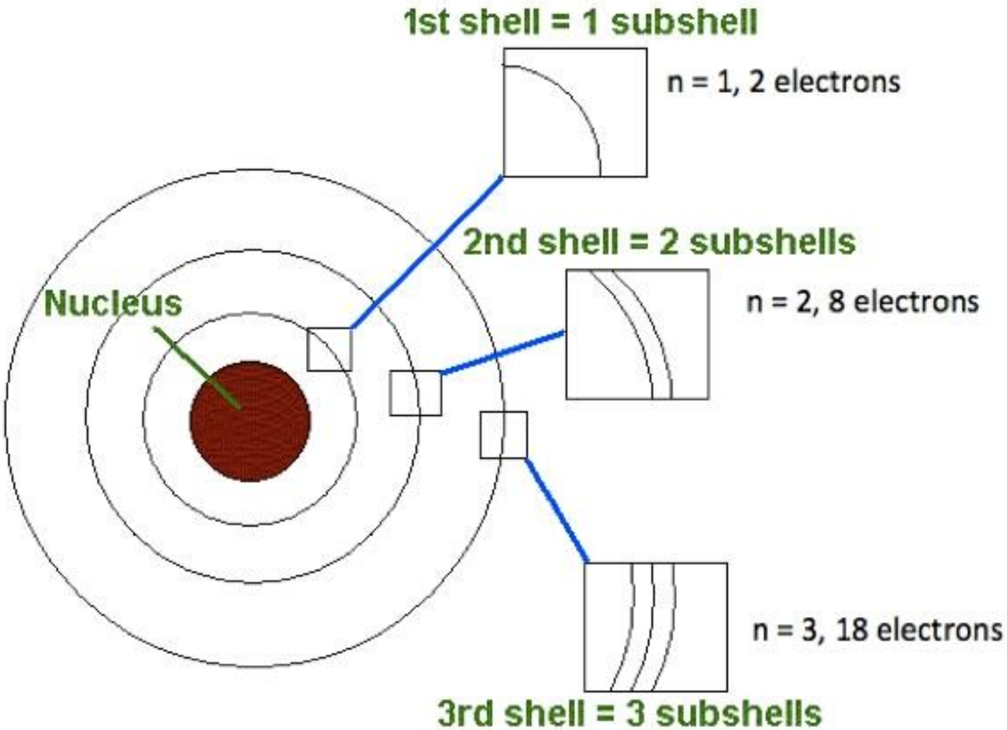

Principal Quantum Number: Subshells and Electrons

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Idea of quatum numbers

Shapes of atomic orbitals

- The atomic orbitals differ in shape.
- The electrons they describe have different probability distributions around the nucleus
- The electron is more likely to be found somewhere inside the spherical boundary surface than outside it.
- An orbital is a wave function for an electron defined by the mainly three quantum numbers, n, ℓ and m_l. ...

There are **four** types of **orbitals**

s **sharp**

p **principle**

d **diffuse**

f **fundamental**

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Quantum numbers often describe specifically the energy levels of electrons in atoms

Four quantum numbers n, ℓ, m_l and m_s which respectively correspond to the electron's energy,angular momentum magnetic quantum number spin quantum number

Each such orbital can be occupied by a maximum of two electrons, each with its own spin quantum number *s*.

s orbital quantum number $\boldsymbol{\ell = 0}$ spherical shaped

p orbital quantum number $\boldsymbol{\ell = 1}$ dumb-bell shaped five different types of sub-orbitals,labeled by

$\mathbf{m_l = -1, 0\ 1}$

d orbital quantum number $\boldsymbol{\ell = 2}$ double dumb-bell shaped five different types of sub-orbitals, labeled

$\mathbf{m_l = -2, -1, 0\ 1, 2.}$

f orbital quantum number $\boldsymbol{\ell = 3}$ seven different types of sub-orbitals, labeled by

$\mathbf{m_l = -3-2, -1, 0\ 1, 2,3.}$

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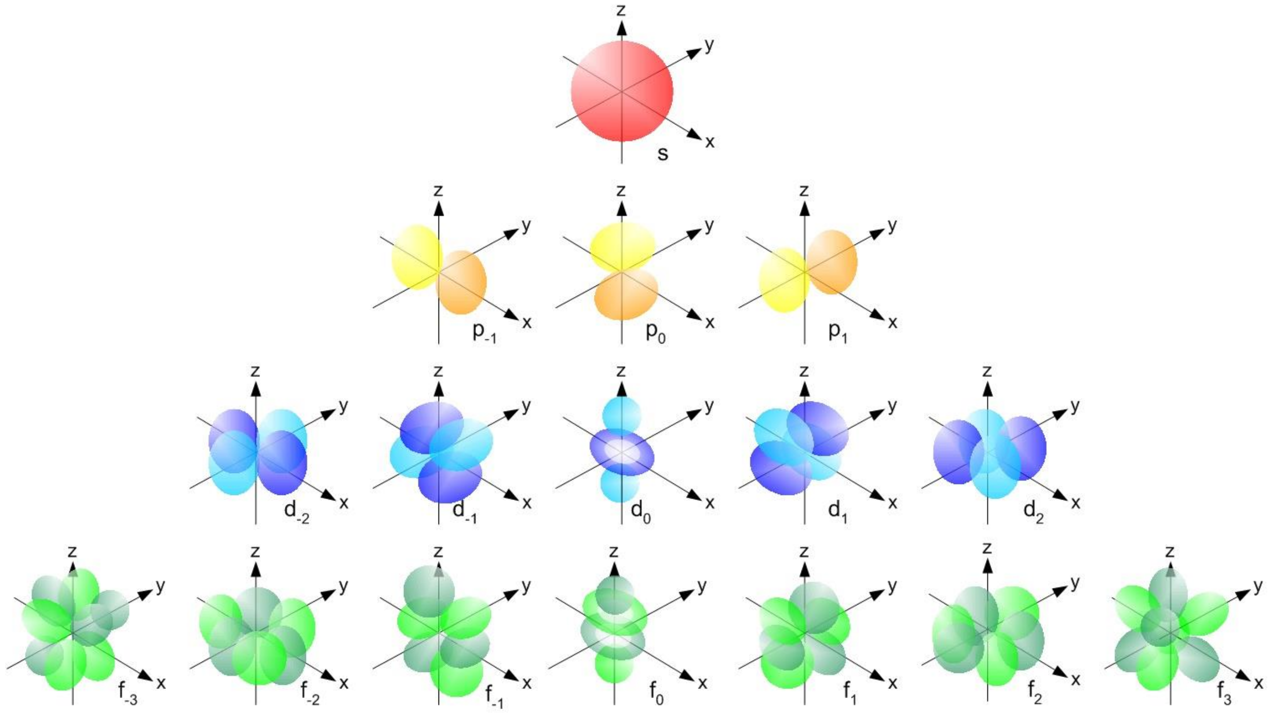

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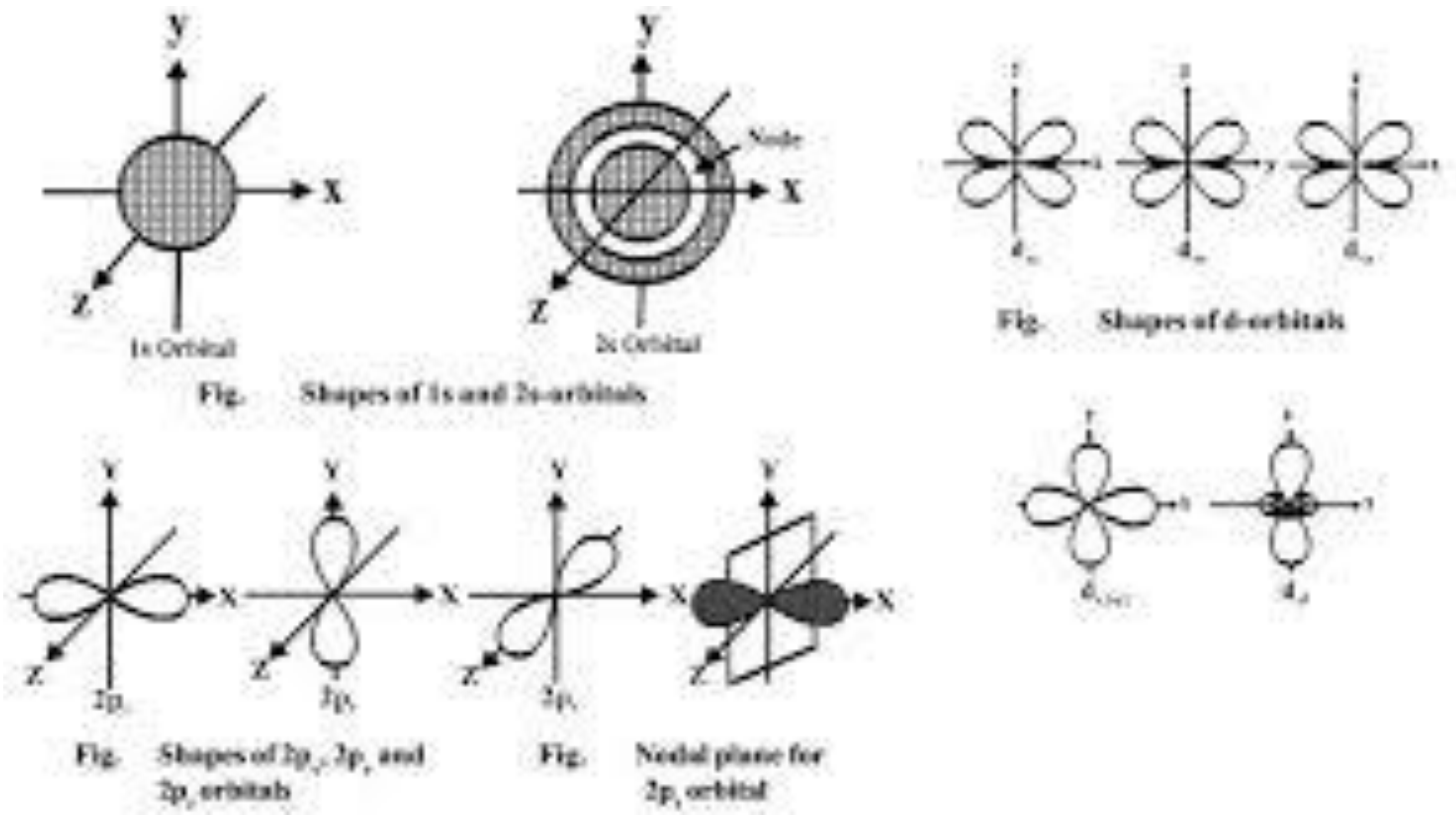

3possible arragement of p- **orbitals** are always perpendicular to each other

5possible arragement of d-**orbital**

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Labelling idea of quantum numbers

- A **quantum number** is a value that is used to describe the energy levels available to atoms and molecules.
- Used to completely **describe** an electron in an atom, four quantum numbers have been given

Significance of quantum numbers

- Used to determine the electron configuration of an atom and the probable location of the atom's electrons.
- Used to determine other characteristics of atoms, such as ionization energy and the atomic radius

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Principal quantum number numer (represented by n) :

Describes the electron shell or energy level of an atom and size of the orbital.

$$n = 1, 2, ...$$

Angular momentum quantum number l (represented by ℓ):

The number of subshells or l, describes the shape of the orbital and also the magnitude of the orbital angular momentum through the relation

$$L^2 = \hbar^2 \ell (\ell + 1)$$

$$\ell = 0, 1, 2, ..., n - 1$$

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Azimuthal quantum nnumber m (represented by m_ℓ):

Describes the specific orbital (or "cloud") within that subshell or describe orital orietation

m_ℓ range from $-\ell$ **to** ℓ,

Spin quantum number s (represented by m_s):

Describes the spin of the electron within that orbital or defines electron spin direction

$$m_s = -s, -s+1, -s+2, ..., s-2, s-1, s$$

where m_s **±1/2**, spin of electron

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Pauli Exclusion Principle :

In 1925 Austrian physicist **Wolfgang Pauli** formulated this priciple for electrons

- It states that, no two electrons in an atom or molecule can have the identical set of four quantum numbers.
- An orbital can contain a maximum of only two electrons, the two electrons must have opposite spins
- every electron must be in its own unique state

For example, if the orbital have two electrons then their ***n***, ***ℓ***, and m_ℓ values are the same, but their m_s must be different, and thus the electrons must have opposite half-integer spin 1/2 and −1/2.

Application:

Pauli exclusion principle is applied solely to electrons.

Importance

- Helps to explain a wide variety of physical phenomena.
- Helps to explain a variety of chemical elements and their chemical combinations.

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Hunds rule

- In 1927 German physicist Friedrich Hund gave a set of rule
- Every orbital in a subshell is singly occupied with one electron before any one orbital is doubly occupied, and all electrons in singly occupied orbitals have the same spin.
- Used to determine the term symbol that corresponds to the ground state of a multi-electron atom.

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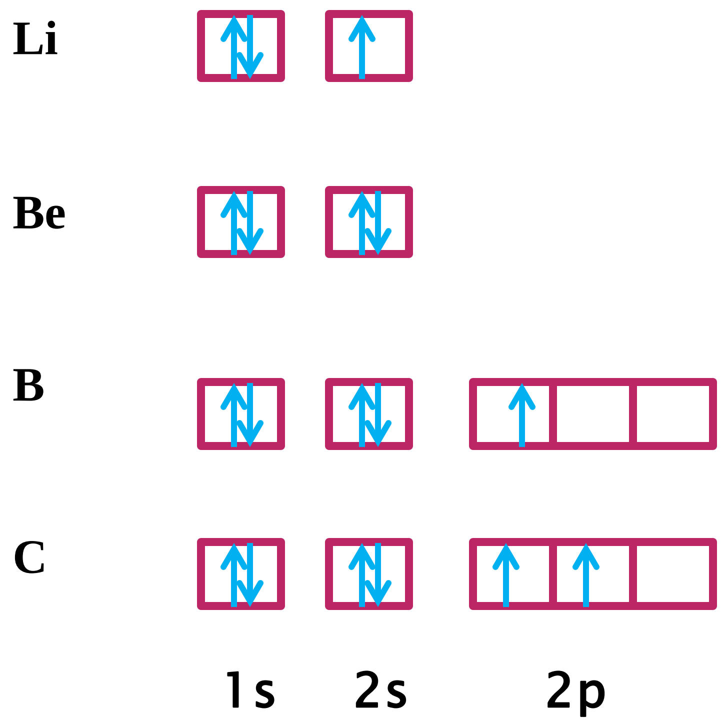

The third electron of lithium is not allowed in the 1s orbital because of pauli exclusion principle
In B and C the 2p orbital gets progressively filled because of Hund's rule pairing of electrons does not take place until each orbital is singly filled.

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Rules are:

- For a given electronic configuration ,the term with maximum multiplicity has the lowest energy.
- The multiplicity is equal to **2S+1** where S total spin angular momentum for all electrons. The multiplicity is also equal to the number of unpaired electrons plus one..

- For a given multiplicity, the term with the largest value of the total orbital angular momentum quantum number L has the lowest energy.
- For a given term, in an atom with outermost subshell half-filled or less, the level with the lowest value of the total angular momentum quantum number J(for the operator =L+S lies lowest in energy. If the outermost shell is more than half-filled, the level with the highest value of J is lowest in energy.

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A German scientist ***Aufbauprinzip*** gave the **aufbau rule**(which means "built up“)

This principle states that in the ground stat of an atom or ion, electrons fill atomic orbitals of the lowest available energy levels before occupying higher levels i.e lower electron orbitals is filled before higher orbitals

Thus orbitals are filled in the order of increasing energy, using two general rules to help predict electronic configurations:

1. Electrons are assigned to orbitals in order of increasing value of $(n+\ell)$.

2. For subshells with the same value of $(n+\ell)$, electrons are assigned first to the sub shell with lower n.

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Exception of Aufbau principle

- According to the **Aufbau principle**, these electrons should always fill shells and subshells according to increasing energy levels.
- Elements such as copper and chromium are **exceptions** because their electrons fill and half-fill two subshells, with some electrons in the higher energy level shells
- Like most rules, there are exceptions. Half-filled and completely filled d and f subshells add stability to atoms, so the d and f block elements don't always follow the principle. For example, the predicted Aufbau configuration for Cr is $4s^2 3d^4$, but the observed configuration is actually $4s^1 3d^5$. This actually reduces electron-electron repulsion in the atom, since each electron has its own seat in the subshell.

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The order in which the energies of the orbitals increase

Hence,the order in which the orbitalsare filled is as follows:

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

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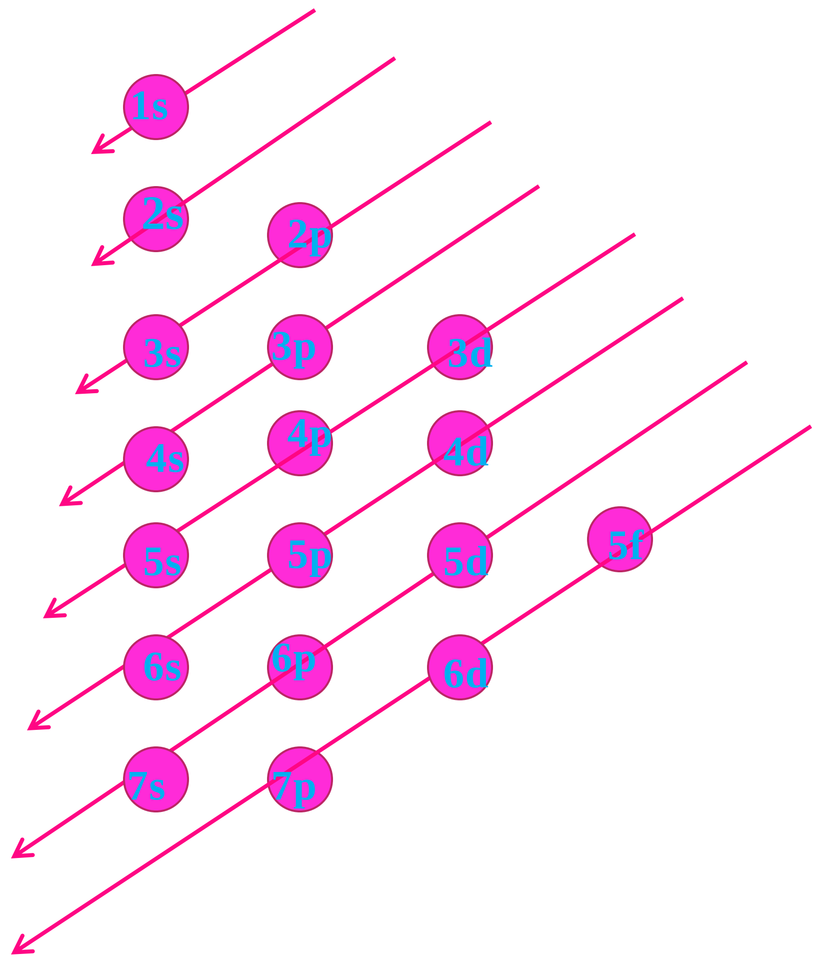

Order of filling of orbitals

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- Aufbau principle, electrons are added to orbitals as protons are added to an atom.
- The Aufbau principle is used to determine how electrons organize into shells and subshells around the atomic nucleus.
- Electrons go into the subshell having the lowest possible energy.
- Electrons obey Pauli exclusion principle, an orbital can hold at most 2 electrons
- Electrons obey Hund's rule, which states that pairing of electrons doesnnot take place unless they are singly filled, if there are two or more energetically equivalent orbitals (e.g., p, d).

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1.Problem for practice:

What is the total number of oritals associated with the principle quantum number

a) n=2

b) n=3

c) n=4

2. Using s,p,d,f notation,describe the orbital

a) n=4,l=2

b) n=4,l=3