

Aufbau Principle :-

According to Aufbau rule electrons first occupy the lowest energy orbital then enter into higher energy orbitals.

Energy of orbitals is defined by $(n+l)$ value, where n is Principal quantum number or number of shell and l is azimuthal quantum number.

For example $n=1$ for 1st shell
 $n=2$ for 2nd shell
 $n=3$ for 3rd shell - - - etc.

And value of l is

0 for s - sub shell
 1 for p, sub-shell
 2 for d, sub-shell
 & 3 for f sub-shell

The maximum number of electrons in s-sub-shell is 2.
 " " " " p, sub-shell is 6.
 " " " " d, sub-shell is 10.
 " " " " f, sub-shell is 14.

(2) If the value of $(n+l)$ is same for two orbitals, then the electron will be filled first which has lower value of n .

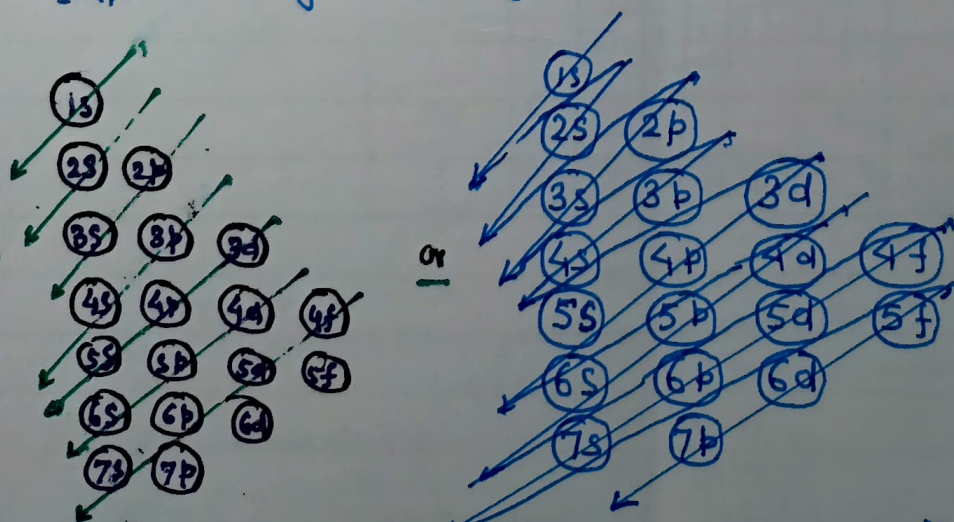
For example, 3p and 4s orbital are present both orbitals have $(n+l)$ value same. i.e 4.

$$3p \rightarrow (n+l) \rightarrow (3+1) = 4$$

$$4s \rightarrow (n+l) \rightarrow (4+0) = 4$$

Then electrons will be enter in 3p first than 4s.

Important diagram regarding Aufbau rule is illustrated below.



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

We have found the sequence of lower to higher order of energy level i.e. 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s

After substituting the maximum number of electron in above sub-shell, we get $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}, 5p^6, 6s^2, 4f^{14}, 5d^{10}, 6p^6, 7s^2$

The above str. is very helpful in writing the electronic configuration of atoms sub-shell wise.

Pauli Exclusion Principle: - No two electrons in an atom can have the same set of all four quantum numbers.

If $n = 1$, Maximum number of electrons = $\frac{2n^2}{n=1} = 2 \times 1^2 = 2$

Q. No.	l_1	l_2
n	1	1
l	0	0
m	0	0
s	$+\frac{1}{2}$	$-\frac{1}{2}$

If $n = 1$
 l value = 0 to $(n-1) = 0$ to $(1-1) = 0$ to $0 = 0$
 m value = $-l$ to $+l = -0$ to $+0 = 0$

If $n = 2$, Maximum no of electron = $\frac{2n^2}{n=2} = 2 \times 2^2 = 2 \times 4 = 8$

It means in 2nd shell, two sub-shell s and p are present containing 2 and 6 electrons, hence sum of these are eight.

$n = 2$

Quantum Number	Subshell s		Subshell p					
	l_1	l_2	l_3	l_4	l_5	l_6	l_7	l_8
n	2	2	2	2	2	2	2	2
l	0	0	1	1	1	1	1	1
m	0	0	-1	-1	0	0	+1	+1
s	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$

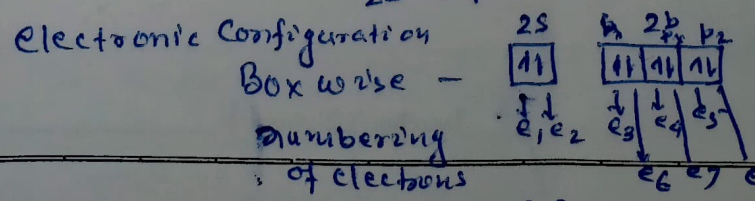
For $p \neq l = 1$
 $m = -1, 0, +1$
 $p_x \quad p_y \quad p_z$

-1	0	+1
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Each box contains two electrons filled by Hund's rule

Eight electron in 2nd shell
 It's electronic configuration sub-shell wise.

$1s^2 2s^2 2p^6$ [Two electrons of s and six electrons of p-sub-shell]



$e_1 e_2, e_3 e_6, e_4 e_7, e_5 e_8$ [According to Hund's rule]

Maximum Number of Electrons in Sub-shell is governed by $(4l+2)$, where l is Azimuthal quantum number

l value	Name of sub-shell
0	s
1	p
2	d
3	f

Number of maximum electrons in sub-shells by $(4l+2)$.

For s, No of electrons = $(4 \times 0 + 2) = (0 + 2) = 2$

For p, No of electrons = $(4 \times 1 + 2) = (4 + 2) = 6$

For, d, No. of electrons = $(4 \times 2 + 2) = (8 + 2) = 10$

for, f, No of electron = $(4 \times 3 + 2) = (12 + 2) = 14$

It may be written as, s^2, p^6, d^{10}, f^{14}

Hund's rule of maximum multiplicity.

Hund's rule of maximum multiplicity or simply Hund's rule states that electron pairing will not take place in orbitals of same energy (same sub-shell) until each orbital is singly filled.

Importance of this principle is in guiding the filling of 'p', 'd' and 'f' orbital by electrons, because they have more than one kind of orbitals.

For example there are three p orbitals (p_x, p_y and p_z) of the p sub-shell

According to Hund's rule each of the three p orbitals must get one electron of parallel spin before any one of them receives the second electron of opposite spin.

For example:- Hydrogen, H, Atomic number = 1, $1s^1$, $\begin{matrix} 1s \\ \boxed{1} \end{matrix}$
 Helium, He, Atomic number = 2, $1s^2$, $\begin{matrix} 1s \\ \boxed{1} \\ \boxed{1} \end{matrix}$
 Lithium Li, " Z = 3, $1s^2 2s^1$, $\begin{matrix} 1s & 2s \\ \boxed{1} & \boxed{1} \\ \boxed{1} & \end{matrix}$
 Carbon, C, Z = 6, $1s^2 2s^2 2p^2$

Electronic Configuration of C is $1s^2 2s^2 2p^2$

Boxwise Configuration

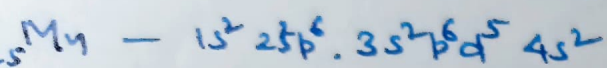
$\begin{matrix} 1s & 2s & 2p \\ \boxed{1} & \boxed{1} & \boxed{1} \ \boxed{1} \end{matrix}$ — Normal state

$\begin{matrix} 1s & 2s & 2p_x & 2p_y & 2p_z \\ \boxed{1} & \boxed{1} & \boxed{1} & \boxed{1} & \end{matrix}$ — Excited state

So, it is also helpful to explain the tetravalency of Carbon and etc.

In term of multiplicity Hund's rule may be explained as follows
 they have the tendency to remain unpaired so as it have maximum multiplicity minimum energy and maximum stability

This rule clearly understood by the following example



$$\text{Spin multiplicity} = (2S+1)$$

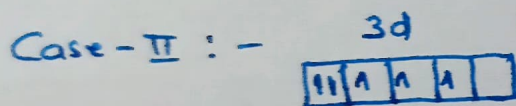
where S is total spin

The distribution of d electrons of Mn may be as follows



In this case Total spin of d electron = $5 \times \frac{1}{2} = \frac{5}{2}$ [\because Five electrons of d orbitals are unpaired]
 i.e $S = \frac{5}{2}$

$$\text{Spin multiplicity} = (2S+1) = (2 \times \frac{5}{2} + 1) = (5+1) = 6$$



In this case II Total spin of d electrons = $3 \times \frac{1}{2} = \frac{3}{2}$ [\because Three electrons are unpaired]

$$\therefore \text{Spin multiplicity} = (2S+1) = (2 \times \frac{3}{2} + 1) = (3+1) = 4$$



In case III Total spin of d electrons = $1 \times \frac{1}{2} = \frac{1}{2}$

$$\text{Spin multiplicity} = (2S+1) = (2 \times \frac{1}{2} + 1) = 2$$

In all the above three cases of distribution of d electrons of Mn in Case I is valid because it has maximum spin multiplicity value i.e Six, so it has minimum energy and maximum stability.