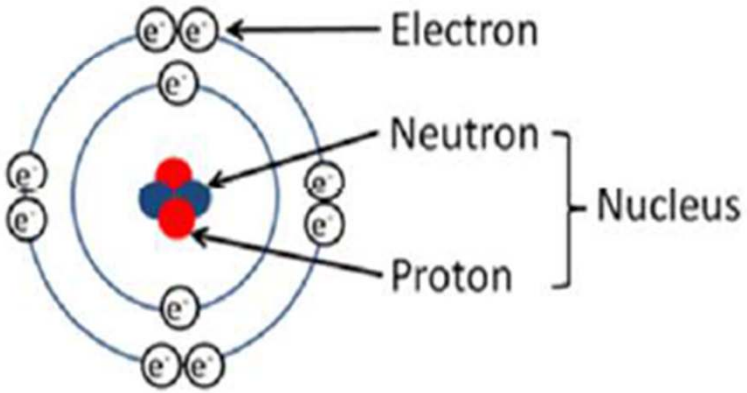
Inorganic Pharmaceutical Chemistry

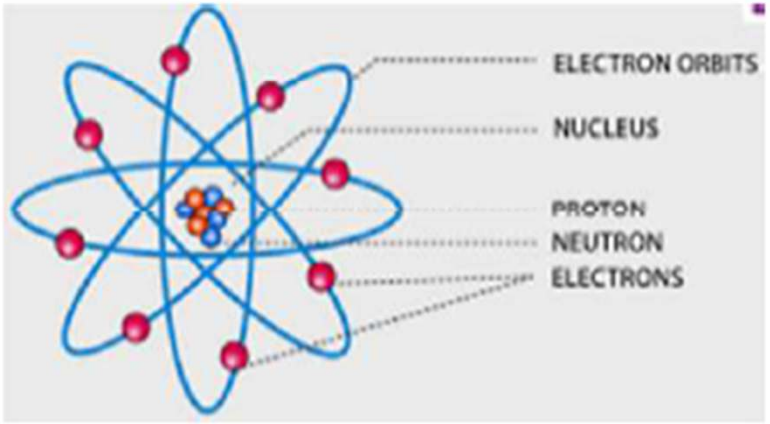
3rd Stage – 1st Semester

Lecture 7

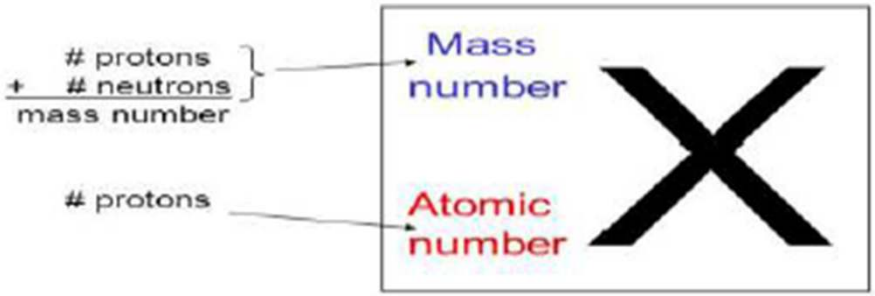
Atomic Structure:

Atoms composed of central nucleus in which the protons (positively charged) and neutrons (neutral) are present. The negatively charged particles called electrons surround the nucleus and occupy discrete regions of space.





In neutral atom, number of electrons is equal to number of protons. The atomic number is the number of protons in the nucleus of an atom. While the atomic mass number is the total number of protons and neutrons in an atomic nucleus. The mass number is different for each different isotope of a chemical element because isotopes of an element have the same number of protons but differ in number of neutrons in each atom.



$^{4}_{2}He$

$^{12}_{6}C$

Atomic Orbitals:

Atomic Orbital is the space or region around the nucleus where the electrons are present. It is a mathematical function describing the location and behavior of an electron in an atom. This function can be used to calculate the probability of finding any electron of an atom in any specific region around the atom's nucleus. Each orbital is denoted by a number and a letter. The number denotes the energy level of the electron in the orbital. Thus (1) refers to the energy level closest to the nucleus; (2) refers to the next energy level further out, and so on.

- The electrons are described by a set of four numbers called "quantum numbers".
- The number of protons determines the identity of the element.
- The number of electron determines the charge.
- The number of neutrons determines the isotope.

Heisenberg (uncertainty) Principle states that it is not possible to fix simultaneously the momentum and the position of an electron. This makes it impossible to know exactly where an electron is traveling in an atom. Heisenberg's uncertainty principle is a key principle in quantum mechanics. According to the Heisenberg Uncertainty Principle, we cannot precisely measure the momentum and position of an electron at the same time. As the momentum of the electron is more and more certain, the position of the electron becomes less certain, and vice versa.

Since it is impossible to know where an electron is at a certain time, a series of calculations are used to approximate the volume and time in which the electron can be located (i.e) in which Atomic Orbitals, also known as the quantum states of the electrons,. Therefore, the location, volume and time of the electrons in atoms and molecules be determined in term of probability. The four quantum numbers set the probability limits within which an electron can be found.

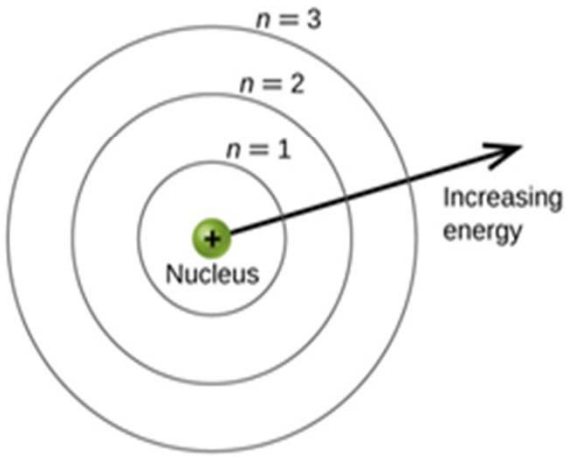
The four quantum numbers:

1- The Principal Quantum Number (n):

Describes the energy of an electron and the most probable distance of the electron from the nucleus. In other words, it refers to the size of the orbital and the energy level an electron is placed in.

Quantum theory states that electrons in atoms exist in discrete energy levels. indicates the shell or energy level in which the electron is found. It determines the distance of the electrons from nucleus. The energy associated with the electron increases as it locate farther from the nucleus. Because (n) describes the most probable distance of the electrons from the nucleus, the larger the number (n) is, the electron is farther from the nucleus, the larger size of the orbital and the more energy level. (n) can be any positive integer number starting at 1, n=1,2,3,4…

The first principal shell is called the ground state or lowest energy state (n =1). (n = 2) indicates the second principal shell. (n = 3) indicates the third principal shell. (n = 4) indicates the fourth principal shell, and so on.



2- The Angular Momentum Quantum Number (l):

It also called as Suborbital Quantum Number, and Azimuthal Quantum Number. This number determines the shape of an orbital, and therefore the angular distribution. It can be an integer number starting at 0, $l = 0,1,2,3,4\ldots$,

Angular Momentum Quantum Number (l)	Subshell
0	s
1	p
2	d
3	f

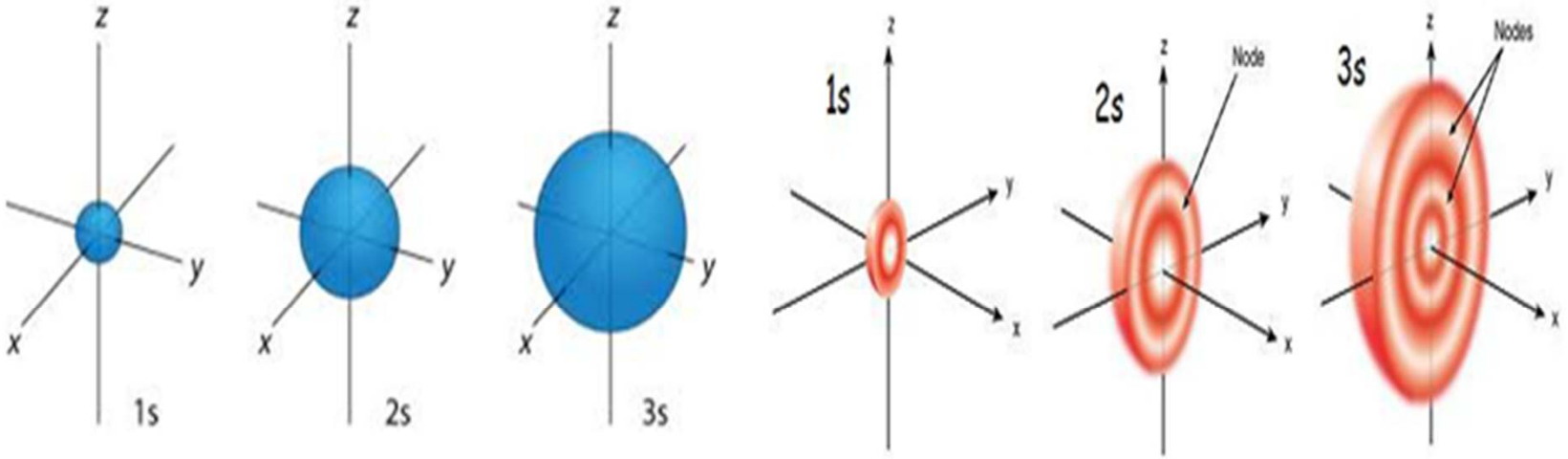
The angular momentum quantum number values range from 0 to (n - 1), and cannot be greater than (n) (i.e) max. (n - 1)

(n)	(l) Range 0- (n-1)	Subshell
1	0	s one subshell
2	0 1	s p two subshells
3	0 1 2	s p d three subshells
4	0 1 2 3	s p d f four subshells

Different shapes of orbitals are drawn depending on the possibility of finding electrons around the nucleus. The shapes of these orbitals are discussed below:

I- s-orbitals shape:

s-orbitals are spherical with the nucleus at the center, symmetrical and non-directional. The size of an orbital increases as the principal quantum number increases, thus a 2s-orbital is larger than 1s-orbital. A 2s-orbital differs from 1s-orbital in having a nodal surface. A nodal surface is the region in space where the probability of finding electron is zero.

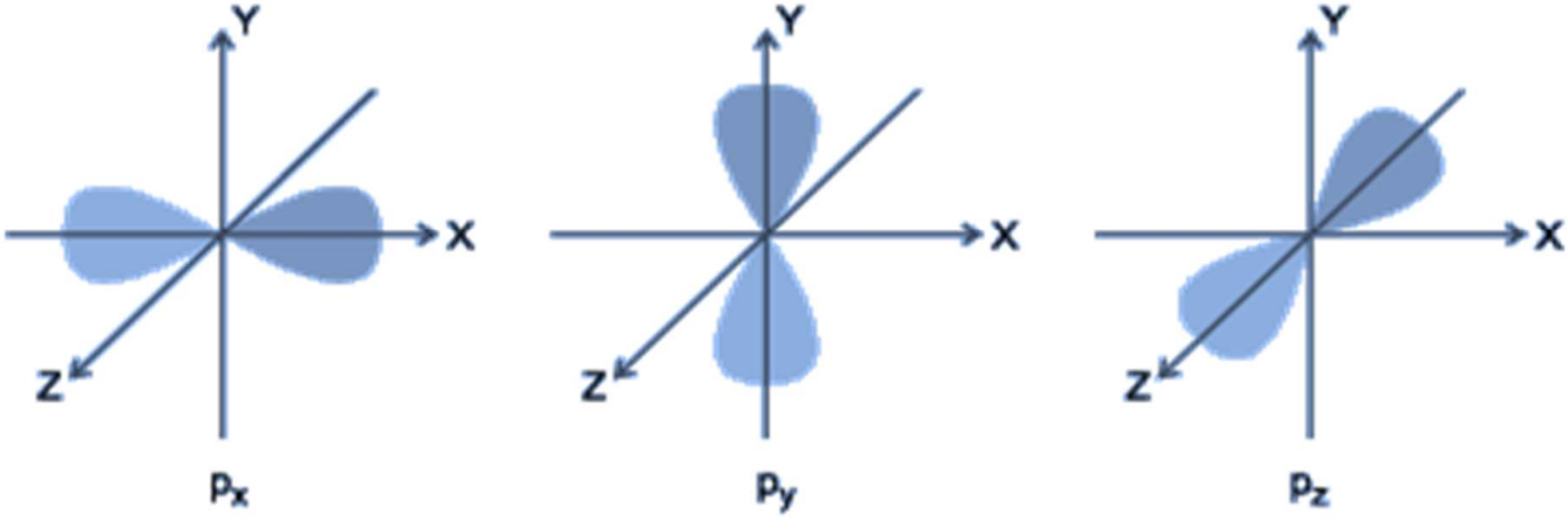


- Value of $l = 0$.
- Radius of sphere increases with increasing value of n.

II- p Orbitals shape: (Shaped like two balloons tied together)

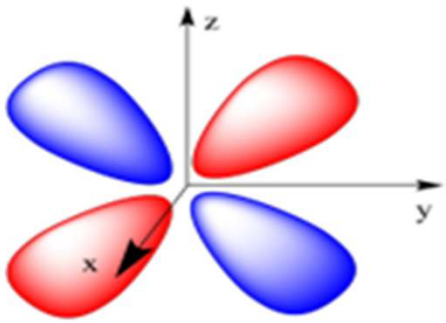
There are 3 orbitals in a p subshell that are denoted as px, py, and pz orbitals. These are higher in energy than the corresponding s orbitals. The probability of finding an electron is maximum in two lobes on opposite side of the nucleus. Unlike s-orbitals, p-orbitals are directional in nature.

- Value of $l = 1$
- Have two lobes with a node between them.
- All the three p-orbitals have same energy and thus are called degenerate orbitals.
- For each p-orbital, there is a plane passing through the nucleus where the probability of finding electron is zero. This is called nodal plane. For example, in orbital, node is in the yz plane; in orbital, node is in the xz plane and in orbital, node is in the xy plane.

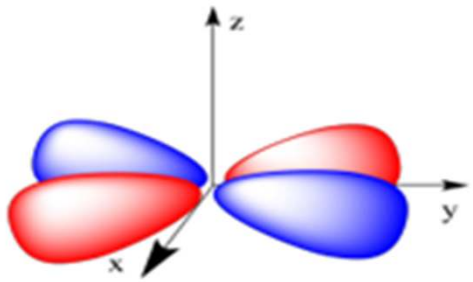


III-d-Orbitals Shape:

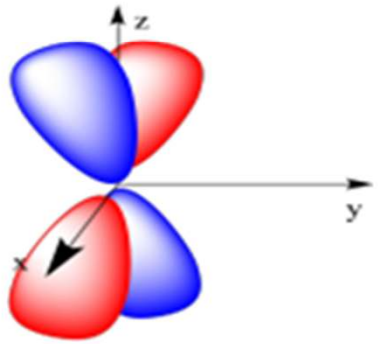
The d subshell is divided into 5 orbitals (d_{XY}, d_{XZ}, d_{YZ} , d_{Z^2} and $d_{X^2-Y^2}$). These orbitals have a very complex shape and are higher in energy than the S and P orbitals. These five d-orbitals which are directional and of same energy. Four of the five d-orbitals are double dumbbell shaped. They are also said to have a clover-leaf shape:



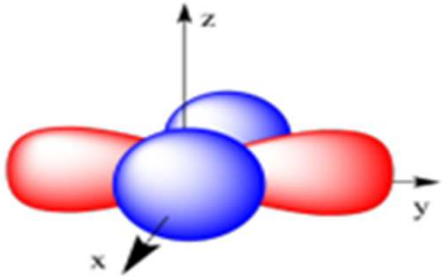
d_{yz}



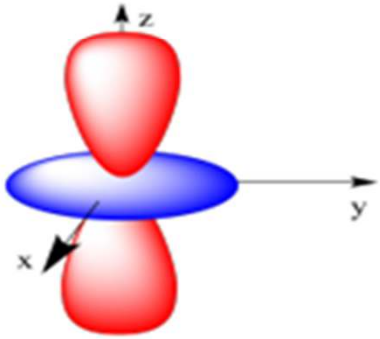
d_{xy}



d_{xz}



$d_{x^2-y^2}$

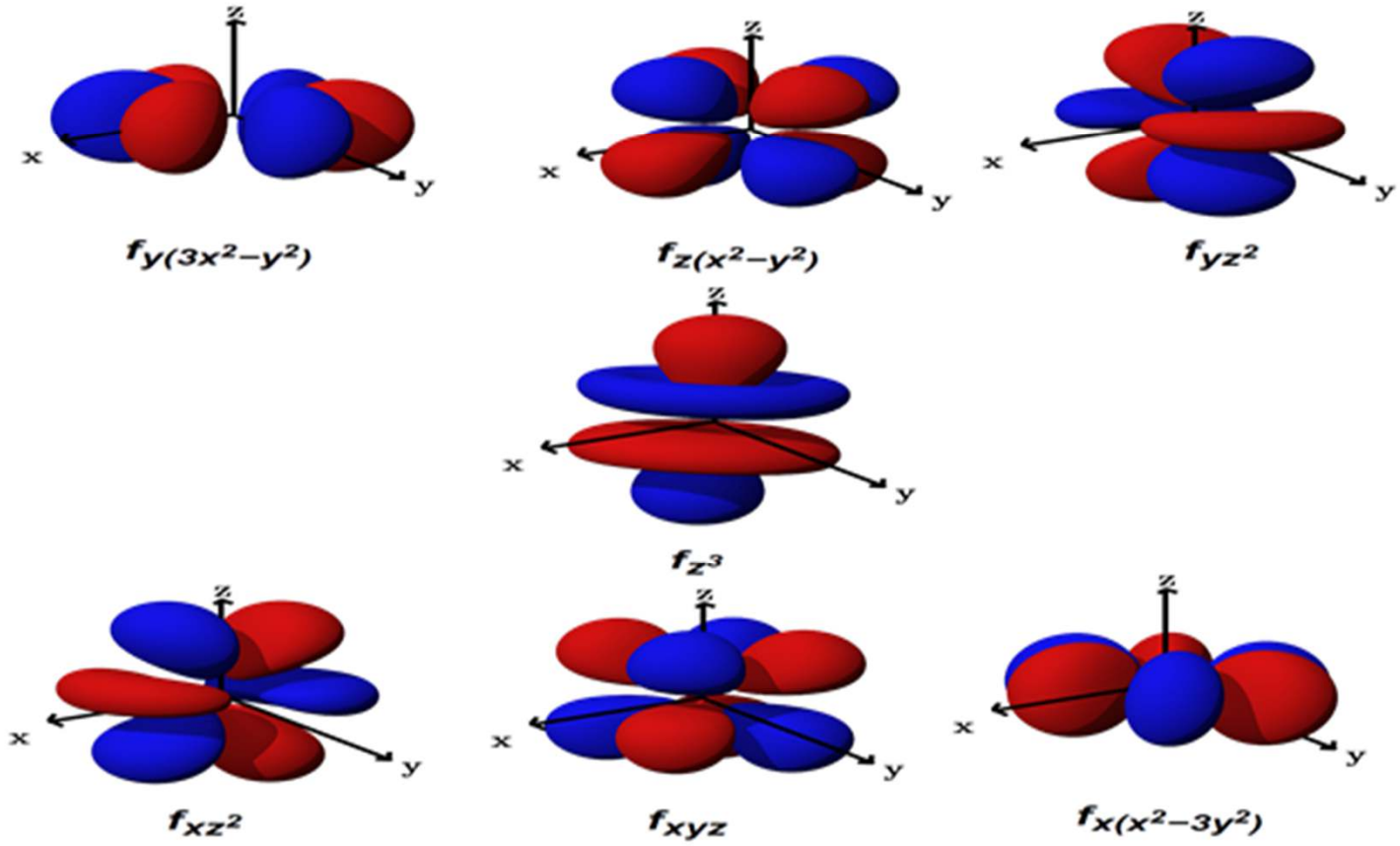


d_{z^2}

- Value of *l* is 2

IV- f- Orbitals Shape:

The f subshell is divided into 7 orbitals {fxyz, fx2, fy2, fz2, fx2, fx (y2-z2), fy(z2-x2), fz (x2-y2)}.These orbitals have a very complex shape and are higher in energy than the s , p and d orbitals. These 7 orbitals have same energy.



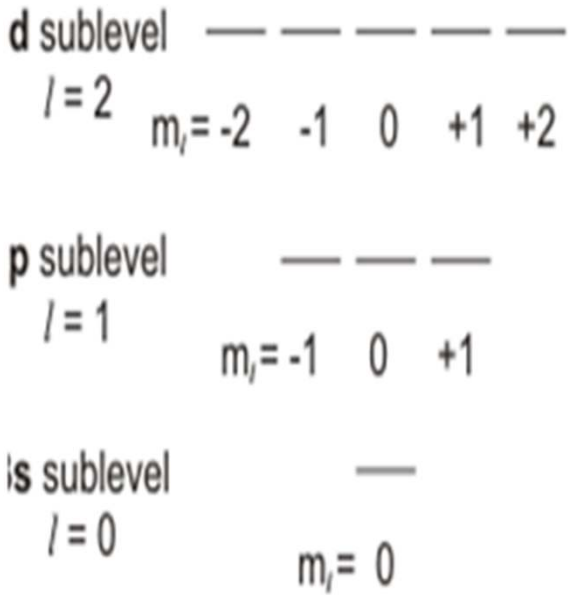
Value of (*l*) is 3

3- The Magnetic Quantum Number (*ml*):

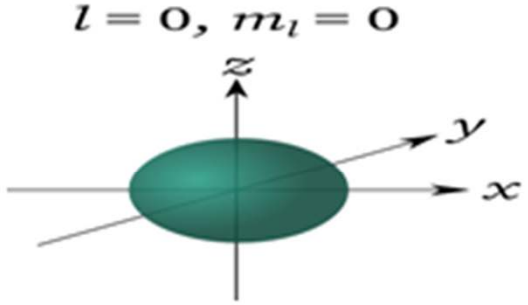
The magnetic quantum number determines the number of orbitals and their orientation within a subshell (the spatial orientation of an orbital). It describes the configuration of the orbitals according to a set of axes in three dimensions. Consequently, its value depends on the orbital angular momentum quantum number. At a certain (l) , (ml) is an interval ranging ($-l$ to $+l$), so it can be zero, a negative integer or a positive integer. There are ($2l+1$) orbitals in each subshell. Thus the s subshell has only one orbital, p subshell has three orbitals and so on.

$$Orbitals = 2\ell + 1$$

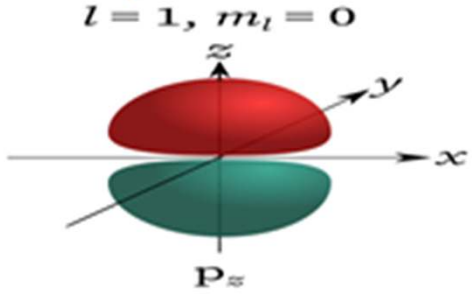
Possible values of $m_\ell = -\ell, \ldots 0 \ldots, +\ell$

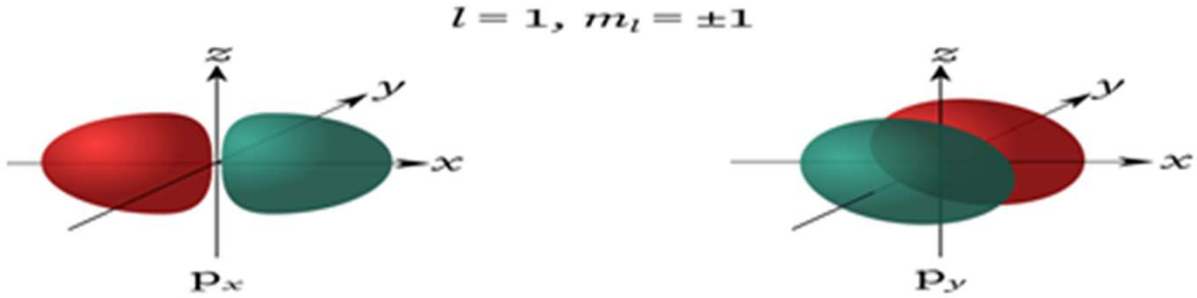


For $l = 0$, $ml = 0$. This represents an s orbital, which is spherical in shape. For an s orbital, the orbital angular momentum is zero and it does not point in any specific directions.



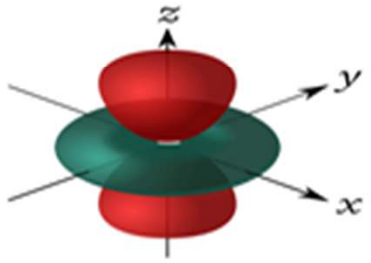
For $l = 1, ml = \{-1, 0, 1\}$. Each value represents a p orbital. When $ml = 0$, it is the pz orbital. It is aligned along the z-direction having each lobe on either of the origin. $ml = \pm 1$ are the px and py orbitals. px and py rest on x- and y-axes.





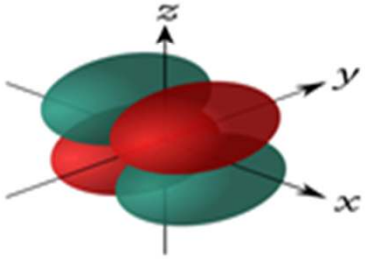
$l = 2$ is the d subshell and it has five orbitals. The magnetic quantum numbers for d subshell are −2, −1, 0, 1, and 2. $ml = 0$ is the dz2 orbital, which is oriented along the z-axis. The orbitals dxz and dyz have $ml = \pm 1$ and lie in the xz and yz planes. $ml = \pm 2$ corresponds to dxy and dx2 − y2; both lie in the xy plane.

$l = 2,\ m_l = 0$

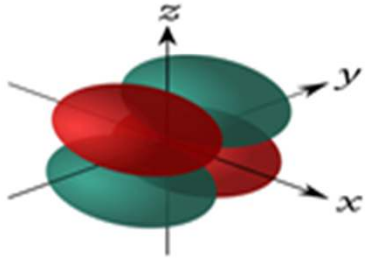


$\mathbf{d}_{z^2}$

$l = 2,\ m_l = \pm 1$

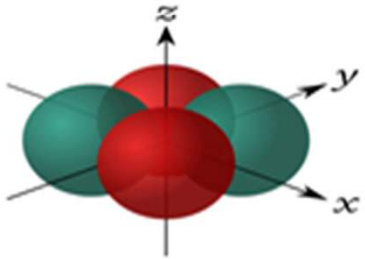


$\mathbf{d}_{xz}$

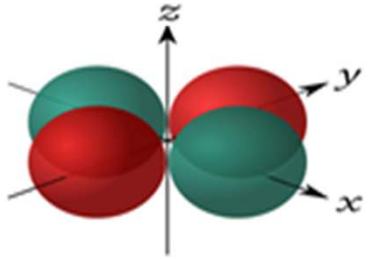


$\mathbf{d}_{yz}$

$l = 2,\ m_l = \pm 2$



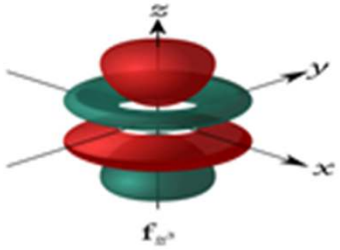
$\mathbf{d}_{xy}$



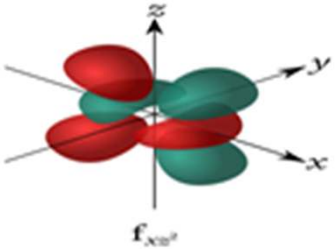
$\mathbf{d}_{x^2-y^2}$

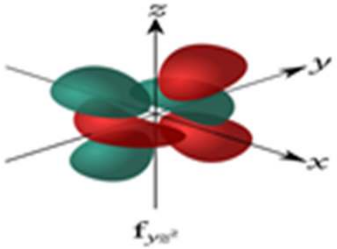
l for f subshell is 3 and it has seven orbitals: fz3, fxz2, fyz2, fxyz, fz(x2 − y2), fx(x2 − 3y2), and fy (3x2 − y2). And *ml* with these orbitals are −3, −2, −1, 0, 1, 2, and 3.

$l = 3,\ m_l = 0$

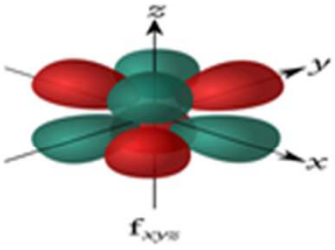


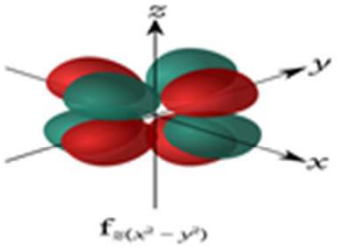
$l = 3,\ m_l = \pm 1$



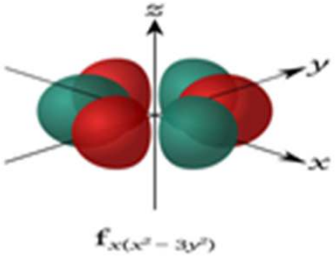


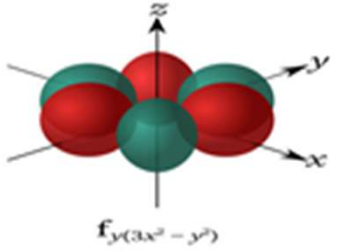
$l = 3,\ m_l = \pm 2$





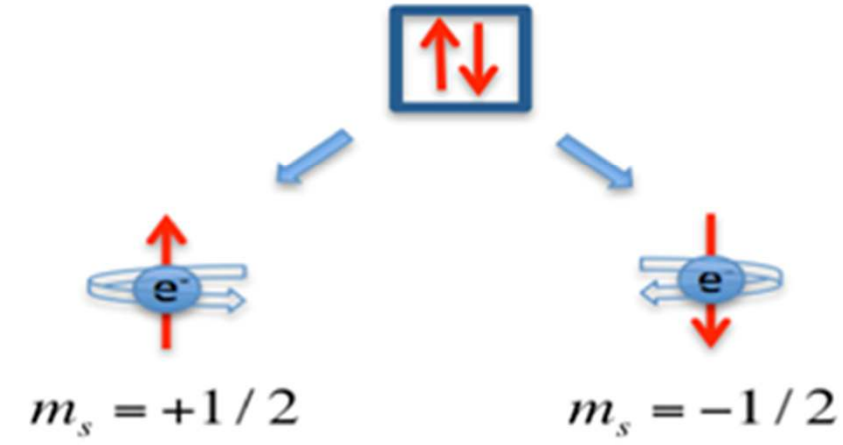
$l = 3,\ m_l = \pm 3$





4- The Electron Spin Quantum Number (ms):

ms does not depend on another quantum number. It designates the direction of the electron spin and may have a spin of +1/2, represented by ↑, or −1/2, represented by ↓. This means that when ms is positive the electron has an upward spin, which can be referred to as "spin up". When it is negative, the electron has a downward spin, so it is "spin down". Each electron in any individual orbital must have different spins. Due to the spinning of the electron, it generates a magnetic field. In general, an electron with ms = + 1/2 is called an alpha electron, and one with ms = - 1/2 is called a beta electron. No two paired electrons can have the same spin value. The significance of the electron spin quantum number is its determination of an atom's ability to generate a magnetic field or not. (Electron Spin)



The following table is very important:

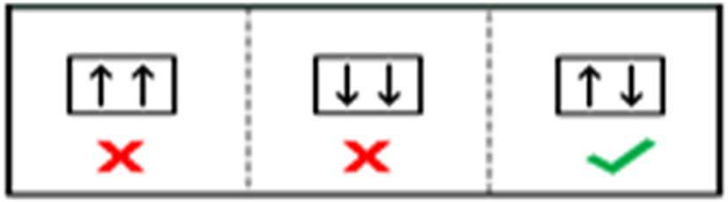
Number	Symbol	Possible Values
Principal Quantum Number	n	$1, 2, 3, 4, \ldots$
Angular Momentum Quantum Number	ℓ	$0, 1, 2, 3, \ldots, (n-1)$
Magnetic Quantum Number	m_l	$-\ell, \ldots, -1, 0, 1, \ldots, \ell$
Spin Quantum Number	m_s	$+1/2, -1/2$

Rules And Order Of Filling Orbitals :

There are a set of general rules that are used as guide to determine the structure of any particulate atom. Aufbau Process or Principle (Build-up Process) describes buildup of atoms by filling the empty orbitals with electrons. Aufbau Principle states that in the ground state of an atom or ion, electrons fill atomic orbitals of the lowest available energy levels before occupying higher levels.

Before the process can be properly employed, there are some fundamental rules must be followed:

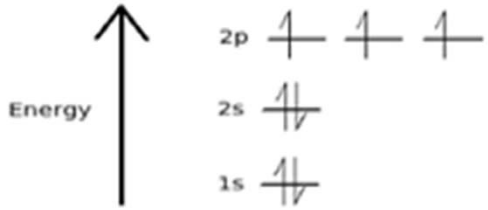
A. Pauli Exclusion Principle : only two electrons can occupy a single orbital and these two electrons must be of opposite spin.



B. Hund's Rule:

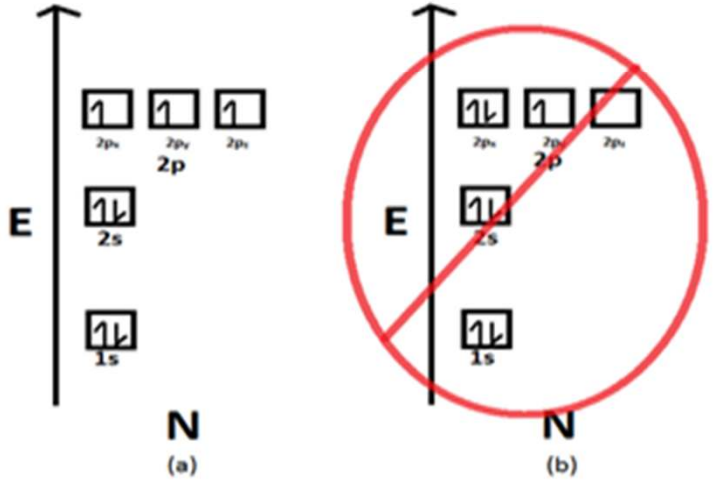
1- In the ground state of any atom, an electron may enter only the vacant orbital of lowest energy levels before occupying higher levels. For example, the 1s subshell is filled before the 2s subshell is occupied. The 2s subshell is filled before the 2p subshell is occupied.

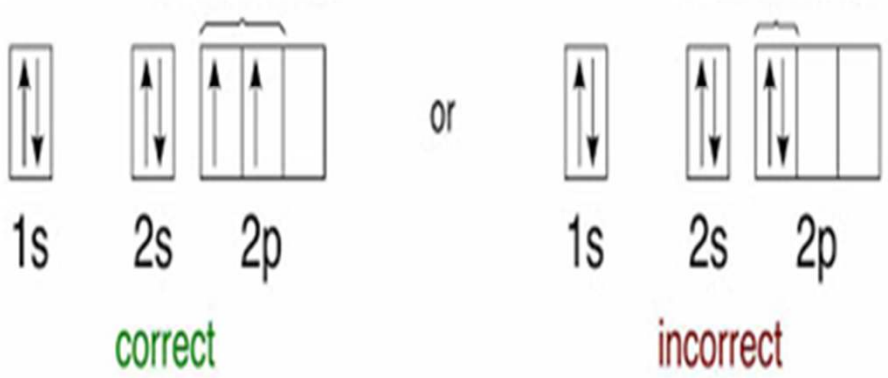
incorrect



correct

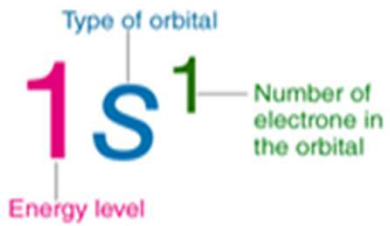
2- Electrons must enter degenerate orbitals (orbitals of same energy), e.g. $2p_x$, $2p_y$ and $2p_z$ singly and with parallel spin. Electrons should remain unpaired in degenerate orbitals as long as possible.



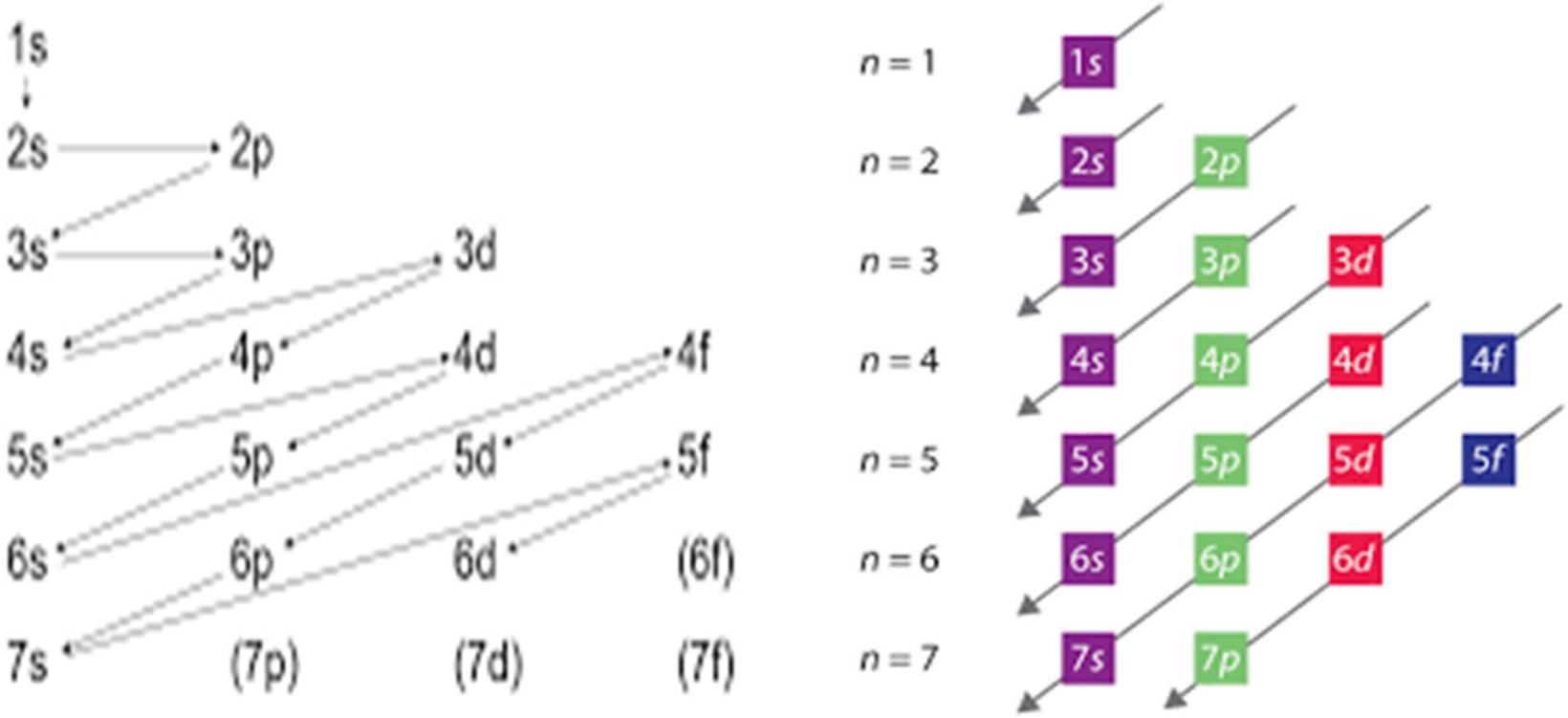


Electron Configuration:

The electron configuration of an element describes how electrons are distributed in its atomic orbitals. It is also called electronic structure and includes the arrangement of electrons in energy levels around an atomic nucleus. Electron configurations of atoms follow a standard notation in which all electron-containing atomic subshells (with the number of electrons they hold written in superscript)



The electrons around an atomic nucleus have discrete energy levels called shells. The lowest energy level is closest to the nucleus, and it has room for only two electrons in a subshell called the s subshell. The next shell has room for eight electrons in two subshells, the s and the p subshells. The third shell has room for 18 electrons in three subshells, the s, p and d subshells. The fourth shell has four subshells, adding the f subshell. The lettered subshells always have room for the same number of electrons: two for the s subshell, six for p, 10 for d and 14 for f. Each subshell consist of orbitals. Each orbital contains not more than two electrons with different spin. Maximum number of electrons that can be in a shell = $2\ n^2$. Maximum number of electrons that can be in a subshell = $2(2\ l + 1)$.



The 3s and 3p subshells fill up with two and six electrons, but the next electrons go into the 4s subshell, not the 3d subshell as expected. The 4s subshell has a lower energy level than 3d subshell and therefore fills up first, that follow Aufbau principle because the electron subshells fill up according to their energy levels.

Bismuth (atomic Number = 83):
$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^3$

There are less common exceptions to the Aufbau principle, for example:
Chromium (atomic Number = 24):
$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6 3d^5\ 4s^1$

Copper (atomic Number = 29):
$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6 3d^{10}\ 4s^1$

Of Chromium 's total of 24 electrons, they fill up the energy levels with two in 1s, two in 2s, six in 2p, two in 3s and six in 3p for a total of 18 in the lower levels. The remaining six electrons should go into the 4s and 3d subshells, with two in 4s and four in 3d. Instead, because the d subshell has room for 10 electrons, the 3d subshell takes five of the six available electrons and leaves one for the 4s subshell. Now both the 4s and 3d subshells are half full, a stable configuration but an exception to the Aufbau principle. Similarly, Copper has 29 electrons with 18 in the lower shells and 11 left over. By Aufbau principle, two electrons should go into 4s and nine into 3d. But 3d can hold 10 electrons so only one goes into 4s to make it half full and 10 go into 5d to fill it. Exceptions occur when subshells are half-full or full, because a completely full or half full d sub-level **is** more stable than a partially filled d sub-level, so an electron from the 4s orbital **is** excited and rises to a 3d orbital.

Orbitals and Electron Capacity of the First Four Principle Energy Levels				
Principle energy level (n)	**Type of sublevel**	**Number of orbitals per type**	**Number of orbitals per level(n^2)**	**Maximum number of electrons ($2n^2$)**
1	s	1	1	2
2	s	1	4	8
	p	3		
3	s	1	9	18
	p	3		
	d	5		
4	s	1	16	32
	p	3		
	d	5		
	f	7		

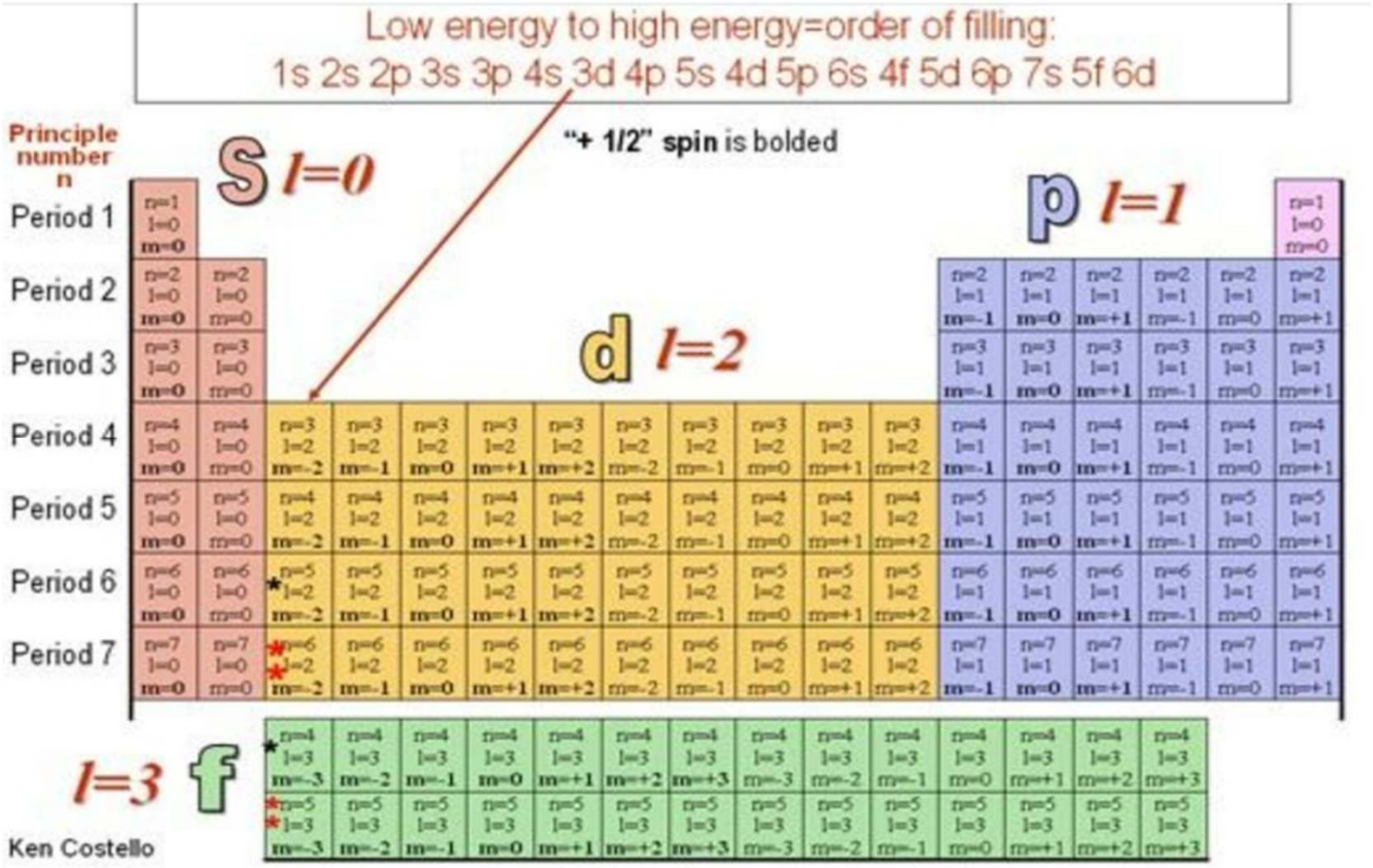
Electron Configurations are useful for:

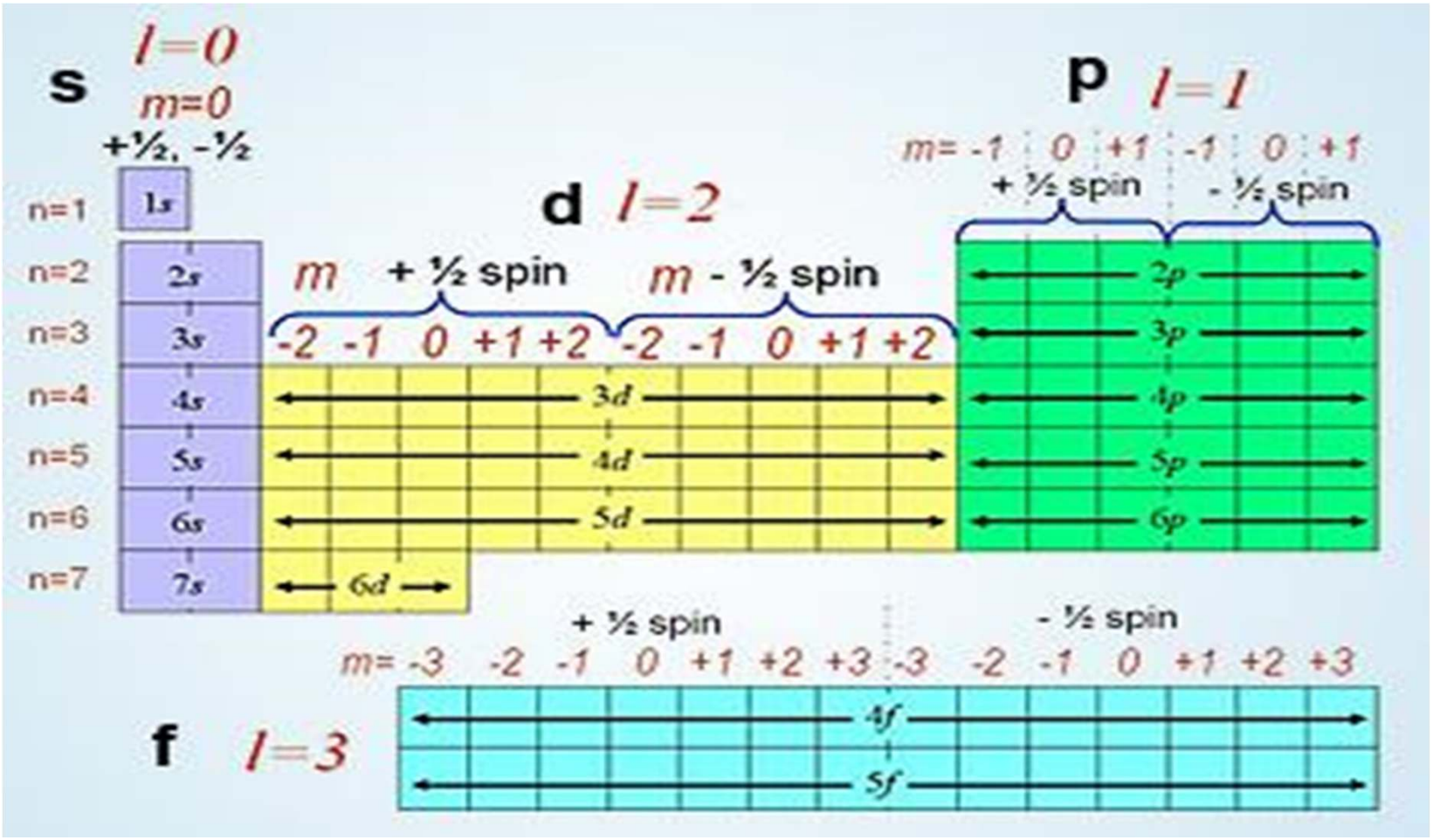
a. Determining the valency of an element.

b. Predicting the properties of a group of elements (elements with similar electron configurations tend to exhibit similar properties)

c. Interpreting atomic spectra.

Periodic Table and Quantum Numbers :




s l=0
m=0
+½, -½
p l=1
m= -1 0 +1 -1 0 +1
+ ½ spin
- ½ spin
d l=2
m + ½ spin
m - ½ spin
-2 -1 0 +1 +2 -2 -1 0 +1 +2
n=1
n=2
n=3
n=4
n=5
n=6
n=7
1s
2s
3s
4s
5s
6s
7s
2p
3p
4p
5p
6p
3d
4d
5d
6d
+ ½ spin
- ½ spin
m= -3 -2 -1 0 +1 +2 +3 -3 -2 -1 0 +1 +2 +3
f l=3
4f
5f

Shorthand Notation For Configuration:

Shorthand Notation For Configuration includes the electron configuration starts with the symbol of the noble gas (in the far right column of the periodic table) in the previous period followed by the additional configuration of the electrons for the given element. It also called condensed electron configuration. The neutral aluminum atom has 13 electrons. The electron configuration of aluminum can be written two ways. Its full electron configuration is $1s^2 2s^2 2p^6 3s^2 3p^1$. The part of the electron configuration that is blue is the electron configuration of neon, the noble gas in the previous period. Aluminum is in period (3) and the noble gas at the end of the period (2) is neon. Its shorthand electron configuration is [Ne] $3s^2 3p^1$.

Scandium element has the same configuration as argon, except with electrons in two extra orbitals. The shorthand form is therefore: [Ar] $4s^2$ $3d^1$

because the configuration of argon is: $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$

Notice that the symbol of the noble gas is in brackets, followed by the configuration of the additional electrons in the element.

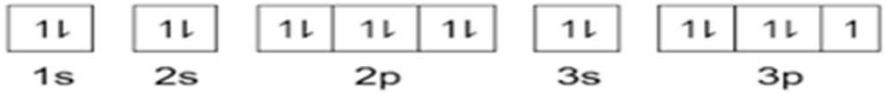
Electron configuration diagram (Orbitals Filling Diagram) :

Element	Total Electrons	Orbital Diagram								Electron Configuration
		1s		2s		2p			3s	
Li	3	↿⇂		1						$1s^2 2s^1$
Be	4	↿⇂		↿⇂						$1s^2 2s^2$
B	5	↿⇂		↿⇂		1				$1s^2 2s^2 2p^1$
C	6	↿⇂		↿⇂		1	1			$1s^2 2s^2 2p^2$
N	7	↿⇂		↿⇂		1	1	1		$1s^2 2s^2 2p^3$
Ne	10	↿⇂		↿⇂		↿⇂	↿⇂	↿⇂		$1s^2 2s^2 2p^6$
Na	11	↿⇂		↿⇂		↿⇂	↿⇂	↿⇂	1	$1s^2 2s^2 2p^6 3s^1$

Example : What are the quantum numbers for chlorine, iron, and tin with atomic numbers 17, 26 and 50 respectively? (Note : For last electron)

Chlorine (17)

$1s^2 2s^2 2p^6 3s^2 3p^5$,



n=3

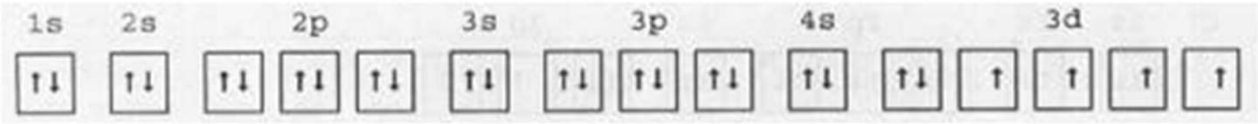
l =1 (p orbital)

ml may be −1,0,+1 (because l =1), ml =0 (since there are 5 electrons, you count five, so −1,0,+1,−1,0 which means the last electron has ml =0.

ms = −1/2

Iron (26)

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



n=3,

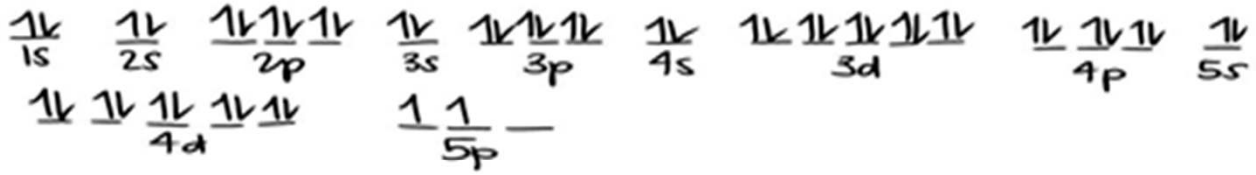
l =2 (because it is the d orbital),

ml may be −2,−1,0,+1, +2 (because l =2), so ml = ,−2 (since there are 6 electrons, you count six, so ml = −2)

ms = − 1/2.

Tin (50)

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^2$



n= 5

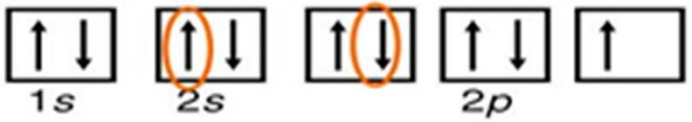
l = 1 (p orbital)

m*l* may be −1,0,+1 (because *l* =1), m*l* =0 (since there are two electrons, you count 2, so −1,0 which means the last electron has m*l* =0.

ms = + 1/2

Example: write a set of quantum numbers for the third electron and a set for the eighth electron of F (9)?

$1s^2\ 2s^2\ 2p^5$



Up arrow = +1/2
Down arrow = -1/2

The third electron is in the 2*s* orbital. Its quantum numbers are:

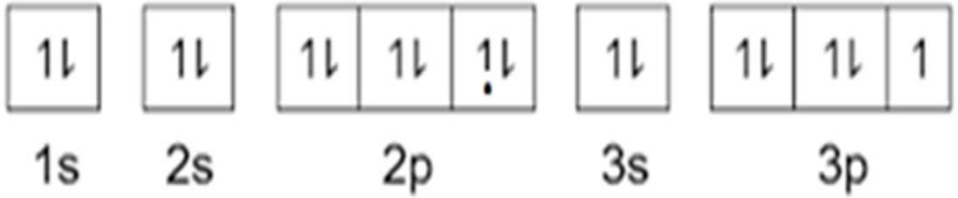
$n = 2$ $l = 0$ $m_l = 0$ $m_s = +1/2$

The eighth electron is in a 2*p* orbital. Its quantum numbers are:

$n = 2$ $l = 1$ $m_l = -1$ $m_s = -1/2$

What are the quantum numbers for the 7^{th} electron in chlorine ?

$1s^2 2s^2 2p^6 3s^2 3p^5$,



<u>the quantum numbers for the 7^{th} electron</u>

n= 2

l =1 (p orbital)

ml may be −1,0,+1 (because l =1), ml = +1 (since there are 3 electrons, you count 3, so −1,0,+1,−1,0 which means the 7^{th} electron has ml = + 1.

ms = + 1/2

Valence Shell and Valence Electrons:

The outermost shell of an atom is called valence shell, and the electrons in the valence shell are valence electrons (electrons in the outermost energy level). The valence electrons can be gained, lost, or shared to form chemical bonds, while inner electrons (those not in the valence shell) typically don't participate in chemical bonding and reactions. For this reason, elements with the same number of valence electrons tend to have similar chemical properties, since they tend to gain, lose, or share valence electrons in the same way.

Atomic Number	Element Symbol	Electron Configuration	Number of Valence Electrons
1	H	$1s^1$	1
2	He	$1s^2$	2
3	Li	$1s^2 2s^1$	1
4	Be	$1s^2 2s^2$	2
5	B	$1s^2 2s^2 2p^1$	3
6	C	$1s^2 2s^2 2p^2$	4
7	N	$1s^2 2s^2 2p^3$	5
8	O	$1s^2 2s^2 2p^4$	6
9	F	$1s^2 2s^2 2p^5$	7
10	Ne	$1s^2 2s^2 2p^6$	8

The periodic table is organized into columns (groups) and rows (periods).

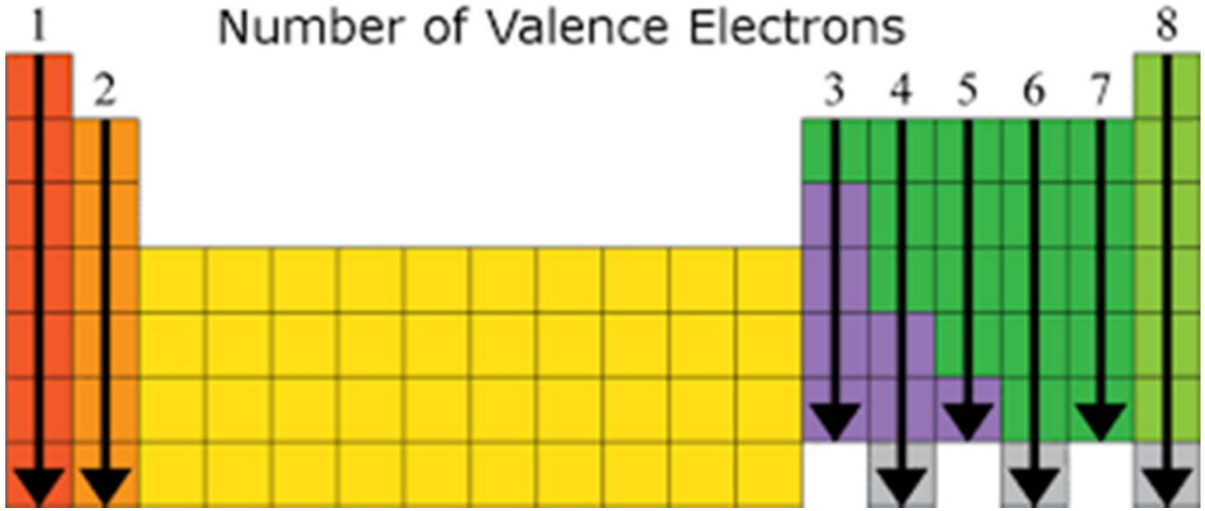
The number of protons in the nucleus increases when reading the periodic table from right to left.

Each row represents an energy level.

The elements in each column share similar properties and the same number of valence electrons.

The number of valence electrons in an atom is reflected by its position in the periodic table of the elements (see the periodic table in the Figure below).

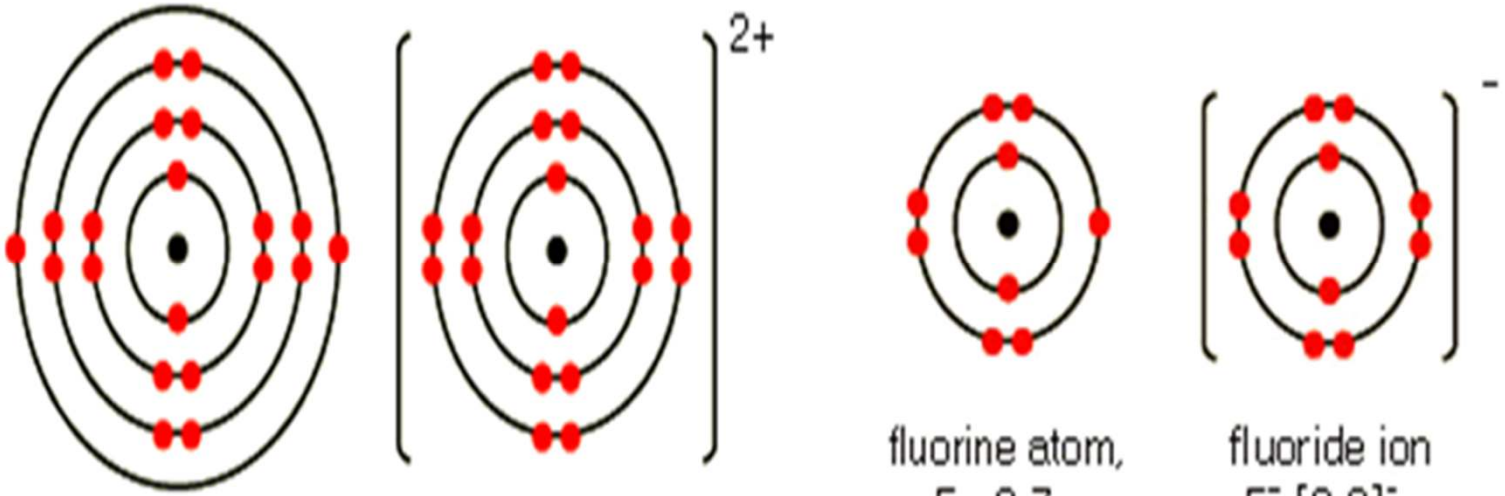
Across each row (period) of the periodic table, the number of valence electrons in groups 1–2 and 13–18 increases by one from one element to the next.



For elements in groups 3–12, determining the number of valence electrons is more complicated (called Transition Elements or Metals). Why (H.W. with definition , examples and properties). (i.e) The general method for counting valence electrons is generally not useful for transition metals. Instead the modified d electron count method is used. Except for helium, which has only two valence electrons.

Ionization:

When the neutral atom loses electron (s), it becomes positively charged (less electrons than protons) and called cation **and becomes** smaller than the original atom. While when the neutral atom gains an electron (s), it becomes negatively charged (more electrons than protons) and called an anion and becomes larger than the original atom.



calcium atom,
Ca 2,8,8,2

calcium ion,
Ca^{2+} $[2,8,8]^{2+}$

fluorine atom,
F 2,7

fluoride ion
F^- $[2,8]^-$

The atomic number of calcium is 20. This means that in a neutral calcium atom, there are 20 protons in its nucleus. A neutral calcium atom also has 20 electrons. The electron configuration of a neutral calcium atom is:

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

While the electron configuration of calcium cation is:
$1s^2 2s^2 2p^6 3s^2 3p^6$

Calcium atom has lost two valence electrons, and now has 18 electrons. The electron configuration is isoelectronic with the noble gas Argon.

The atoms tend to form compounds in ways that give them eight valence electrons and thus the electron configuration of a noble gas to be less reactive and more stable because of saturation of last shell with electrons, this is called **Octet Rule**

The atomic number of fluorine is 9. This means that in a neutral fluorine atom, there are 9 protons in its nucleus. A neutral fluorine atom also has 9 electrons.

The electron configuration of a neutral fluorine atom is:

$1s^2 2s^2 2p^5$

While the electron configuration of fluoride anion is:
$1s^2 2s^2 2p^6$

Fluorine atom has gain one electron, and now has 10 electrons. The electron configuration is isoelectronic with the noble gas Neon.

The elements can be classified :

1- Metals:

- good conductors of heat and electricity
- malleable (can be hammered into sheets)
- ductile (can be drawn into wire).
- Most of the metals are solids at room temperature, with a characteristic silvery shine (except for mercury, which is a liquid).

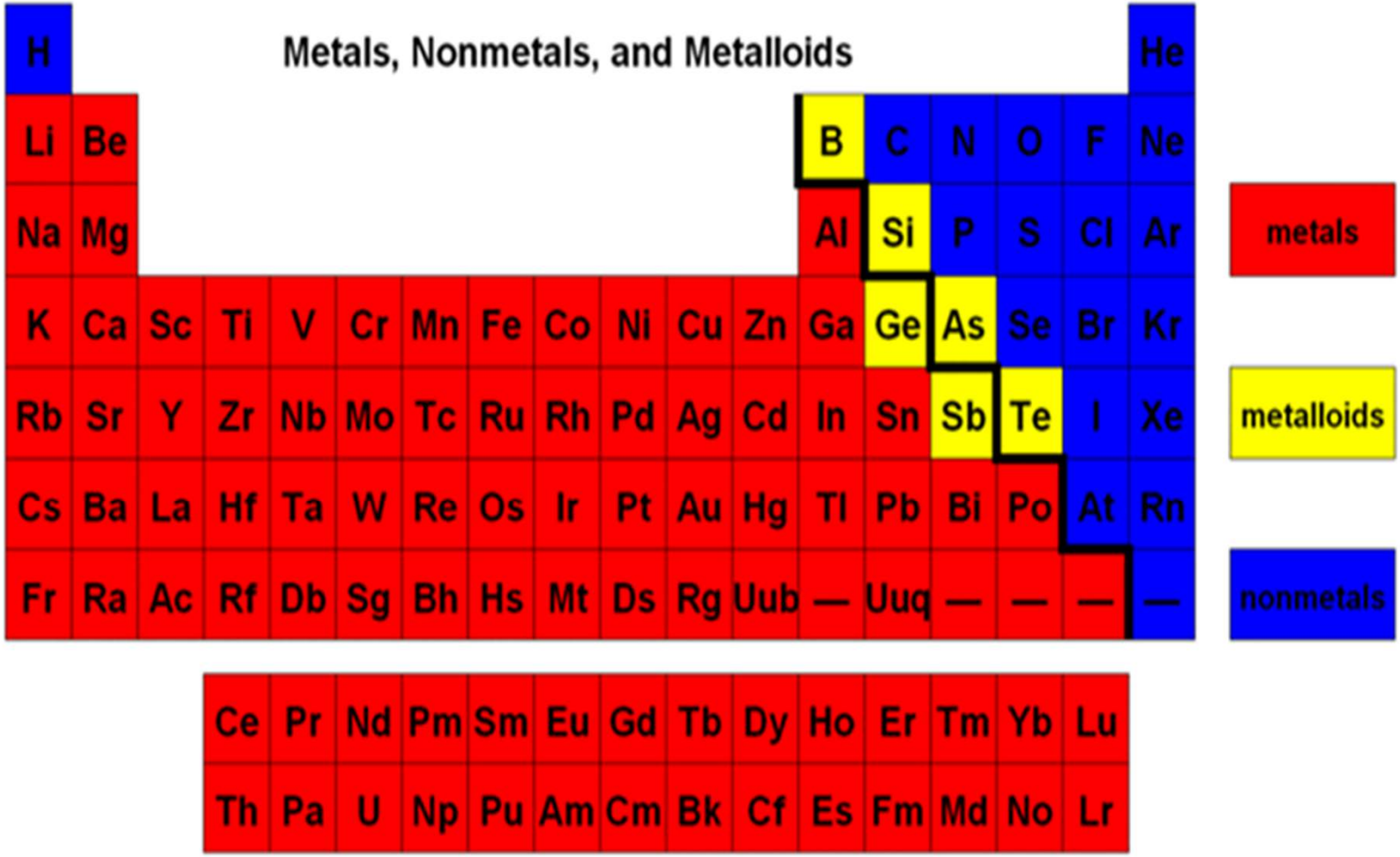
2- Nonmetals:

- (usually) poor conductors of heat and electricity
- not malleable
- not ductile
- many of the nonmetals are gases at room temperature, while others are liquids and others are solids.

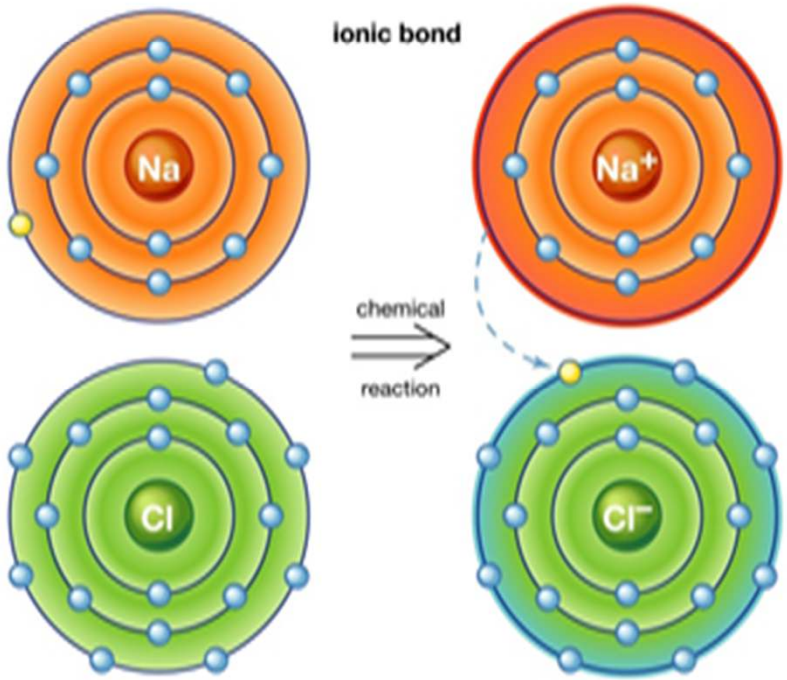
3- The metalloids:

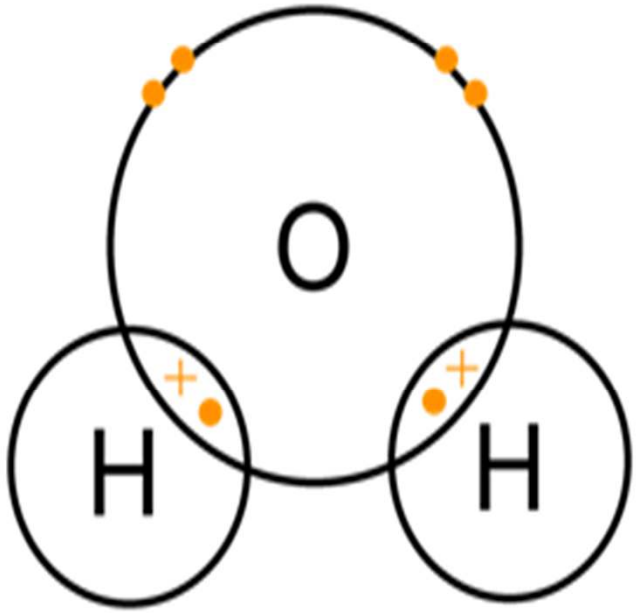
- intermediate in their properties. In their physical properties, they are more like the nonmetals, but under certain circumstances, several of them can be made to conduct electricity.
- These semiconductors are extremely important in computers and other electronic devices.

In the periodic Table, metals are to the left of the line (except for hydrogen, which is a nonmetal), nonmetals are to the right of the line, and the elements immediately adjacent to the line are the metalloids. A zigzag line that separates metals from metalloids.



When elements combine to form compounds, there are two major types of bonding that can result. **Ionic Bonds** form when there is a transfer of electrons from one species to another, producing charged ions which attract each other very strongly by electrostatic interactions, and **Covalent Bonds**, which result when atoms share electrons to produce neutral molecules. In general, metal and nonmetals combine to form ionic compounds, while nonmetals combine with other nonmetals to form covalent compounds (molecules).

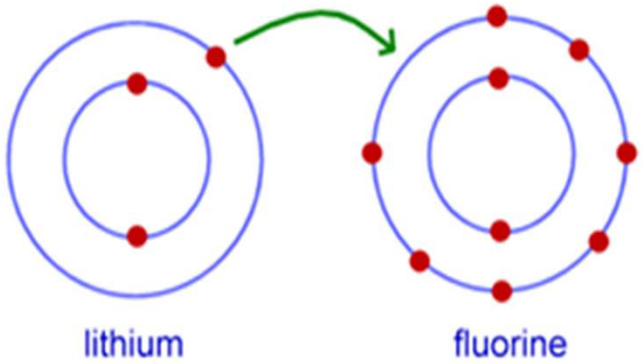




Covalent Bond

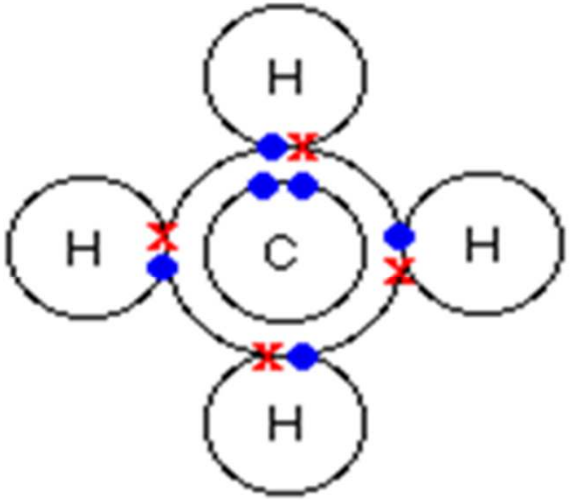
Metals have low ionization energies (the amount of energy that is required to remove an electron from a mole of atoms in the gas phase) and low electron affinities (the energy change which accompanies the addition of an electron to an atom in the gas phase to produce a negatively charged anion), so they lose electrons relatively easily and gain them with difficulty. They also have relatively few valence electrons, and can form ions (and thereby satisfy the octet rule) more easily by losing their valence electrons to form positively charged **cations**.

Nonmetals have high ionization energies and high electron affinities, so they gain electrons relatively easily, and lose them with difficulty. They have a larger number of valence electrons, and are already close to having a complete octet of eight electrons. The nonmetals gain electrons until they have the same number of electrons as the nearest noble gas (Group 8A), forming negatively charged **anions**. The Group 8A elements already have eight electrons in their valence shells, and have little tendency to either gain or lose electrons, and do not readily form ionic or molecular compounds.



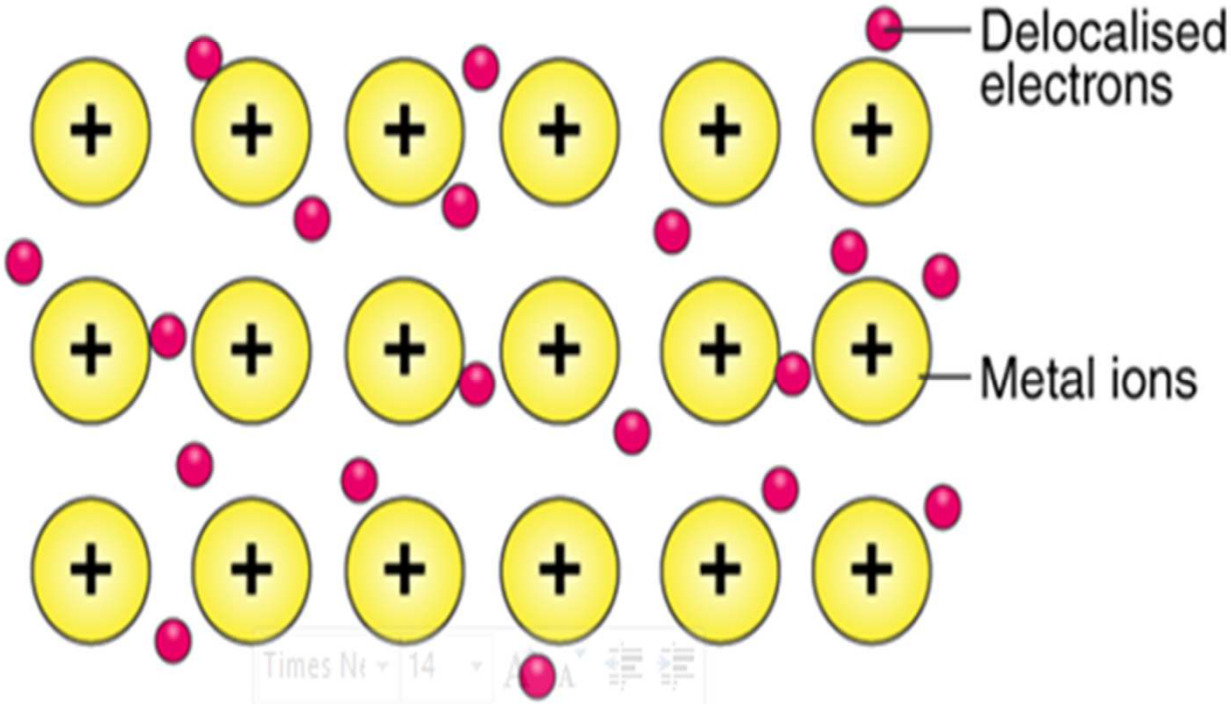
lithium fluoride

When nonmetals combine with other nonmetals, they tend to share electrons in covalent bonds instead of forming ions, resulting in the formation of neutral molecules.



methane

When metals combine with each other, the bonding is usually described as **metallic bonding**. In this model, each metal atom donates one or more of its valence electrons to make an electron sea that surrounds all of the atoms, holding the substance together by the attraction between the metal cations and the negatively charged electrons. Since the electrons in the electron sea can move freely, metals conduct electricity very easily, unlike molecules, where the electrons are more localized.



Orbital Hybridization:

It is the concept of overlapping or mixing atomic orbitals into new hybrid orbitals (with different energies , shapes and other properties than the component atomic orbitals. (i.e) Hybridization includes redistribution of the energy of orbitals of individual atoms to give orbitals of equivalent energy. The new formed orbitals are known as hybrid orbitals. Hybrid orbitals are useful in the explanation of molecular geometry and atomic bonding properties. Hybridization need excitation or promotion of electron to transfer or jump from an orbital to a higher orbital.

Types of Hybridization are based on the types of orbitals involved in mixing:

1- sp^1 Hybridization:

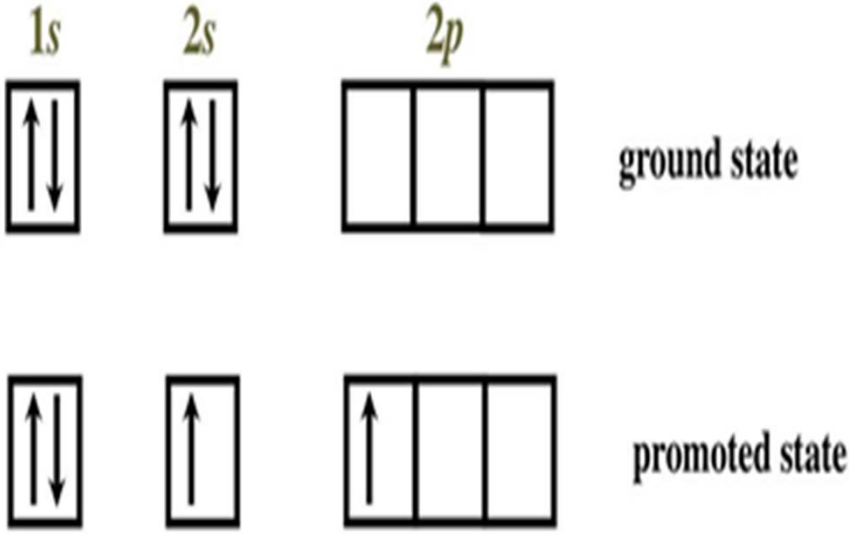
sp^1 hybridization is observed when one s orbital and one p orbital in the same main shell of an atom mix to form two new equivalent orbitals. The new orbitals formed are called sp^1 hybridized orbitals. It forms linear molecules with an angle of 180°.

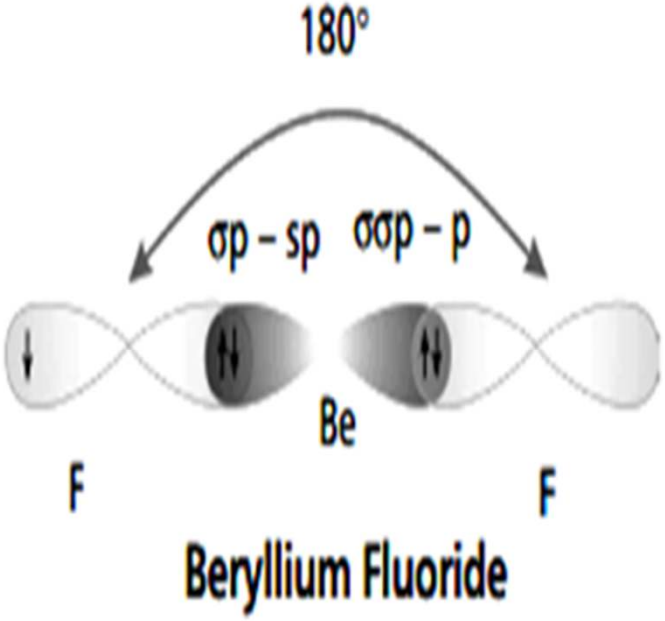
Examples:

- All compounds of beryllium (i.e) BeF_2, BeH_2, $BeCl_2$
- All compounds of carbon-containing triple Bond. (i.e) C_2H_2

BeF_2

Be (4): $1s^2 2s^2$





2- sp^2 Hybridization:

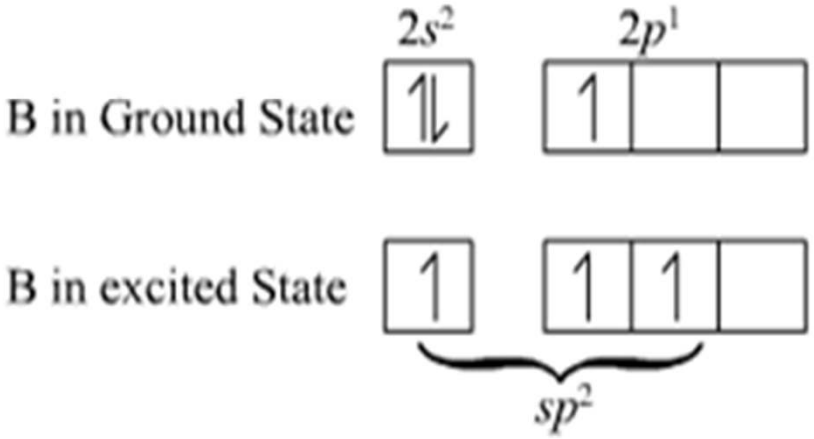
sp^2 hybridization is observed when one s orbital and two p orbitals of the same shell of an atom are mix to form 3 equivalent orbital. The new orbitals formed are called sp^2 hybrid orbitals. It forms trigonal molecules with an angle of 120°. The molecules in which the central atom is linked to 3 atoms forming a triangular planar shape.

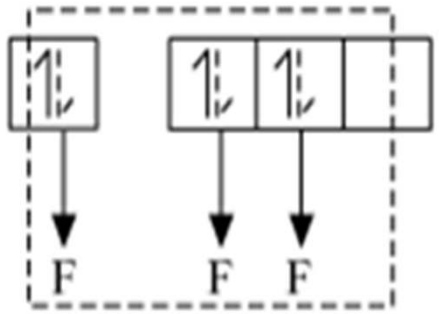
Examples:

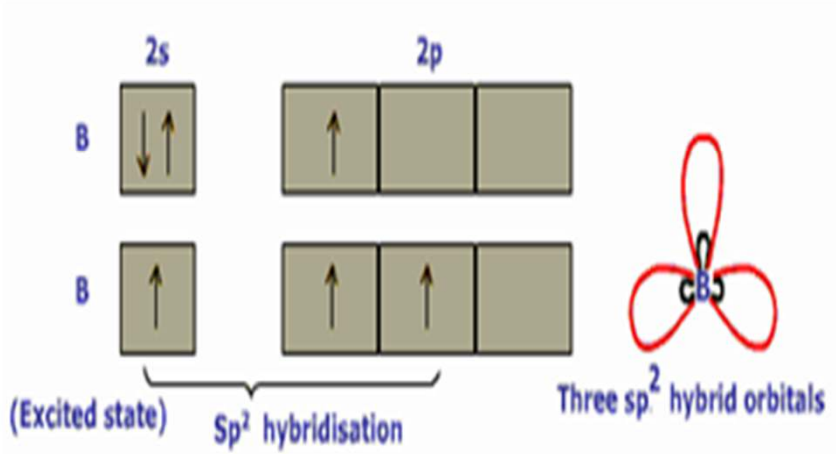
- All the compounds of Boron (i.e.) BF_3, BH_3
- All the compounds of carbon containing a carbon-carbon double bond, Ethylene (C_2H_4)

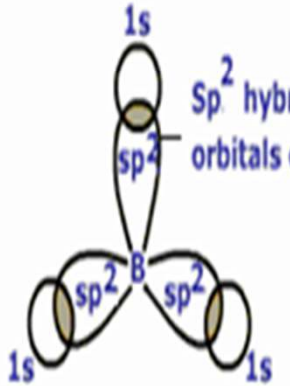
BF_3 and BH3

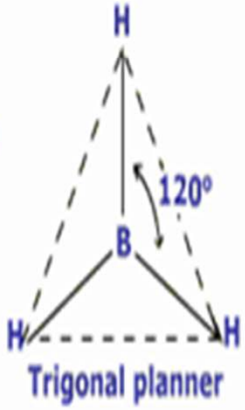
Boron (5): $1s^2 2s^2 2p^1$











3- sp^3 Hybridization:

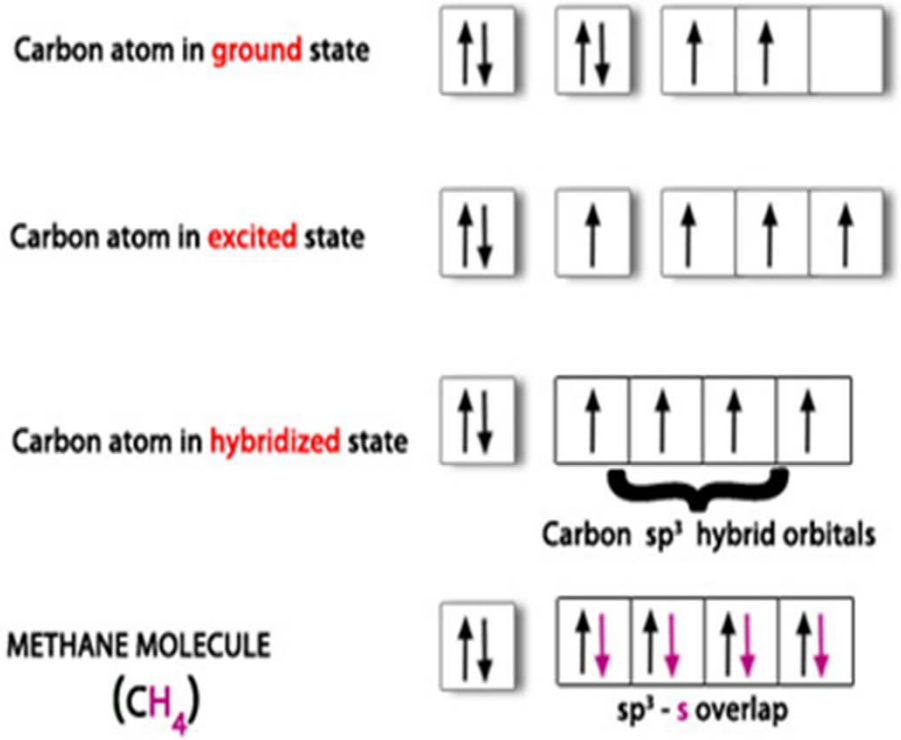
When one 's' orbital and 3 'p' orbitals belonging to the same shell of an atom mix together to form four new equivalent orbital, the type of hybridization is called a tetrahedral hybridization or sp^3. The new orbitals formed are called sp^3 hybrid orbitals. It forms tetrahedron molecules with an angle of 109.5°.

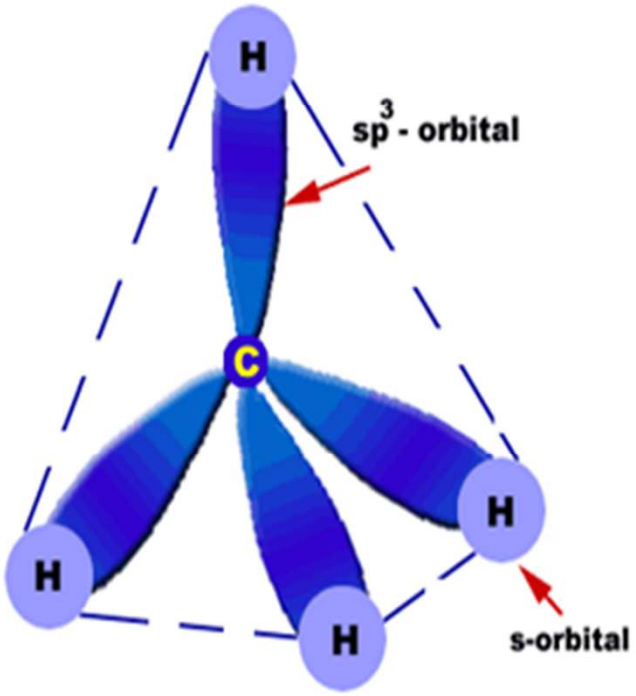
Example:

methane (CH4), ethane (C_2H_6)

CH_4

Carbon (6) : $1s^2\ 2s^2\ 2p^2$





4- sp^3d Hybridization

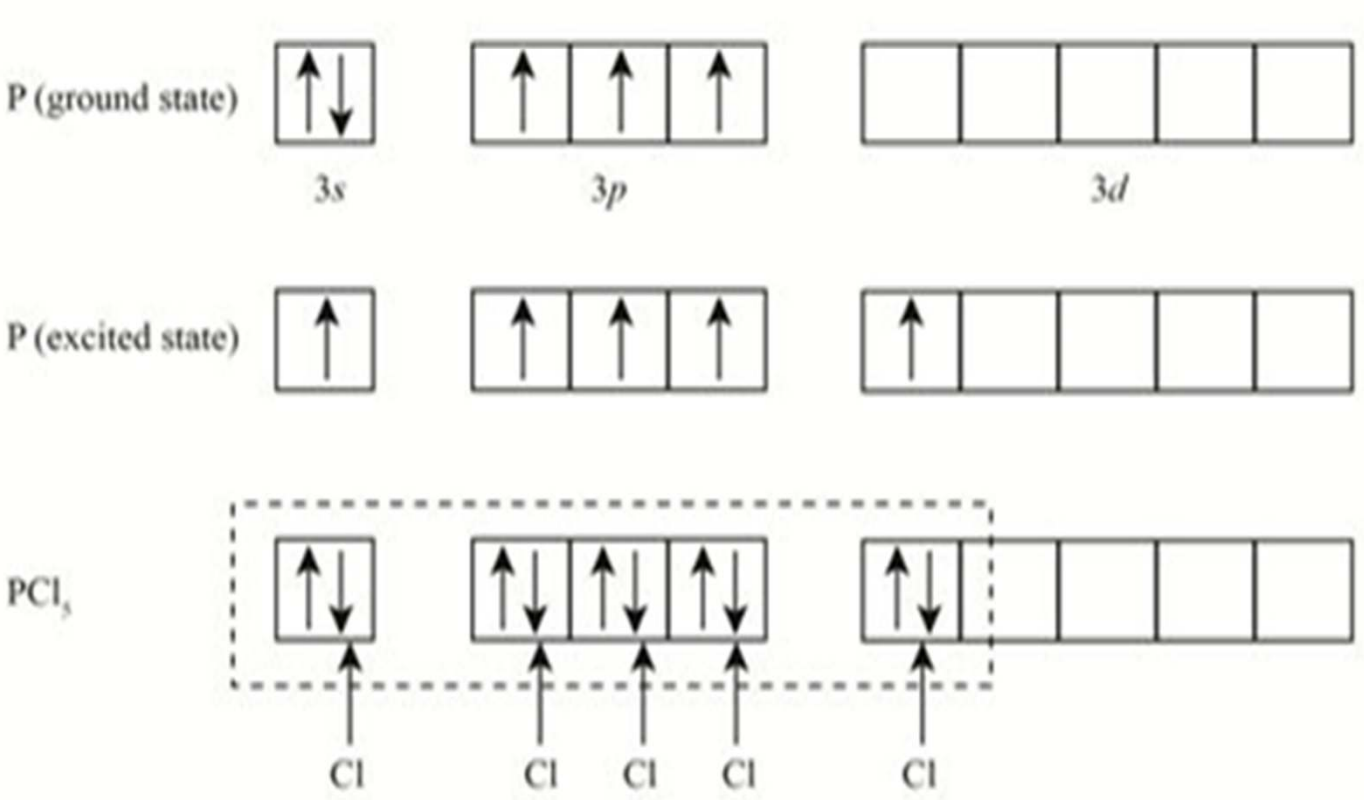
It involves the mixing of 1s, 3p orbitals and 1d orbital to form 5 sp3d hybridized orbitals of equal energy. They have trigonal bipyramidal geometry. Three hybrid orbitals lie in the horizontal plane inclined at an angle of 120° to each other known as the equatorial orbitals. The remaining two orbitals lie in the vertical plane at 90 degrees plane of the equatorial orbitals known as axial orbitals.

Example:

Phosphorus pentachloride (PCl_5)

Phosphorus pentachloride (PCl_5)

P (15): $1s^2 2s^2 2p^6 3s^2 3p^3$



5- sp^3d^2 Hybridization:

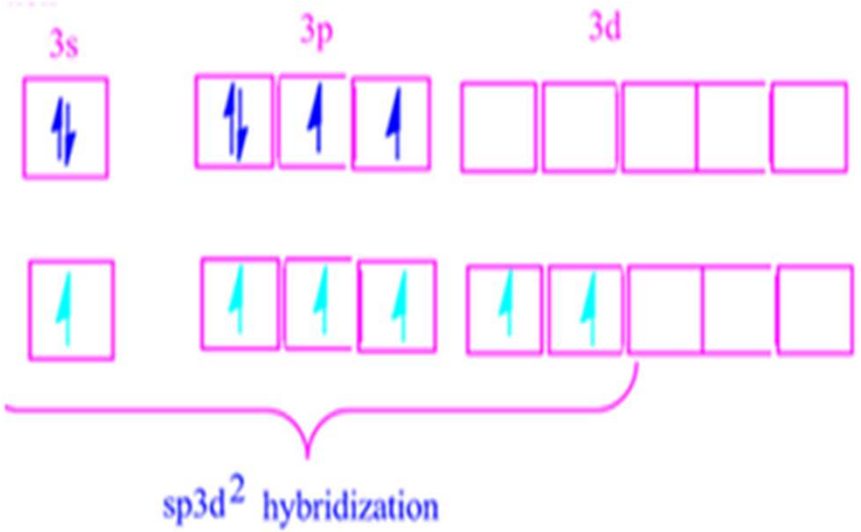
It involves the mixing of one s orbital , 3p orbitals and 2d orbitals, to form 6 identical sp^3d^2 hybrid orbitals. These 6 orbitals are directed to wards the corners of an octahedron. They are inclined at an angle of 90 degrees to one another.

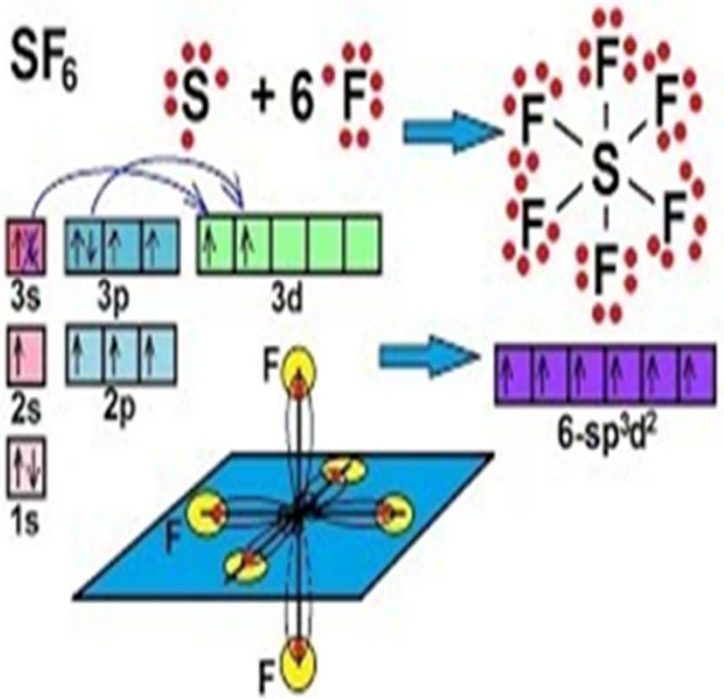
Example:

Sulfur hexafluoride SF_6

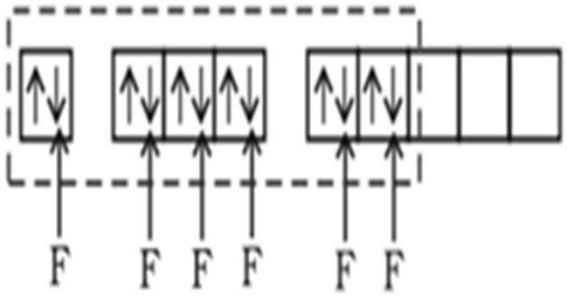
Sulfur hexafluoride SF_6

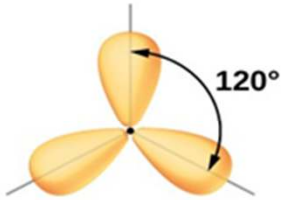
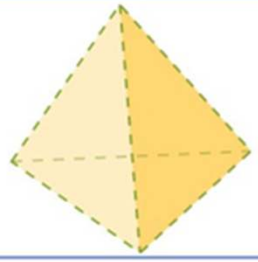
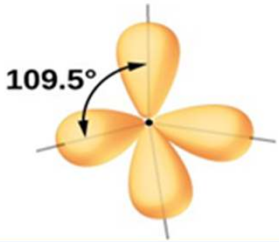
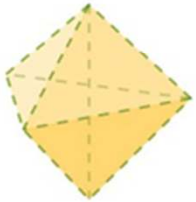
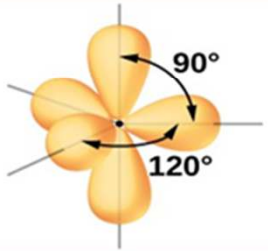
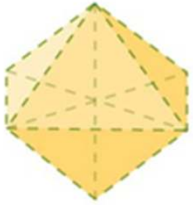
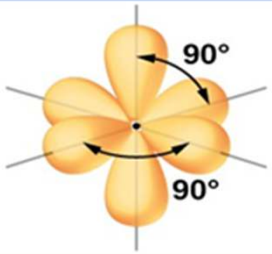
S (16): $1s^2 2s^2 2p^6 3s^2 3p^4$





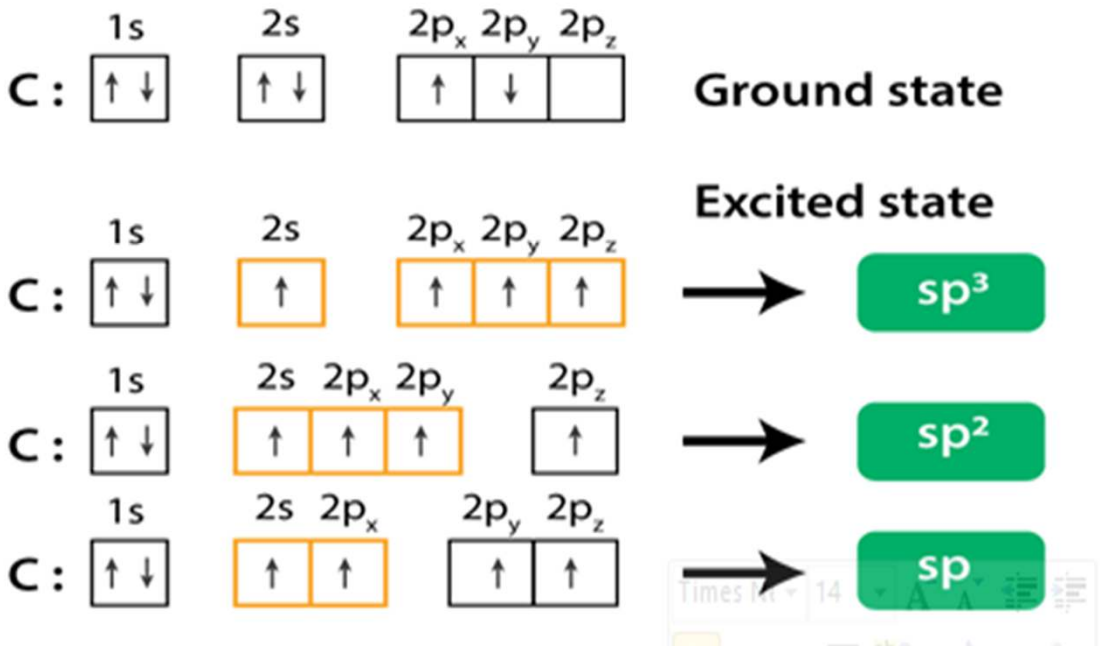
SF_6



Arrangement		Hybridization	
	linear	sp	
	trigonal planar	sp^2	
	tetrahedral	sp^3	
	trigonal bipyramidal	sp^3d	
	octahedral	sp^3d^2	

Hybridization of Carbon atom:

Carbon is one of the important and most common chemical element that is essential for organic connections. Carbon atoms usually form bonds by mixing different orbitals and can contribute to the formation of different structures and properties. Most of the time the s and p orbitals of the second shell in carbon combine together during hybridization. In essence, carbon can use different hybridization to form different compounds.



1. sp Hybridization

Carbon can have an sp^1 hybridization when it is bound to two other atoms with the help of two double bonds or one single and one triple bond. When the hybridization occurs the molecules have a linear arrangement of the atoms with a bond angle of 180°.

Example:

Hybridization of alkynes and CO_2

In an alkyne bond, the two carbon atom are sp hybridized so they each have two unhybridized p orbitals and two sp hybrid orbitals.

2. sp^2 Hybridization

Carbon atom is sp^2 hybridized when bonding takes place between 1 s-orbital with two p orbitals. There is a formation of two single bonds and one double bond between three atoms. The hybrid orbitals are placed in a triangular arrangement with 120° angles between bonds.

Example:

Hybridization of alkenes

one 2s, and three 2p (2px, 2py, 2pz) but with the difference that one of the 2p orbitals does not participate in the hybridization. the net result is that there is three sp2 hybrid orbitals and one p orbital per atom of carbon.

3. sp^3 Hybridization

Example:

Hybridization of alkanes

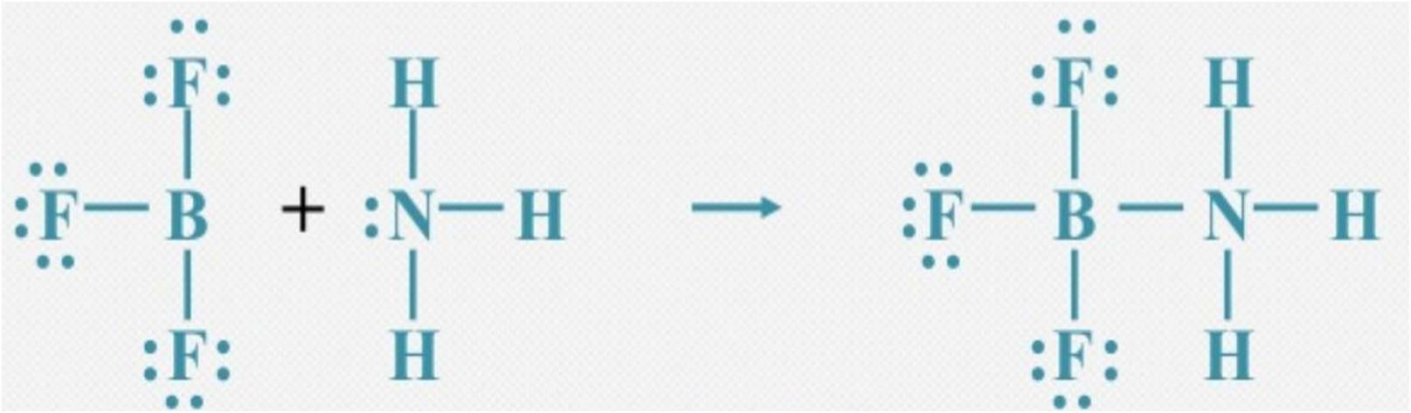
CH_4 (Methane), formation of 4 single bonds with 4 hydrogen atoms

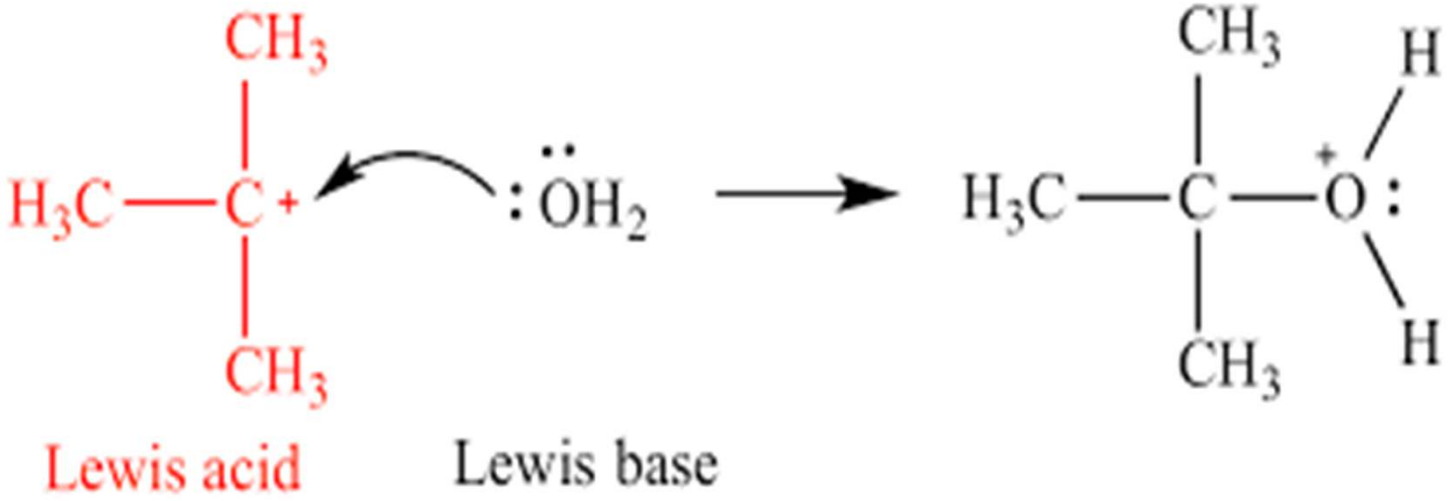
Lewis Acids and Bases

- Lewis acid is a substance that accepts a pair of electrons to form a covalent bond.
- Lewis base is a substance that donates a pair of electrons to form a covalent bond.

So, a Lewis acid-base reaction is represented by the transfer of a pair of electrons from a base to an acid.

It also defines the nature of bond and position of atoms of the molecule which are connected in the molecule.

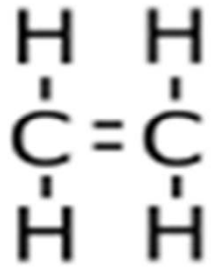



Lewis acid
Lewis base

- Lewis symbols use dots to visually represent the valence electrons (the electrons present in the outer shell) of an atom.
- These symbols are known as Electron Dot Symbols and the structure of the compound is known as Lewis Dot Structure.
- It defines the nature of bond and position of atoms of the molecule which are connected in the molecule.

How to Draw a Lewis Structure?

- The symbol of the chemical element is written surrounded by dots each point representing one electron and every two adjacent points are an electronic pair. These points are distributed to the four sides surrounding the symbol so that do not exceed two points on each side.
- The electrons will be arranged similar to the noble gas (which has eight electrons in its outer shell except helium who has only two electrons). "Octet Rule“ . Note : put the real number of valence electrons and do not exceed.

Hydrogen		
Carbon		
Water		
Ethylene		
Acetylene		

Water molecule (H_2O) the electronic configuration of an atom (H) is 1H: $1s^1$
Lewis symbol of atom (H) is

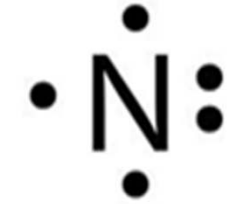
H •

(O) atom is $1s^2\ 2s^2\ 2p^4$
Lewis symbol of atom (O) is

Lewis symbol of water molecule is

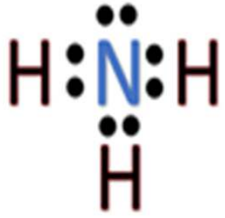
Ammonia molecule (NH_3)
The electronic configuration of an atom (N) is: $1s^2\ 2s^2\ 2p^3$

Lewis symbol of Nitrogen is:



and the hydrogen atom as mentioned above.

Lewis symbol for the ammonia molecule is:



Octet Rule is not applicable for all the atoms in the molecules as in the PCl_5 and BF_3.
It notes that the central phosphorus atom was surrounded by ten electrons, as for the boron atom is surrounded by six electrons, so it does not agree with rule of eight.