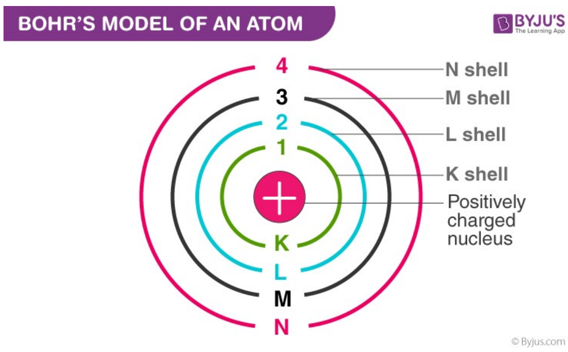
What is Mineral or Inorganic Chemistry?

The word organic refers to the compounds which contain carbon atoms in it. So the branch of chemistry that deals with the study of compounds, which does not consist of carbon-hydrogen atoms in it, is called *'Inorganic Chemistry.'* The substances which do not have carbon-hydrogen bonding are metals, salts, chemical substances, etc.

Reminders on the fundamental notions of atomistics

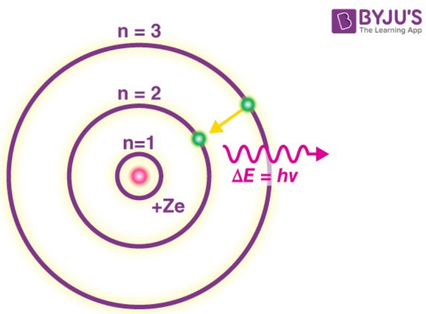
1- Bohr's Model of an Atom

Bohr's model consists of a small nucleus (positively charged) surrounded by negative electrons moving around the nucleus in orbits (shells) and not anywhere in between and he also explained that each orbit (shell) has a fixed energy.



Bohr found that an electron located away from the nucleus has more energy, and the electron which is closer to nucleus has less energy

The electrons in an atom move from a lower energy level to a higher energy level by gaining the required energy and an electron moves from a higher energy level to lower energy level by losing energy.



2- Atomic Structure

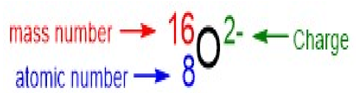
In general, an atom of a hypothetical element X is represented by its symbol $^{A}_{Z}X^{I\,charge}$ as charge where (X is the Element, Z is the atomic number, A is the mass number, and I is an integer equal to charge number and *charge* the sign of the charge number: + or -.

The number of protons, neutrons, and electrons is calculated by using the following formulas:

$$\text{Number of protons} = Z,$$

$$\text{Number of neutrons} = A - Z,$$

$$\text{Number of electrons} = Z - (charge\ I),$$



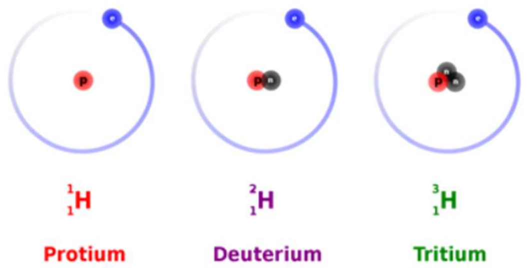
Atomic Structure - nucleus composed of protons and neutrons surrounded by an electron cloud Particle	**Charge**	**Mass**
Proton	+ 1.60 x 10^{-19} Coulombs	m_p= 1.674 x 10^{-27} kg 1.0728 amu
Neutron	Neutral	m_n= 1.672 x 10^{-27} kg 1.00867 amu
Electron	- 1.60 x 10^{-19} Coulombs	m_e= 9.109 x 10^{-31} kg 0.000545 amu

3- What are Isotopes?

Isotopes can be defined as: all atoms of the same element have the same number of protons and electrons, but a different number of neutrons.

In other words, isotopes are variants of elements that differ in their nucleon (The total number of protons and neutrons) numbers due to a difference in the total number of neutrons in their respective nuclei.

Example: Isotopes of hydrogen have neutrons equal to 0, 1, and 2, respectively.



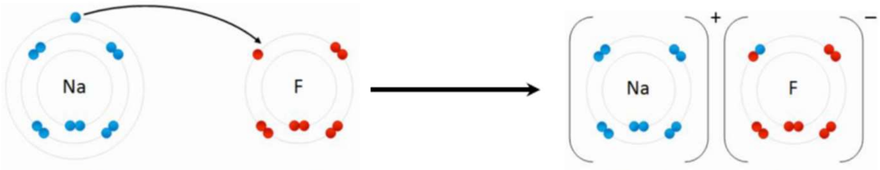
Isotopes of hydrogen

4- What is an ion?

An ion is an atom or group of atoms that has an electric charge. Ions with a positive charge are called cations. Ions with a negative charge are called anions.

A neutral atom can lose some electrons and become a positively charged particle, called a **cation**.

An atom can gain electrons and become a negatively charged particle, called an **anion**.



Symbol:	${}^{23}_{11}Na$	${}^{19}_{9}F$	${}^{23}_{11}Na^{1+}$	${}^{19}_{9}F^{1-}$
Protons	11	9	11	9
Neutrons	12	10	12	10
Electrons	11	9	10	10

Chapter 1: The Periodic Table

1- Quantum Numbers and Atomic Orbitals

1-1. Quantum Numbers

The Bohr model was a one-dimensional model that used one quantum number to describe the distribution of electrons in the atom. The only information that was important was the *size* of the orbit, which was described by the *n* quantum number. Schrödinger's model allowed the electron to occupy three-dimensional space. It therefore required three coordinates, or three **quantum numbers**, to describe the orbitals in which electrons can be found.

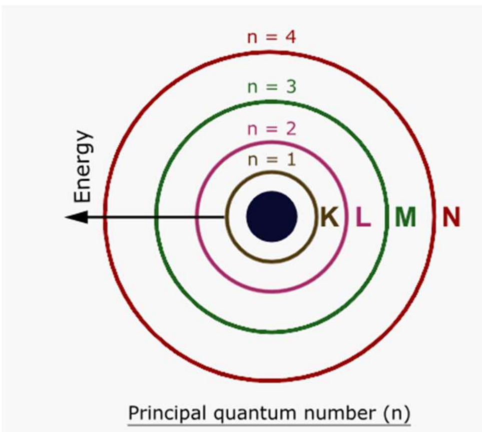
Each electron in an atom is described by four different quantum numbers. The first three (n, l, ml) specify the particular orbital of interest, gives the probability of finding the electron at various points in space called an atomic orbital. An atomic orbital is pictured qualitatively by describing the region of space where the probability of finding the electrons is maximum.and the fourth (ms) specifies how many electrons can occupy that orbital.

a. Principal Quantum Number (n):

This quantum number (*n*) describes the electron shell or energy level of an atom. The value of n ranges from 1 to the shell containing the outermost electron of that atom. n takes the values of $n = 1, 2, 3, \ldots, \infty$. Or K,L,M,N,O,P….

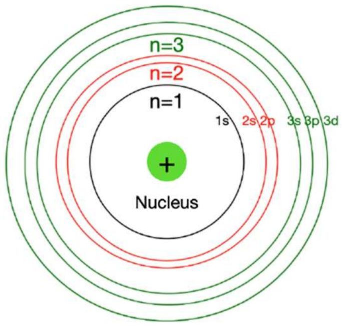
This number has a dependence only on the distance between the electron and the nucleus (i.e. the radial coordinate r). It gives the following information:

- It gives the average distance of the electron from the nucleus.
- It determines the energy of the electron.
- The maximum number of electron present in any principal shell is given by **$2n^2$** where n is the number of principal shell.



b. Angular Momentum (Secondary, Azimunthal) Quantum Number (l):

the angular momentum quantum number (ℓ) is related to the shape of atomic orbitals. It has integral values **ℓ = 0, 1, 2,…., n – 1** for each value of n. This quantum number divides the shells into smaller groups of orbitals, called **subshells (sublevels).** For a particular orbital, the value of ℓ **0,1,2,3,4,…** is commonly assigned by a letter **s,p,d,f,g**…



ℓ describes the shape of the orbital. Orbitals have shapes that are best described as spherical ($l = 0$), polar ($l = 1$), or cloverleaf ($l = 2$). They can even take on more complex shapes as the value of the angular quantum number becomes larger.

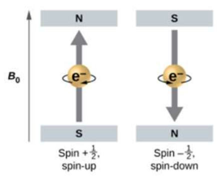
If n = 1 ,	then l = 0	s orbital	1s
If n = 2 ,	then l = 0	s orbital	2s
	and l = 1	p orbital	2p
If n = 3 ,	then l = 0	s orbital	3s
	and l = 1	p orbital	3p
	and l = 2	d orbital	3d

c. Magnetic Quantum Number (ml):

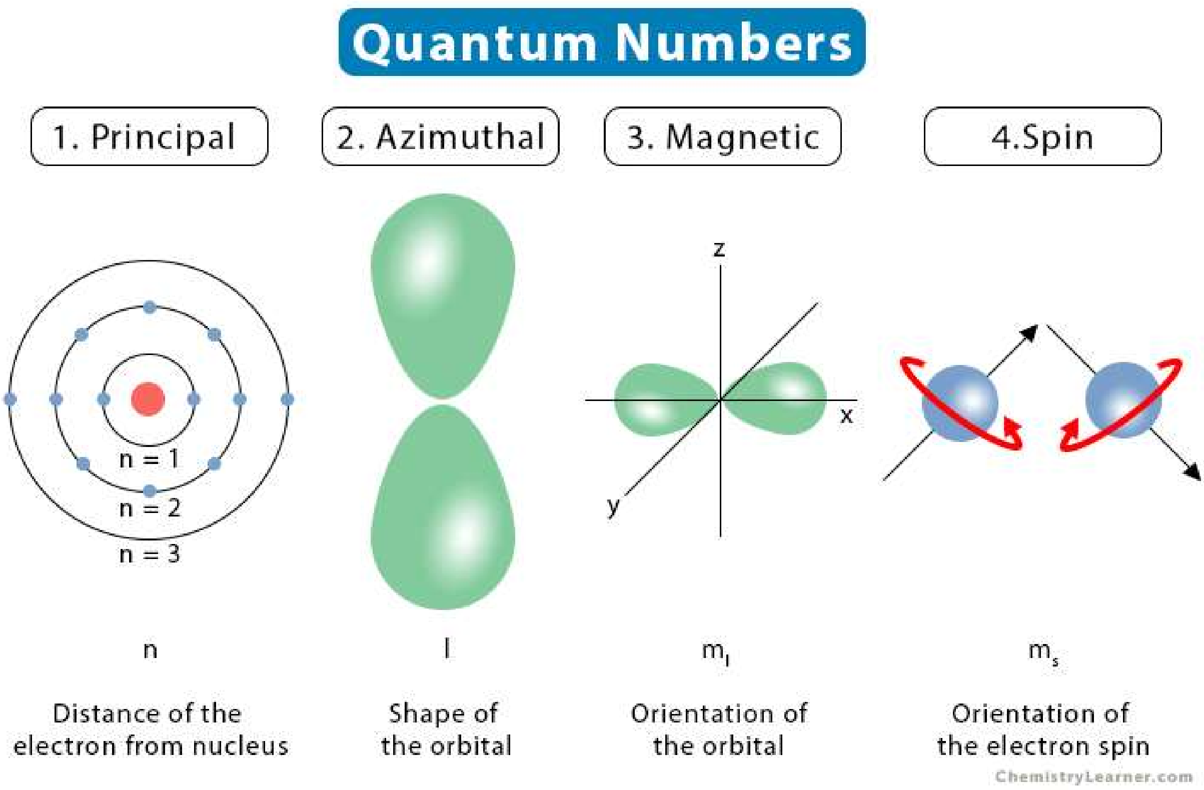
Specifies the orientation in space of an orbital of a given energy (n) and shape (l). ml takes the values of **ml = -l, ..., 0, ..., +l**. This number divides the subshell into individual orbitals which hold the electrons; there are **2l+1** orbitals in each subshell.

d. Spin Quantum Number (ms):

ms = +½ or -½. Specifies the orientation of the spin axis of an electron. An electron can spin in only one of two directions (sometimes called up and down). What this means is that no more than two electrons can occupy the same orbital,



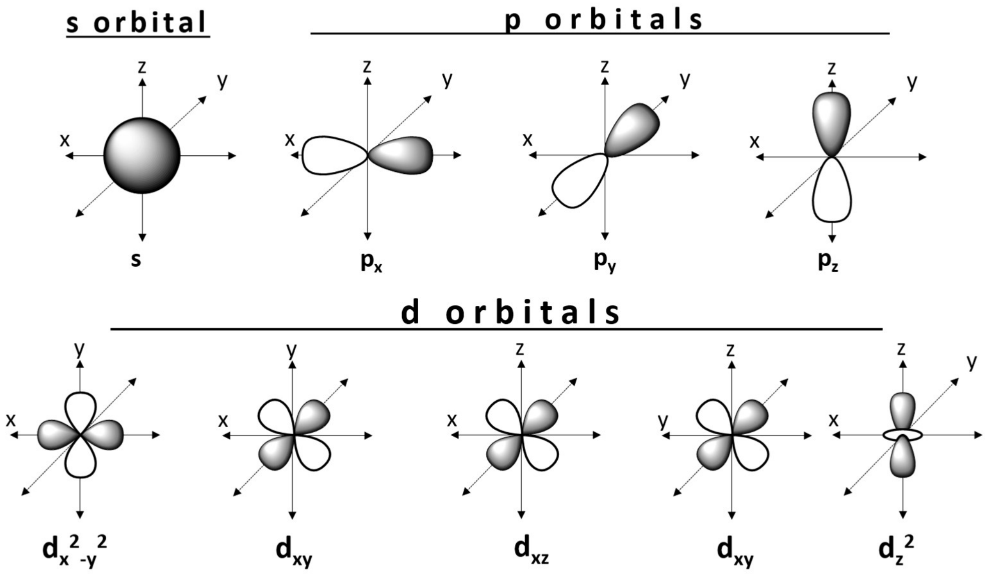
Name and Symbol	Meaning and Possible Values
Principal quantum number, n	Electron shell, $n \geq 1$
Azimuthal quantum number, l	Subshells (s=0, p=1, etc.) , $(n-1) \geq l \geq 0$
Magnetic quantum number, m_l	Total number and orientation of orbitals, $l \geq m_l \geq -l$
Electron spin quantum number, m_s	The direction of electron spin, $m_s = \pm½$



1-2. Atomic Orbitals

An atomic orbital is a mathematical function that describes the wave-like behavior of either one electron or a pair of electrons 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.

There are four different kinds of orbitals, denoted s, p, d and f each with a different shape. Of the four, s and p orbitals are considered because these orbitals are the most common in organic and biological chemistry. An s-orbital is spherical with the nucleus at its centre, and a p-orbitals is dumbbell-shaped and four of the five d orbitals are cloverleaf shaped. The fifth d orbital is shaped like an elongated dumbbell with a doughnut around its middle. The orbitals in an atom are organized into different layers or electron shells.



The Shape of s ,p and d Orbitals

1- S orbitals:

The s orbitals are characterized by l = 0 and m = 0, which are presented by a single orbital box diagram. S □

All s (ns) orbitals; are spherically symmetric because the probability of the electron's presence varies equally in all directions around the nucleus. The size of these orbitals increases with the value of n.

2- p orbitals:

For $l = 1 \Rightarrow m = -1, 0 \text{ or } 1 \Rightarrow 3$ p orbitals, which are represented by three degenerate orbital box diagrams: p □□□

We are talking about the p_x, p_y and p_z orbitals having the same shape, but each is elongated on one of the three perpendicular axes.There are three possible orientations for the p orbitals. This plane passes through the nucleus. The size of the p orbitals increases with the value of n.

3- d orbitals:

If $l = 2 \Rightarrow m = -2 ; -1 ; 0 ; 1 ; 2 \Rightarrow 5$ d orbitals, which are presented by five degenerate orbital box diagrams: d

d orbitals come in two basic forms: four of the five d orbitals have four lobes oriented along the axes shown (d_{xz}, d_{yz}, d_{xy}, and d_{x2-y2}). The fifth orbital, d_{z^2}, has a special form: two lobes are oriented along the z axis, on either side of a ring.

4- f orbitals:

If $l = 3 \Rightarrow m = -3 ; -2 ; -1 ; 0 ; 1 ; 2 ; 3 \Rightarrow 7$ f orbitals, which are presented by seven orbital box diagrams: f

There are seven different orientations for the f orbitals that are very complicated.

The orbital Notation

A particular state (or orbital) of the electron is designated by the value of the quantum number n accompanied by a lowercase letter linked to the value of the azimuthal quantum number l: ns, np, nd,….

The value of the quantum number m is specified as a subscript which is a function of the symmetry of the orbitals. We thus have: $\psi_{n,l,m}(r,\theta,\phi)$ = orbital: **n (letter) m**

Example:

What are the values of n, l and m for an electron associated with the orbital denoted $3d_{+1}$?

Answer:

3: indicates the value of n where n = 3

d: represents the value 1 for l = 2

+1: represents the value of m where m = + 1

What are the possible values of (n, l, ml , MS) for an electron in a 2s orbital and write all the possible sets of quantum numbers?

For an electron in 2s orbital, there are two possible set of quantum numbers:

n = 2, l = 0, ml = 0, ms = +1/2

n = 2, l = 0, ml = 0, ms = -1/2

2- Electron configuration and periodic table

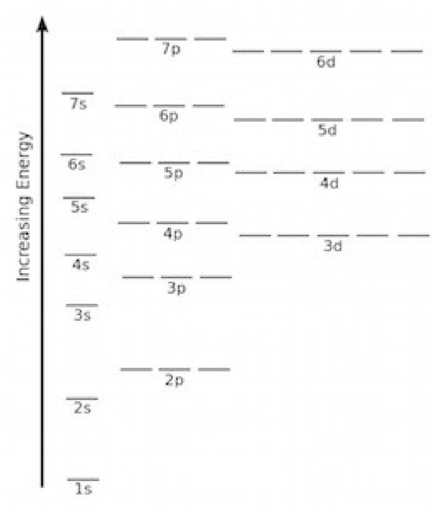
2-1. Electron configuration

Various elements have different numbers of electrons, these electrons are configured around the nucleus in the atom, this order is called the electron configuration. Therefore, atoms of every element have unique electron configuration whereby the electrons are ordered in the atoms in such a way that the total energy is at the minimum, and the following rules are considered when electron are ordered in levels:

Rule 1: Aufbau Principle

The word "Aufbau" comes from the German meaning "construction" or 'building up', also called the building-up principle,

The Aufbau principle dictates the manner in which electrons are filled in the atomic orbitals of an atom in its ground state. According to the Aufbau principle, the available atomic orbitals with the lowest energy levels are occupied before those with higher energy levels. they follow the “n+l” rule.



Atomic orbital energy diagram

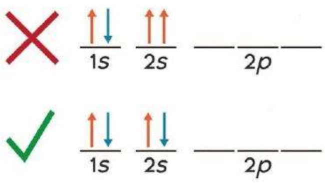
Rule 2: The Pauli Exclusion Principle

The Pauli Exclusion Principle states that, in an atom or molecule, no two electrons can have the same four electronic quantum numbers (n, l, m_l, and m_s). As an orbital can contain a maximum of only two electrons, the two electrons must have opposing spins. This means if one electron is assigned as a spin up (+1/2) electron, the other electron must be spin-down (-1/2) electron.

There are two salient rules that the Pauli exclusion principle follows:

- Only two electrons can occupy the same orbital.

- The two electrons that are present in the same orbital must have opposite spins, or they should be antiparallel.



Since an orbital cannot contain more than two electrons,

- s subshell can contain a maximum of two electrons,

- p subshell six electrons,

- d subshell ten electrons

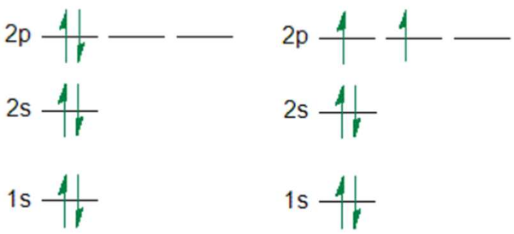
- f subshell fourteen electrons.

Therefore, there is a maximum number of electrons for each shell. It is equal to **$2n^2$**.

Rule 3: The HUND's rule

If orbitals of equal energy (*i.e.* degenerate orbitals) are being filled, the electrons are placed into each orbital in the degenerate set before they are spin paired with another electron in the same orbital

In simple terms, Hund's rule requires single occupancy before pairing.



Incorrect violates Hund's rule   **Correct** satisfies Hund's rule

Rule 4: KLECHKOWSKI's rule

Subshells are filled in ascending order of **n+l** values. For two equal values, the sublayer with the smallest n is filled first.

For example,

1- for 3d and 4s,

3d: n + l = 3 + 2 = 5

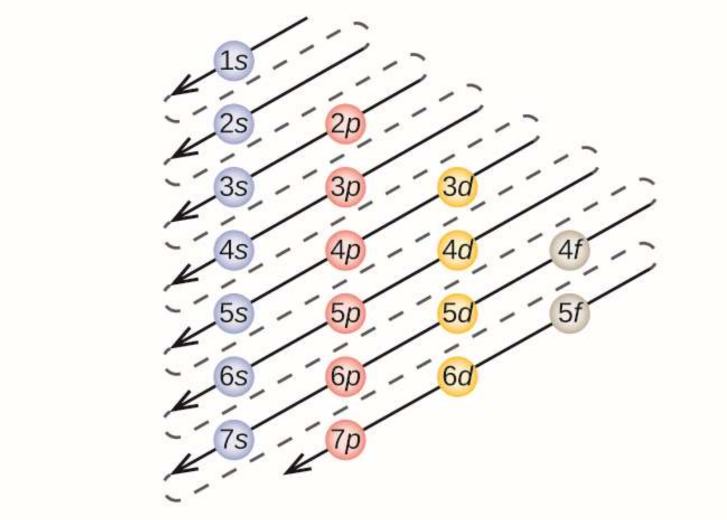
4s: n + l = 4 + 0 = 4; so 4s is filled first, and then 3d.

2- for 2p and 3s,

2p: n + l = 2 + 1 = 3

3s: n + l = 3 + 0 = 3; so 2p is filled first (smaller n), and only then 3s.

The order in which the sublayers are filled can be represented as follows:



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

Exceptions to the Aufbau Principle

It is important to note that there exist many exceptions to the Aufbau principle such as chromium and copper. These exceptions can sometimes be explained by the stability provided by half-filled or completely filled subshells.

$(n-1)d^4\ ns^2$ → which will transform into $(n-1)d^5\ ns^1$

$(n-1)d^9\ ns^2$ → which will transform into $(n-1)d^{10}\ ns^1$

the resulting configuration will be more stable than the initial configuration.

These exceptions occur due to small differences in energy levels between two subshells. Due to this small difference, the electrons transfer to a higher level shell to make the shell half filled or fulfilled. It increases the stability of the atom.

2-2. Periodic table

a- Periodic Table History

The Periodic Table has 118 elements which organized on the basis of atomic number and grouped based on similarity in chemical properties. The first element is Hydrogen (H) with atomic number 1 and the last element is Oganesson (Og) with atomic number 118.

The periodic table wasn't always like today's. The periodic table has been through several iterations of attempted systemization before we reached the one we use now. The first attempt was by Antoine Lavoisier in 1789 when he published a list of 33 chemical elements. He grouped them into gases, metals, nonmetals and earth.

The first edition of the modern periodic table was published by Mendeleev in 1871. Mendeleev's periodic table had eight columns, each column containing elements with similar properties. The columns were numbered I to VIII and also had empty cells for elements that hadn't been discovered yet, but Mendeleev predicted they should exist. As chemists discovered more and more elements, these gaps were filled.

b- Periodic Table Grouping Method

1- Groups

The 18 vertical columns of the table are called Groups. The number of electrons in the outermost shell of the atom, i.e. valence shell, is equal for all elements in the same group. The leftmost group contains alkali metals and the rightmost contains noble gases.

Elements in the same column exhibit similar chemical properties and display periodicity with an increase in atomic number. Elements in the same group tend to show patterns in atomic radius, ionisation energy, and electronegativity.

The groups are numbered 1 to 18 from left to right. Earlier, naming conventions differed in Europe and America. However, after the IUPAC naming was put in place in 1988, old names went out of use.

As we move down a group:

- Atomic radius increases
- Electronegativity decreases (except for group 11)
- Ionization energy decreases

2- Periods

The 7 horizontal rows are called periods of the periodic table. they contain a variable number of elements. A period is characterized by the filling of the OAs: ns, (n-2)f, (n-1)d, np.

Lanthanides and actinides in the f block display more similarity in the same period than in the same group.

On moving left to right in a period:

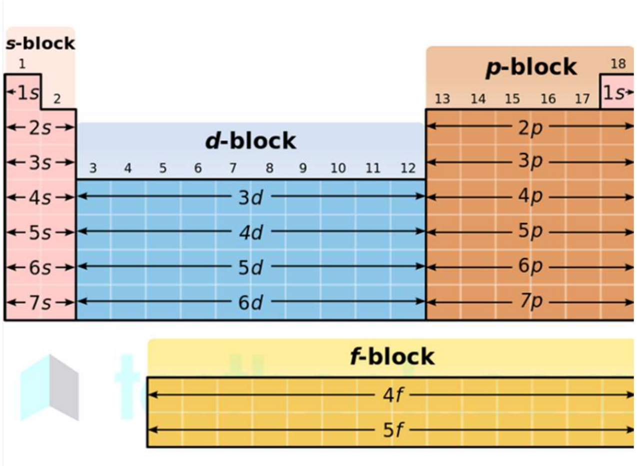
- Atomic size decreases due to stronger nuclear force
- Ionisation Energy increases
- Electronegativity increases
- Electron affinity increases (except for noble gases)

3- Blocks

Sections of the table are called blocks. Each block gets its name from the letter of the outermost subshell that receives an electron.

The four blocks are:

- **s-block:** Comprises of alkali metals (group 1) and alkaline earth metals (group 2).
- **p-block:** Contains groups 13 to 18, including the metalloids.
- **d-block:** Consists of groups 3 to 12 and has all the transition metals.
- **f-block**: Home of the lanthanides and actinides, these groups don't have group numbers.



On the basis of their physical and chemical properties, elements are divided into:

• **Metals:** Highly conducting solids that make ionic compounds with other elements. They are also further divided into alkali metals (Group 1), alkaline earth metals (Group 2), lanthanides and actinides (f - block), and post-transition metals. Metals form alloys with each other.

• **Nonmetals:** Colored or colorless solids, liquids or gases that undergo covalent bonding with other elements. They are usually further classified into polyatomic, diatomic and monatomic (inert) nonmetals.

• **Metalloids:** Their properties are a mixture of the properties of metals and nonmetals.

Note: Hydrogen is a special case since it does not belong to any of these regions. It can behave as a metal or a nonmetal depending on the conditions.

The following table summarizes the characteristics of the elements according to their classification into metals and non-metals:

Metals are	Non-metals are
solid (except mercury which is liquid)	solid, liquid or gaseous
fairly dense (density > 2.5 g/cm3)	not very dense (density < 2.5g/cm3)
Shiny	Dull
Malleable	non-malleable
good electrical conductors	poor electrical conductors

valence and core electrons

The electrons of an atom are typically divided into two categories: valence and core electrons. Valence electrons occupy the outermost shell or highest energy level of an atom while core electrons are those occupying the innermost shell or lowest energy levels. This difference greatly influences the role of the two types of electrons in a chemical reaction. Generally, valence electrons can participate in the formation of chemical bonding, but core electrons cannot.

Na $1s^2 2s^2 2p^6 3s^1$ Abbreviation $[Ne]3s^1$

Core electrons ($1s^2 2s^2 2p^6$) Valence electron ($3s^1$)

Example: What are the core and valence electrons in cobalt?

Solution: Start by writing the electron configuration of cobalt with 27 electrons:

Co: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7$

Co: $[Ar]4s^2 3d^7$

The two electrons in the 4s orbital and the seven electrons in the 3d are the valence electrons: all others are core electrons.

Electronic structure of ions: Find the element's electronic configuration: if it's a cation (+), remove one or more electrons; if it's an anion (-), add one or more electrons.

Period determination:

The period corresponds to the highest value of n in the electronic configuration.

Column determination:

- Structure ending with ns^x => Column number = x ;

Exception: Structure $1s^2$ => Column number = 18 (He)

- Structure ending with $ns^x\ np^y$ => Column number = x + y + 10

- Structure ending with $(n-1)\ d^z\ ns^x$ => Column number = x + z

The 18 columns of the periodic table are divided into 9 groups following the classification of columns whose elements have the same external electronic configuration. 8 of them are denoted by Roman numerals I, II, III, …., VIII and the 9^{th} group is denoted 0 (zero). The roman numeral represents the number of valence electrons.

□ Group 0 constitutes the chemical elements of the rare gases (R.G)

□ Groups I to VII are each divided into two subgroups. The first is indexed with the letter A and the second with the letter B.

Group	**I**	**II**	**III**	**IV**	**V**	**VI**	**VII**	**VIII$_B$**	**0 or (VIII$_A$)**
Subgroup	I$_A$, I$_B$	II$_A$, II$_B$	III$_A$, III$_B$	IV$_A$, IV$_B$	V$_A$, V$_B$	VI$_A$, VI$_B$	VII$_A$, VII$_B$		
Column	1- 11	2- 12	13- 3	14- 4	15- 5	16- 6	17- 7	8-9-10	18

The letters A and B indicate the nature of the valence electrons.

Subgroup A: Filling of the s or s and p subshell.

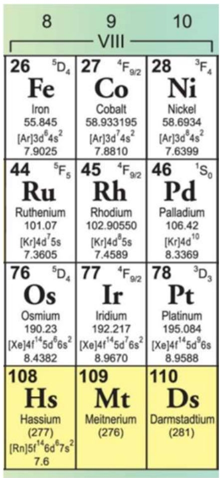
Subgroup B: Filling of the s and d subshell.

Exp:

$_{31}$Ga: [Ar] $3d^{10}4s^{2}4p^{1}$ => group III (3rd valence), subgroup => III$_A$ (or 13)

$_{21}$Sc: [Ar] $3d^{1}4s^{2}$ => group III (3rd valence), subgroup => III$_B$ (or 3)

□ Group VIII$_B$ is formed by three neighboring columns called triads. These elements have similar physicochemical properties in the horizontal and vertical directions.



Note: Number of elements in each period (according to external electronic structures)

Period 1: $1s^{1\to2}$ => 2elements

Period 2: $2\ s^{1\to2}\ 2p^{1\to6}$ => 8 elements

Period 3: $3\ s^{1\to2}\ 3\ p^{1\to6}$ => 8 elements

Period 4: $4\ s^{1\to2}\ 3d^{1\to10}\ 4p^{1\to6}$ => 18 elements

Period 5: $5\ s^{1\to2}\ 4d^{1\to10}\ 5\ p^{1\to6}$ => 18 elements

Period 6: $6\ s^{1\to2}\ 4f^{\ 1\to14}\ 5d^{1\to10}\ 4\ p^{1\to6}$ => 32 elements

Period 7: $7\ s^{1\to2}\ 5f^{\ 1\to14}\ 6d^{1\to10}\ 5\ p^{1\to6}$ => 32 elements

Example: Determine the group, period, and block in which each of the following elements is located in the periodic table.

a. $[Kr]5s^24d^1$

b. $[Ar]4s^23d^{10}4p^3$

c. $[He]2s^22p^6$

d. $[Ne]3s^23p^1$

Answer

a. Group 7, Period 5, d-block

b. Group 13, Period 4, p-block

c. Group 8, Period 2, p-block

d. Group 3, Period 3, p-block

Families in the periodic table

The table is arranged into vertical columns "groups" or "families". There are a number of main groups with similar properties. They are as follows:

Hydrogen: This element does not match the properties of any other group so it stands alone. It is placed above group 1 but it is not part of that group. It is a very reactive, colorless, odorless gas at room temperature. (1 outer level valence electron)

Group 1: Alkali Metals –These metals are extremely reactive and are never found in nature in their pure form. They are silver colored and shiny. Their density is extremely low so that they are soft enough to be cut with a knife. (1 outer level valence electron)

Elements whose external electronic configuration is of the $\mathbf{ns^1}$ type with n= 2, 3,...

Lewis notation: X●

The single electron in the valence shell can be lost easily, according to the ionization reaction:

$$X \rightarrow X^{+} + \acute{e}$$

Group 2: Alkaline-earth Metals –Slightly less reactive than alkali metals. They are silver colored and more dense than alkali metals. (2 outer level valence electrons)

Groups 3 –12: Transition Metals –These metals have a moderate range of reactivity and a wide range of properties. In general, they are shiny and good conductors of heat and electricity. They also have higher densities and melting points than groups 1 & 2. (1 or 2 outer level valence electrons) Lanthanides and Actinides: These are also transition metals Inner Transition Metals that were taken out and placed at the bottom of the table so the table wouldn’t be so wide. The elements in each of these two periods share many properties. The lanthanides are shiny and reactive. The actinides are all radioactive and are therefore unstable.

Group 13: Boron Group –Contains one metalloid and 4 metals. Reactive. Aluminum is in this group. It is also the most abundant metal in the earth's crust. (3 outer level valence electrons)

Group 14: Carbon Group –Contains on nonmetal, two metalloids, and two metals. Varied reactivity. (4 outer level valence electrons)

Group 15: Nitrogen Group –Contains two nonmetals, two metalloids, and one metal. Varied reactivity. (5 outer level valence electrons)

Group 16: Oxygen Group –Contains three nonmetals, one metalloid, and one metal. Reactive group. (6 outer level valence electrons)

Groups 17: Halogens –All nonmetals. Very reactive. Poor conductors of heat and electricity. Tend to form salts with metals. Ex. NaCl: sodium chloride also known as "table salt". (7 outer level valence electrons)

Their external electronic configurations are of type ns^2np^5 with n=2, 3,…..

Lewis notation: $|\overline{\underline{X}}\bullet$:

They lack one electron to have a complete valence shell. They can therefore easily capture an electron, according to the reaction: $X + é \rightarrow X^-$

Groups 18: Noble Gases –Unreactive nonmetals. All are colorless, odorless gases at room temperature. All found in earth's atmosphere in small amounts. (8 outer level valence electrons, except helium which has 2 valence electrons)

Periodic properties and their trends

The properties of the elements are directly or indirectly related to the electronic configuration of their atoms and show gradation (increases or decreases) in moving down a group or a longer period.

The common physical properties of the elements are melting points, boiling points, density, enthalpy of fusion and vaporization etc. But we shall focus our attention mainly on the properties which are based on electronic configuration these are:

- Atomic and ionic radii
- Ionization energy
- Electrons affinity
- Electronegativity

1- Atomic and ionic radius

a- Atomic Radius

Atomic radius is the distance between the centre of the nucleus of an atom to its outermost shell.

The periodic trend of atomic radius across a period – As we move from left to right in a period, atomic radius gradually decreases.

Reason – As we move left to right in a period the atomic number of the elements increases so nuclear charge increases while the number of shells in elements remains the same.

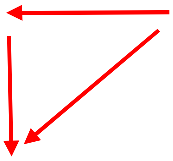
Across a Group – on moving top to bottom in a group, atomic radius gradually increase as nuclear charge and number of shells also increase.

Example:

Along the Period – Li> Be > B > C > N > O > F

Down the Grp – Li < Na < K < Rb < Cs

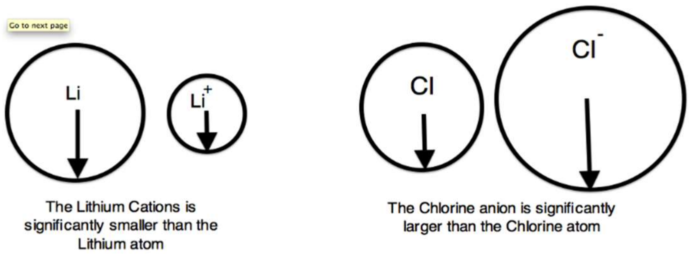
Atomic radius increases R_a



b- Ionic Radius

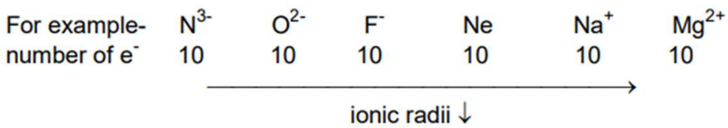
The ions formed by the loss of one or more electrons from the neutral atom are known as cation (positive ion) when the electrons added to the neutral atom form an anion (negative ion). The effective distance from the centre of the nucleus of the ion upto which it exerts its influence on the electron cloud is known as the ionic radius.

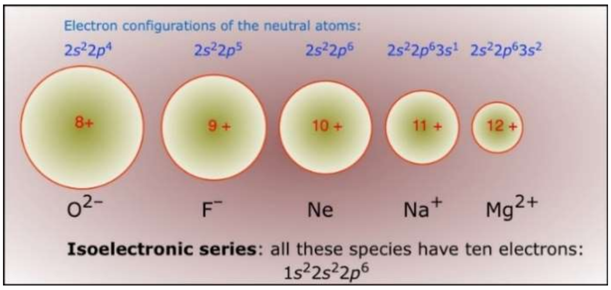
The ionic radius change in the same trend as atomic radius. It decreases along the period from left to right and increases down the group from top to bottom. size of cation and anion of any natural atom as: **cation< neutral atom < anion**



c- Isoelectric Series

A series of atoms, ions and molecules in which each species contains same number of electrons but different nuclear charge is called isoelectronic series. In an isoelectronic series atomic size decrease with the increase of charge.





2- Ionisation Energy IE

Ionisation energy is the amount of energy required to remove one electron from an atom in its neutral or gaseous state.

The first ionization energy is the energy required to remove the first electron and convert M to M^+ ; the second ionization energy is the energy required to remove the second electron and convert M^+ to M^{+2} the third ionization energy converts M^{2+} to M^{3+}, and so on.

$$M \longrightarrow M^+ + 1e^- \quad 1^{st} \text{ ionization energy}$$

$$M^+ \longrightarrow M^{+2} + 1e \quad 2^{nd} \text{ ionization energy}$$

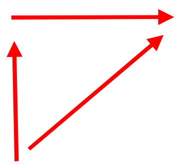
$$1^{st}\ IE < 2^{nd}\ IE < 3^{rd}\ IE < \ldots\ldots$$

The periodic trend of ionisation energy across a period – As we move from left to right in a period, ionisation energy gradually increases.

Reason – As we move left to right in a period atomic size or atomic radius decreases while nuclear charge increases

Across a Group – on moving top to bottom in a group, ionisation energy gradually decreases as atomic radius increases.

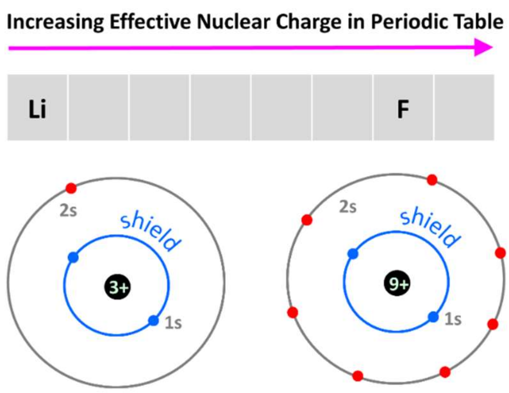
Ionisation energy increases IE



Various Factors that Affect the Ionization Energy Levels

- **Nuclear Charge**

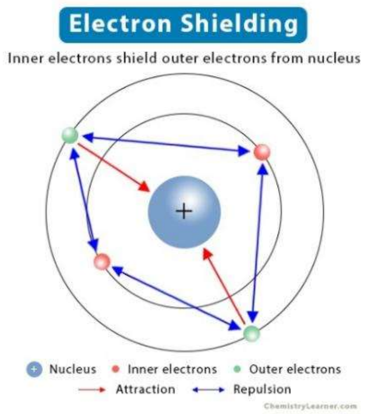
Lower the nuclear charge lower is the force of attraction between the nucleus and valence electrons, thus low ionization energy.



- **Shielding Effect**

The screening effect or shielding effect is the phenomenon of the reduction of the force of attraction of the nucleus on the outermost valence electrons due to the presence of the inner shell electrons.

Shielding effect increases as nuclear charge increases, thus with an increase in shielding effect the ionization energy also increases.



- **Atomic Radius**

As the atomic radius increases the force of attraction between the nucleus and valence electrons also decreases. Thus, with an increase in atomic radius the ionization decreases.

3- Electron Affinity *A*

The amount of energy required to add an electron to an atom is called the electron affinity of that atom.

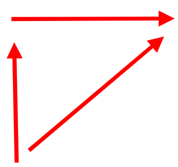
$$M + 1e^{-} \longrightarrow M^{-}$$

The periodic trend of electron affinity across a period – As we move from left to right in a period, electron affinity gradually increases.

Reason – As we move left to right in a period atomic size or atomic radius decreases while nuclear charge increases.

Across a Group – on moving top to bottom in a group, electron affinity gradually decreases.

Electron Affinity increases EA



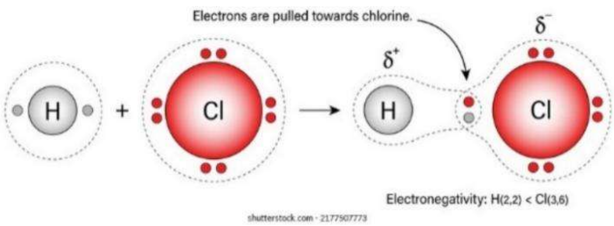
4- Metallic character of the elements

Across a Period – As we move left to right across a period in the periodic table, the metallic character of elements decreases.

Across a Group – As we move top to bottom in a group of the periodic table, the metallic character of elements increases.

5- Electronegativity χ

Electronegativity is a measure of the ability of an atom or molecule to attract pairs of electrons in the context of a chemical bond.

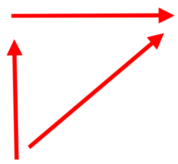


Across A Period – As we move left to right across a period, electronegativity increases in the periodic table. Fluorine is the most electronegative element.

Reason – As the nuclear charge increases of an atom, its electron loving character also increases.

Across A Group – As we move top to bottom in a group, electronegativity decreases

Electronegativity increases E



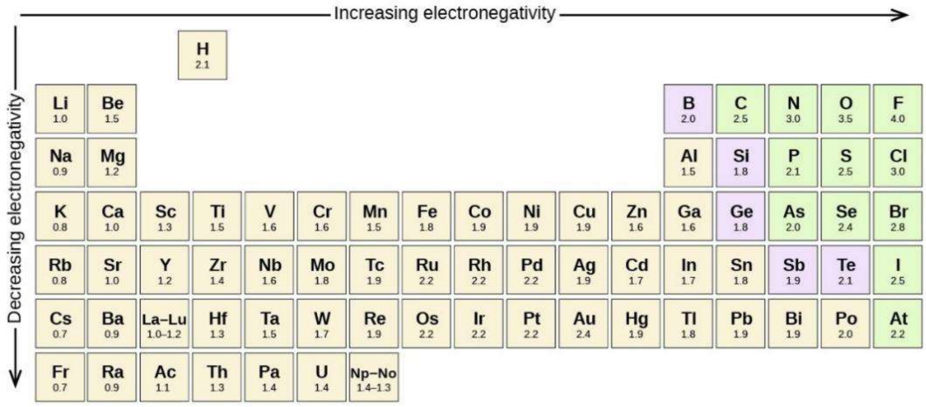
There are a few different 'types' of electronegativity which differ only in their definitions and the system by which they assign values for electronegativity.

Mulliken Electronegativity Scale: Developed by Robert S. Mulliken, this scale calculates electronegativity values based on the average ionization energy and electron affinity of an atom. The Mulliken electronegativity values are similar to the Pauling scale but may differ for certain elements.

$$X_m = \frac{\text{Ionisation Potential} + \text{Electron Affinity}}{2}$$

Pauling Electronegativity Scale: Proposed by Linus Pauling, this scale assigns electronegativity values to elements based on their chemical behaviour and bond energies. The Pauling electronegativity values range from approximately 0.7 for cesium (Cs) to 4.0 for fluorine (F), with fluorine being the most electronegative element.

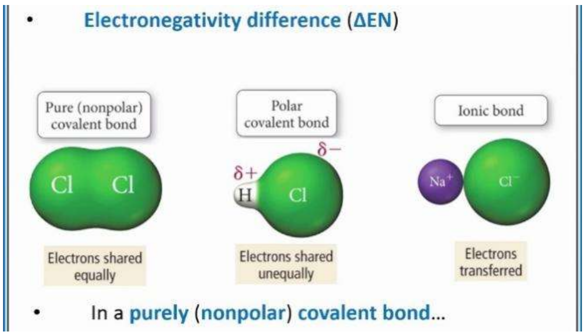
$$\Delta = X_A - X_B = 0.208\sqrt{E_{A-B} - \sqrt{E_{A-A} \times E_{B-B}}}$$

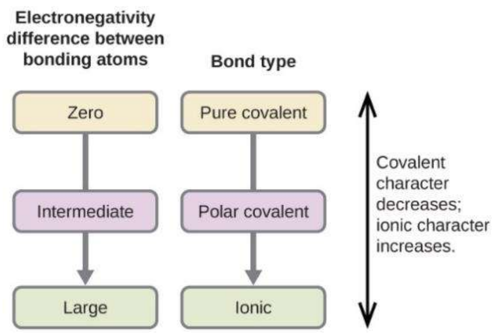


- Electronegativity allows us to distinguish metals from non-metals:
  Non-metals have $\chi > 2.2$, metals have: $\chi < 1.8$, semi-metals have $2.2 > \chi > 1.8$.

Electronegativity and Bond Type

The absolute value of the difference in electronegativity (ΔEN) of two bonded atoms provides a rough measure of the polarity to be expected in the bond and, thus, the bond type. When the difference is very small or zero, the bond is covalent and nonpolar. When it is large, the bond is polar covalent or ionic. The absolute values of the electronegativity differences between the atoms in the bonds H–H, H–Cl, and Na–Cl are 0 (nonpolar), 0.9 (polar covalent), and 2.1 (ionic), respectively. The degree to which electrons are shared between atoms varies from completely equal (pure covalent bonding) to not at all (ionic bonding)





Bond Type	Electronegativity Difference
pure covalent	< 0.4
polar covalent	between 0.4 and 1.8
ionic	> 1.8

<u>Exemple</u> : 1) $\chi_C = 2{,}55$ et $\chi_H = 2{,}2$

$$\Delta\chi = \chi_C - \chi_H = 0{,}35 \Rightarrow \text{non polar covalent bond.}$$

Using the table, what type of bond exists between the atoms of the following molecules?

O-H , Mg-Cl , B-F , Cr-O , C-N , Na-I , Ca-O , N-O , Mn-O.

Oxidation-Reduction Reactions

An oxidation-reduction (redox) reaction is a type of chemical reaction that involves a transfer of electrons between two species.

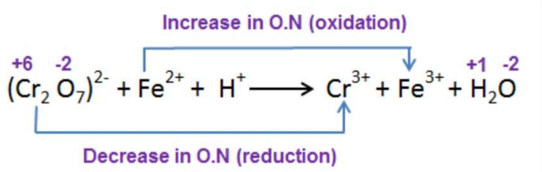
$$2\ Na \rightarrow 2\ Na^+ + 2e^-$$

$$Cl_2 + 2\ e^- \rightarrow 2\ Cl^-$$

oxidation = loss of electrons

reduction = gain of electrons

Redox reactions are comprised of two parts, a reduced half and an oxidized half, that always occur together. The reduced half gains electrons and the oxidation number decreases, while the oxidized half loses electrons and the oxidation number increases.



The two species that exchange electrons in a redox reaction are given special names:

1. The ion or molecule that accepts electrons is called the **oxidizing agent -** by accepting electrons it oxidizes other species.
2. The ion or molecule that donates electrons is called the **reducing agent -** by giving electrons it reduces the other species

$$2\,Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2\,Fe$$

2 Al	Fe_2O_3	Al_2O_3	2 Fe
reducing agent	oxidizing agent	oxidizing agent	reducing agent

reducing agent = species that is oxidized

oxidizing agent = species that is reduced

Example

Determine what is oxidized and what is reduced in the following reaction.

$$Zn + 2\,H^+ \rightarrow Zn^{2+} + H_2$$

Solution

The oxidation state of H^+ changes from +1 to 0, Hence, H^+ ion is reduced and acts as the oxidizing agent.

and the oxidation state of Zn changes from 0 to +2. Hence, Zn is oxidized and acts as the reducing agent and

The oxidation number

The **Oxidation Number** or **oxidation state**, is basically the count of electrons that atoms in a molecule can share, lose or gain while forming chemical bonds with other atoms of a different element.

How to Find Oxidation Number

An oxidation number can be assigned to a given element or compound by following the following rules.

- Any free element has an oxidation number equal to zero.

  Example: ON (Al) = 0

- For monoatomic ions, the oxidation number always has the same value as the net charge corresponding to the ion.

  Example: ON (Al^{3+}) = +3

- The hydrogen atom (H) exhibits an oxidation state of +1. However, when bonded with an element with less electronegativity than it, it exhibits an oxidation number of -1.

- Oxygen has an oxidation of -2 in most of its compounds. However, in the case of peroxides, the oxidation number corresponding to oxygen is -1.

- All alkali metals (group 1 elements) have an oxidation state of +1 in their compounds.

- All alkaline earth metals (group 2 elements) exhibit an oxidation state of +2 in their compounds.

- In the compounds made up of two elements, a halogen (group 17 elements) have an oxidation number of -1 assigned to them.
- In the case of neutral compounds, the sum of all the oxidation numbers of the constituent atoms totals zero.
- When polyatomic ions are considered, the sum of all the oxidation numbers of the atoms that constitute them equals the net charge of the polyatomic ion.

Example

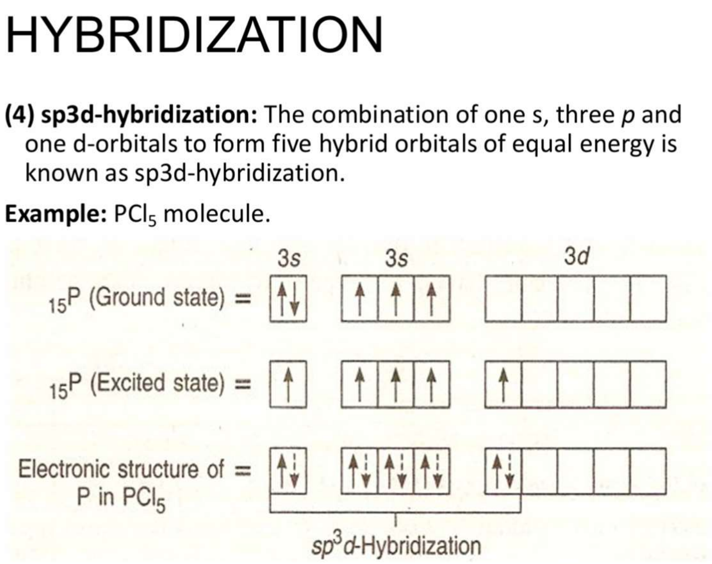
1- What is the oxidation state (number)of the sulphur atom S in Sulphuric acid H_2SO_4
2- Oxidation Number of Nitrogen in Ammonium Nitrate . NH_4NO_3

Hybridization shape and geometry

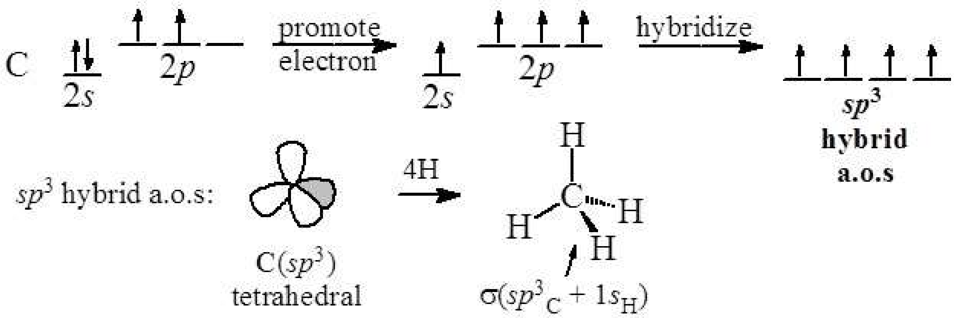
Hybridization Definition

hybridization is defined as the process of combining two atomic orbitals to create a new type of hybridised orbitals. The formation of hybrid orbitals with completely different energies, shapes. It was introduced to explain molecular structure

Hybridization is mostly carried out by atomic orbitals of the same energy level.

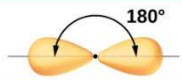
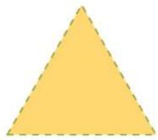
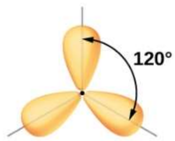
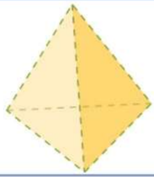
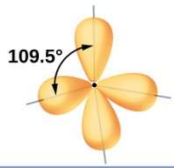
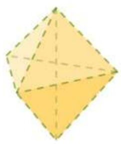
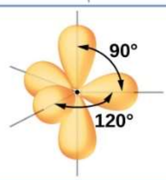
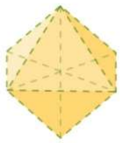
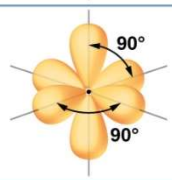


Energy changes occurring in hybridization

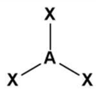
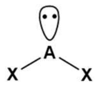
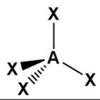
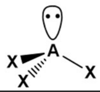
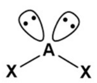
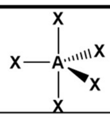
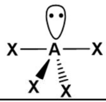
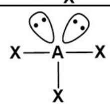
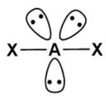
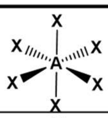
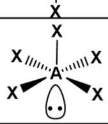


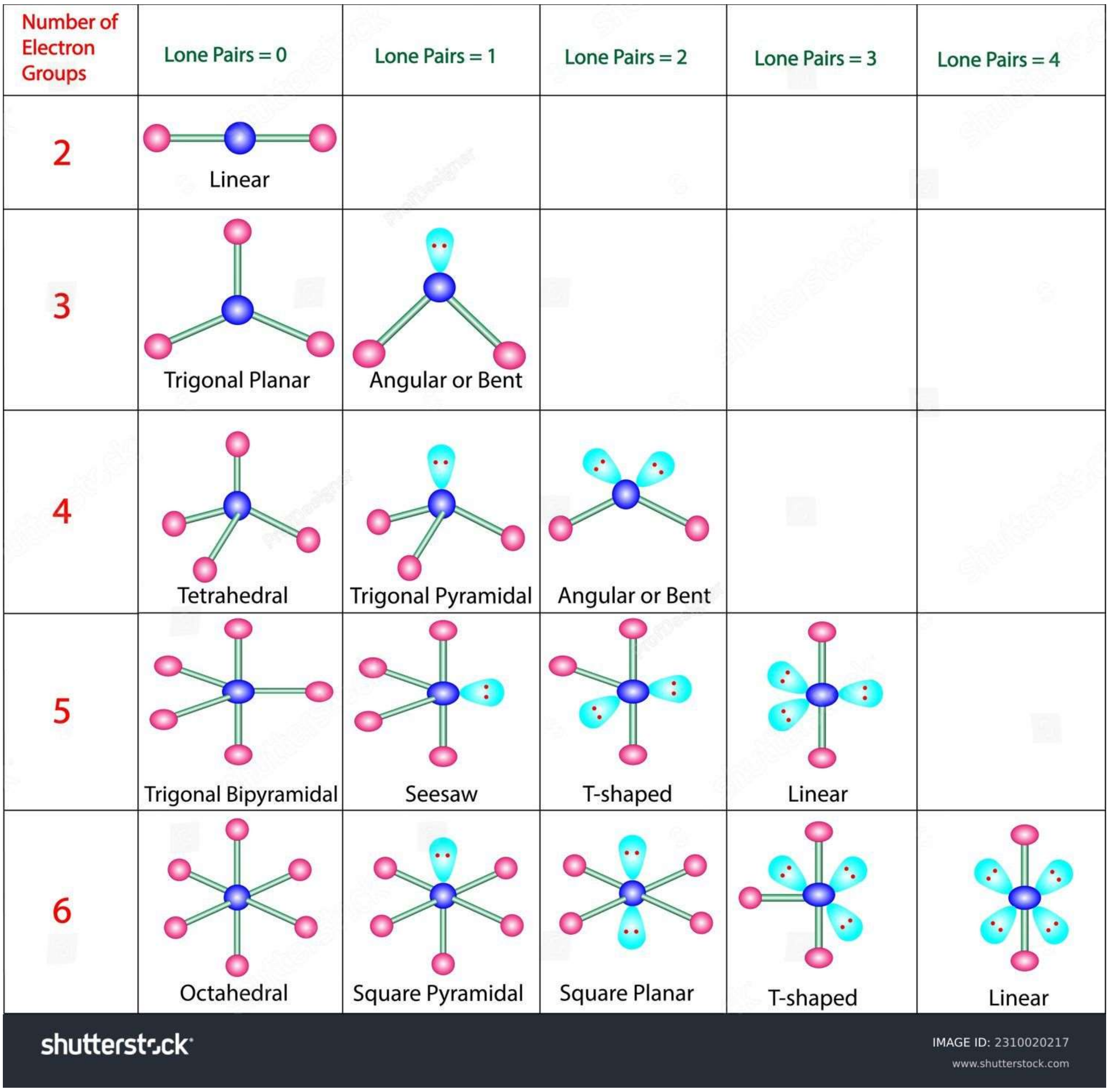
Types of Hybridization

Depending on the types of orbitals included in mixing, hybridisation could be characterised as sp^3, sp^2, sp, sp^3d, sp^3d^2, or sp^3d^3

Regions of Electron Density	Arrangement		Hybridization	
2		linear	*sp*	
3		trigonal planar	sp^2	
4		tetrahedral	sp^3	
5		trigonal bipyramidal	sp^3d	
6		octahedral	sp^3d^2	

Molecular Geometry: Valence-Shell Electron-Pair Repulsion Theory (**VSEPR**) Theory based on the idea that pairs of valence electrons in bonded atoms repel one another.

AXE Formula	Molecular Geometry	Bond Angle	Molecule Shape
AX_2E_0	**Linear**	180°	
AX_3E_0	**Trigonal planar**	120°	
AX_2E_1	Bent	119°	
AX_4E_0	**Tetrahedral**	109.5°	
AX_3E_1	Trigonal pyramidal	107.3°	
AX_2E_2	Bent	104.5°	
AX_5E_0	**Trigonal bipyramidal**	90°, 120°, 190°	
AX_4E_1	See-saw	86.5°,102°, 187°	
AX_3E_2	T-shape	87.5°, 185°	
AX_2E_3	Linear	180°	
AX_6E_0	**Octahedral**	90°	
AX_5E_1	Square pyramidal	84.8°, 180°	


Number of Electron Groups
Lone Pairs = 0
Lone Pairs = 1
Lone Pairs = 2
Lone Pairs = 3
Lone Pairs = 4
2
Linear
3
Trigonal Planar
Angular or Bent
4
Tetrahedral
Trigonal Pyramidal
Angular or Bent
5
Trigonal Bipyramidal
Seesaw
T-shaped
Linear
6
Octahedral
Square Pyramidal
Square Planar
T-shaped
Linear
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